ORIGINAL ARTICLE

Artificial intelligence model of fuel blendings as a step toward the zero emissions optimization of a 660 MWe supercritical power plant performance

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Abstract

Accurately predicting fuel blends' lower heating values (LHV) is crucial for optimizing a power plant. In this paper, we employ multiple artificial intelligence (AI) and machine learning-based models for predicting the LHV of various fuel blends. Coal of two different ranks and two types of biomass is used in this study. One was the South African imported bituminous coal, and the other was lignite thar coal extracted from the Thar Coal Block-2 mine by Sind Engro Coal Mining Company, Pakistan. Two types of biomass, that is, sugarcane bagasse and rice husk, were obtained locally from a sugar mill and rice mill located in the vicinity of Sahiwal, Punjab. Bituminous coal mixture with other coal types and both types of biomass are used with 10%, 20%, 30%, 40%, and 50% weight fractions, respectively. The calculation and model development procedure resulted in 91 different AI-based models. The best is the Ridge Regressor, a high-level end-to-end approach for fitting the model. The model can predict the LHV of the bituminous coal with lignite and biomass under a vast share of fuel blends.

KEYWORDS
artificial neural networks, fuel blending, LHV prediction, machine learning, sustainability, zero emissions

1 | INTRODUCTION

Economic growth is marked by massive electricity consumption, making it a key indicator of economics. Increased population and industrialization have also taken the demands for power to a new high surge in postcovid economy and have also led to a greater need for electricity which is provided by majorly coal-fired power plants, mainly in Asia, with coal standing out among all with 36.7% share in global power generation.

In 2021, high gas prices also increased the demand for coal power generation. According to IEA, tracking report —November 2021, compared with the first quarter of 2020, coal generation in the first quarter of 2021 increased by 15%, and the higher consumption of coal increases carbon emissions and enhances global warming.

The UN Climate Change Conference 2021, also called COP26, emphasized reducing greenhouse gas emissions so the global temperature rise can be restricted to 1.5°C. Nations are directed to phase down unabated coal power. IEA report suggested a few methods toward net zero emissions, namely electrification of transport, deployment of CCUS, hydrogen-derived fuels, and use of bioenergy for power generation. Biofuels are low-carbon fuels available in underdeveloped countries, for example, South Asian countries. Pakistan, India, and Bangladesh's economies are agriculture-based due to the vast fertile lands of sugarcane, rice, wheat, and cotton. The residue of these grains has considerable potential to be recognized as biomass.[1]

Biomass blending with nonrenewable fuels has many advantages in fuel flexibility, less pollutant emission, high combustion efficiency, and carbon neutrality or at least a reduction of carbon footprint.[2–4] This also solves the problem of green waste handling. Combusting biomass in cofiring modes is the most inexpensive method of converting biomass into fuel.[5–8] Besides economic and environmental issues, other technological constraints should also be considered in fuel blending fuels, such as flame stability. For wet coal events, biomass can help boost the plant's capacity and increase flame stability.[2]

A comprehensive evaluation of low-rank fuel compositions obtained using multicriteria decision-making methods can be found in Dorokhov et al.[9] The authors confirmed that adding a small amount of plant biomass (2%–5%) can be considered the most effective way to improve the emission performance of the slurry based on coal slime.

According to the literature, coal plays a minor role in Pakistan's energy mix. Although the country contains an estimated 180 billion tons of proven recoverable reserves, the coal imports are high. In the province of Sindh (Pakistan), the desert of Tharparker, a large deposit of coal reserves with 175 billion tons of good quality has been found. However, several factors have hindered the development of the thar coal reserves, including the depth and moisture level of the lignite reserves, a scarcity of fresh water, and a lack of road and power infrastructure.[10,11] Khan and Dessouky noted that biomass in Pakistan is gaining interest because it produces a similar type of fuel extracted from crude oil. Since biomass energy only depends on the availability of cheap raw materials.

According to Rehman et al., at present, the share of coal in the power generation of Pakistan is lower than 1%. Therefore, the percentage of coal in the Pakistan energy mix could be increased considerably using low-grade coals such as sub-bituminous ones in the Salt Range, Trans Indus Range in Punjab and Baluchistan, and lignites in Thar and Lakhra (Sindh). These low-grade local coals can be blended with better-quality imported coals for higher performance and compliance with environmental regulations. The authors underlined that fluidized bed combustion is one feasible method for small to medium-scale power production. It is flexible enough to utilize low-grade coal while maintaining low sulfur and nitrogen oxide emissions.[12] In the Sahiwal power plant, two types of coal are used, that is, 50% sub-bituminous coal imported from Indonesia and 50% bituminous coal from South Africa. Therefore, shifting toward renewables like biomass might improve the air quality and the ecosystem.[13]

Several techniques have been used to model and predict blended fuel properties. Wang et al.[14] developed models based on linear regression and artificial neural networks (ANN) for estimating the lower heating value (LHV) of municipal solid wastes (MSW). Despite models generated using the two methods showing acceptable performance levels in predicting LHV, the ANN models were more robust in handling data sets of diverse quality.

An interesting ANN-based model with 14 input layers, 26 hidden layers, and 1 output layer was developed for predicting the enthalpy of combustion for various oxygenated fuels.[15] In predicting the enthalpy of combustion, 96.3% accuracy was achieved, so the developed model can be successfully employed to predict the enthalpies of neat compounds and mixtures.

An LHV and higher heating value (HHV) prediction model using regression analysis with the help of bond energies for biodiesel was developed by Erdogan.[16] The model obtained excellent accuracy, and LHV and HHV were estimated with less than 1% error. Li et al. used machine learning (ML) and deep learning in typical fuel property prediction regression problems and compared their predictive performance. The authors underlined that adding too many layers into CNN decreases predictive accuracy because the multiple activation operations result in a vanishing gradient.[17]

In this work, coal of two different ranks and two types of biomass are used in this study. One was the South African imported bituminous coal, and the other was lignite thar coal extracted from the Thar Coal Block-2 mine by Sind Engro Coal Mining Company (SECMC), Pakistan. Two types of biomass, that is, sugarcane bagasse and rice husk, were obtained locally from a sugar mill and rice mill located in the vicinity of Sahiwal, Punjab. Bituminous coal mixture with other coal types and both types of biomass are used with 10%, 20%, 30%, 40%, and 50% weight fractions, respectively.

Three data-driven modeling algorithms, namely Ridge Regressor, Nystroem Kernel SVM Regressor, and

Linear Regressor, are deployed for modeling the lower heat value of the fuel blends against their characterized properties, for example, air-dried moisture (%), ash (%), volatile matter (%), fixed carbon (%) and hydrogen (%). The fuels used in the study, that is, coal of two different ranks and two types of biomass, and the tools used in this study constitute the paper's novelty. The algorithms have demonstrated excellent performance in modeling both lab-scale and enterprise-level systems.

The paper's novelty consists of the selected fuels used in the study and the application of the automated machine learning (AutoML) approach. We utilized the DataRobot application as one of the best software among AutoML tools. To the best of our knowledge, this is the first time this approach and the selected fuels were employed to predict the lower heat value of the fuel blends, contributing to the sustainable development and zero-emissions concepts of the energy processes.

We can test the heating values of pure samples in a bomb calorimeter but cannot test the blended sample of every fraction. Hence, we fit the model to the available data. Without complete elemental analysis (C, H, N, O, and S), we can estimate the accurate heating value of the considered biomass and fuel blend with the developed AI-based model, thereby reducing the testing cost, time-saving approach, and digitalization of the process.

2 | MATERIALS AND METHODS

Zero emissions optimization can be achieved by blending biomass with fossil fuel, which will reduce carbon emissions because of the introduction of green fuels. Therefore we must predict the heating value of the fuel as blending fuels of different natures will have a different heating value compared to the original heating values combined. The constraint we kept in this work is that the power output should be kept the same, so we had a bracket of heating value to work, and based on this heating values prediction, we could suggest the most suitable blend that will help us in reducing the carbon footprint.

Coal of two different ranks and two types of biomass are used in this study. One was the South African imported bituminous coal, and the other was lignite thar coal extracted from the Thar Coal Block-2 mine by SECMC, Pakistan. Two types of biomass, that is, sugarcane bagasse and rice husk, were obtained locally from a sugar mill and rice mill located in the vicinity of Sahiwal, Punjab.

Raw coal and biomass samples were dried in an oven (Laboratory Blast drying oven FFL-70) at 105°C for 60 min. Biomass samples were then chopped (Disc Mill Pulverizer 5S-PC1*100) to reduce their size. After grinding, the samples were passed through standard sieves of mesh number 70 (210 μm) to obtain an average particle size of <0.2 mm. Five samples with different blending ratios were prepared, and to achieve proximate homogeneity, samples were tumbled for 30 min. The standard sample preparation method was followed, as mentioned in the literature.[18,19]

The infrared carbon and hydrogen analyzer SDCHN435, proximate analyzer SDTGA5000a, and sulfur analyzer SDS516 are the main components of the experimental setup (Table 1).

The BSA224S Sartorius weigh balance with a weighing capacity of 220 g was used for sample weighing in different tests. The repeatability of the weighing balance is 0.00001 g (0.1 mg). Balance was placed on a nonmoveable marble table in a room with no interference from the external environment, for example, strong winds or an air conditioner.

The SDTGA5000a Proximate Analyzer consists of the host (internally equipped with Sartorius analytical balance module, gas supplying unit, computer (including display), and printer. The host consists of a sample weighing room, combustion furnace, analytical balance module, and sample introduction device. The analytical balance module (Model: XX85-001) was used for weighing the samples with a measuring range of 0–120 g and a sensitivity of 0.0001 g.

A conventional combustion environment with air provided with a centrifugal fan was used. Coal mixture with other coal types and both types of biomass was used with 10%, 20%, 30%, 40%, and 50% weight fractions, respectively. Samples weighing 1 ± 0.01 g of mixtures were used in testing.

The infrared absorption analytical method is used to measure carbon and hydrogen content. Sample analysis consists of three steps: gas circuit, combustion, and analysis. In the combustion process, the sample is delivered into the combustion tube for oxygen-excess combustion. Generated gases after secondary combustion pass through multistage filtration, collected in a gas collection chamber. During analysis, collected gases flow into the CO_2 infrared sensor and H_2O infrared sensor to detect carbon and hydrogen, respectively.

A synthetic combustion environment with oxygen purity ≥99.5% and pressure 0.18 ± 0.01 MPa and nitrogen gas with pressure range 0.18 ± 0.01 MPa is used during this analysis. Samples weighing 100 mg were used with a precision of ± 0.1 mg, and all the samples were tested twice.

The SDACM4000 Bomb Calorimeter (resolution: 0.0001 K) was used to measure the calorific values of solid and liquid combustibles. The $1 g \pm 0.001$ g sample

TABLE 1 Equipment setup.

Equipment name	Model	Standard	Performance index		
Infrared Carbon and Hydrogen Analyser	SDCHN435	DL/T 568-2013	Repeatability: $C_{ad} \leq 0.5\%$, $H_{ad} \leq 0.15\%$	Measuring range: C_{ad} 0.02%–100%, H_{ad} 0.02%–50%	Weighing sensitivity: 0.0001 g
Proximate Analyser	SDTGA5000a	GB/T 212-2008	Weighing sensitivity: 0.0001 g	Temperature resolution: 1°C	The precision of temperature control ≤10°C
Bomb Calorimeter	SDACM4000	GB/T 213-2008	Resolution: 0.0001 K		
Sulfur Analyser	SDS516	GB/T 214-2007	Repeatability for $St_{,ad} \leq 1.5\%$ is <0.05	Range: 0.01%–40%	The precision of temperature control ≤5°C
Moisture Analyser	YX-WK/SF7330	GB/T 212-2008			

weight was used for all the samples tested with high precision in bombs filled with 99.5% pure oxygen at pressure 2.8–3.2 MPa for 15–60 s. LHVs were measured with the change in water temperature, and LHVs were calculated by adding the required values to the control program.

Proximate, ultimate, and heating value analyses were performed in the quality control lab of a 660 MW$_e$ supercritical coal-fired power generating unit.[20–22] The proximate analyzer was used with a strict temperature resolution. The analysis includes the moisture content (M^{ad}, air-dried basis), the ash content (A^{ad}, air-dried basis), volatile matter (V^{ad}, air-dried basis), and sulfur content (S^{ad}, air-dried basis). The fixed carbon content (F.C.^{ad}, air-dried basis) was not directly obtained but was calculated by linear calculation through constituents because of the correlation with other air-dried constituents. The standard for the volatile matter was ISO 562-12010, and no air/gas was supplied during the tests by the proximate analyzer.

Infrared Carbon and Hydrogen Analyzer with oxygen and nitrogen supply valves were used for measuring carbon content (C^{ad}, air-dried basis) and hydrogen content (H^{ad}, air-dried basis), while sulfur content (S^{ad}, air-dried basis) was measured by coulometric titration in the sulfur analyzer. HHV was obtained first by the bomb calorimeter. with a bomb attached to an oxygen cylinder for oxygen filling. LHV was obtained later by eliminating the latent heat of water vaporization generated during the GCV test using the standard ISO 1928–2009.

The experimental data collected from the chemical characterization of the fuel blends is deployed for constructing an ML model to predict their LHV. ML algorithms can mine the nonlinear and complex dependencies among the observations of the input and output variables which are sometimes difficult to develop by conventional mathematical techniques. The superior modeling capacity of the ML algorithms makes them suitable for experimental studies where the well-developed and robust models backed by domain knowledge provide valuable insight into the relationships and working physics of the operating systems.[22–24]

The measurement and modeling methodology applied in the study is shown in Figure 1.

3 | RESULTS AND DISCUSSION

3.1 | Data analysis

The results of the measurements are shown in Table 2. The air-dried moisture (M^{ad}) of imported coal, thar coal, and biomass samples were tested on the Proximate
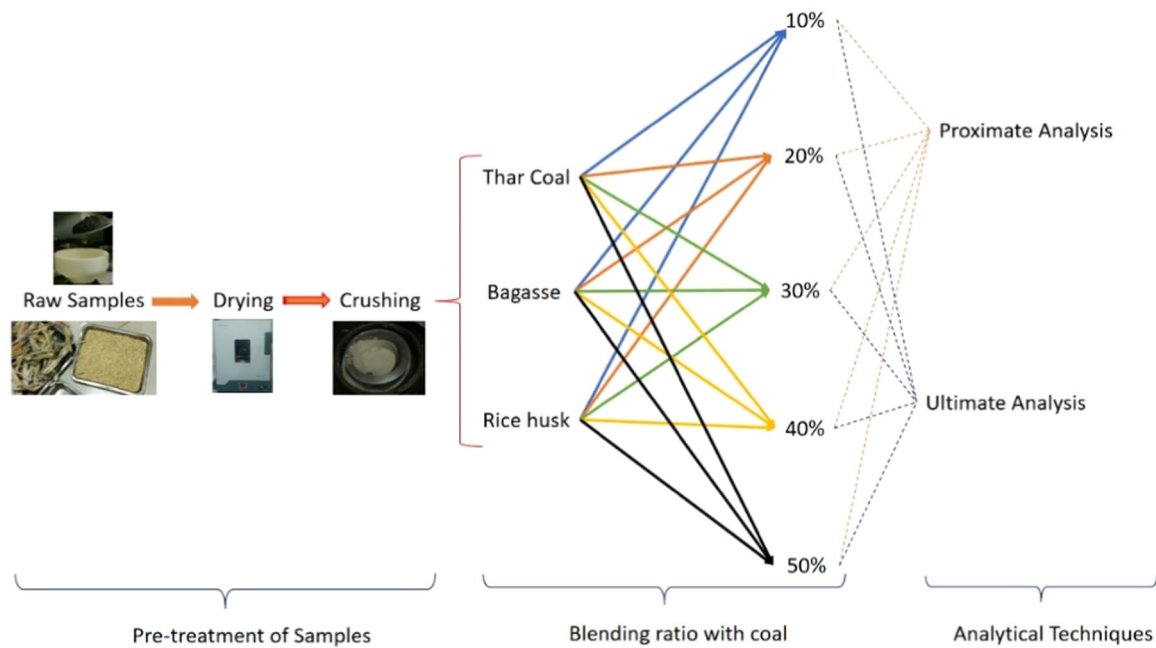
FIGURE 1 The methodology adopted to construct the experiments and modeling of the fuel blends.

TABLE 2 Results of the proximate analysis of the fuel blends.

Sample	Weight fractions (%)	M^{ad}	A^{ad}	V^{ad}	FC^{ad}	H^{ad}	S^{ad}	ID_f	LHV
Imported coal	100	4.58	15.94	23.96	55.52	3.71	0.55	1.00	24.36
Thar coal	100	35.54	6.02	35.06	23.88	5.09	0.68	2.00	13.05
Thar coal + Imported coal	10	5.63	15.22	25.48	53.67	3.77	0.54	2.10	23.20
	20	8.74	14.31	27.12	49.83	3.98	0.58	2.20	22.04
	30	12.75	13.18	27.42	46.65	4.40	0.57	2.30	21.01
	40	16.21	11.96	28.33	43.50	4.70	0.57	2.40	19.80
	50	19.57	11.02	29.19	40.22	4.99	0.60	2.50	18.64
Rice husk	100	6.92	14.87	65.90	12.31	4.98	0.07	3.00	13.70
Rice husk + Imported coal	10	2.94	15.64	28.83	52.59	3.27	0.50	3.10	23.33
	20	3.56	14.96	33.53	47.95	3.51	0.46	3.20	22.10
	30	4.22	14.16	38.16	43.46	3.69	0.43	3.30	21.00
	40	6.42	12.96	42.19	38.43	4.02	0.38	3.40	19.93
	50	6.80	12.28	47.00	33.92	4.23	0.33	3.50	18.775
Bagasse	100	6.05	2.49	84.38	14.29	5.85	0.14	4.00	15.03
Bagasse + Imported coal	10	2.63	14.93	29.33	53.11	3.49	0.51	4.10	23.36
	20	3.09	13.66	34.34	48.91	3.78	0.46	4.20	22.15
	30	3.58	12.33	39.52	44.57	4.00	0.42	4.30	21.070
	40	4.14	10.97	44.70	40.19	4.25	0.39	4.40	20.09
	50	4.33	9.56	54.34	31.77	4.52	0.34	4.50	18.79

Analyser, and it was found that thar coal has the highest moisture content among all other samples. In contrast, imported bituminous coal has the least moisture content among other fuels. The additional ID_f fuel tag in Table 2 identifies the fuel type allowing consideration of the fuel mixture during calculations. The biomass samples, bagasse, and rice husk have almost the same moisture content.

Therefore, when the blended samples of imported coal and thar coal were tested, the moisture content of the composite samples increased along with the increasing content of thar coal (Figure 2). There is a linear trend in the moisture content. The blended sample of imported coal and bagasse, as well as imported coal and rice husk, also possess an increasing trend in the moisture content but the change in moisture content is not too large as the difference in coal moisture content, bagasse, and rice husk is not significant.

The air-dried ash (A^{ad}) content of all the samples tested on the proximate analyzer indicated that imported coal and Rice husk have the highest ash content. At the same time, bagasse has the least ash content (Table 2). As a result, the ash content of imported coal blends with other fuels showed a decreasing trend in the blended mixtures as the average ash content of all row blended fuels is lower than that of imported coal (Figure 3).

The volatile matter test indicated that biomass samples contain a high content of volatile matter (V^{ad}), with bagasse having the highest among the two (Figure 4). In contrast, imported parent coal has the least amount among all considered fuels. Consequently, the V^{ad} of all fuel blends increases with the blending ratio of all constituent fuels.

The highest volatile matter content equal to 54.34% can be obtained for Important coal with 50% of bagasse.

Fixed carbon (FC^{ad}), performed on an elemental analyser, showed that the imported coal has the highest content while the other three fuels have quite less, and that of bagasse and rice husk is close. Since all doped fuels have lower FC than parent bituminous coal, the increase in the blending ratio leads to a decrease in blended fuels (Figure 5).

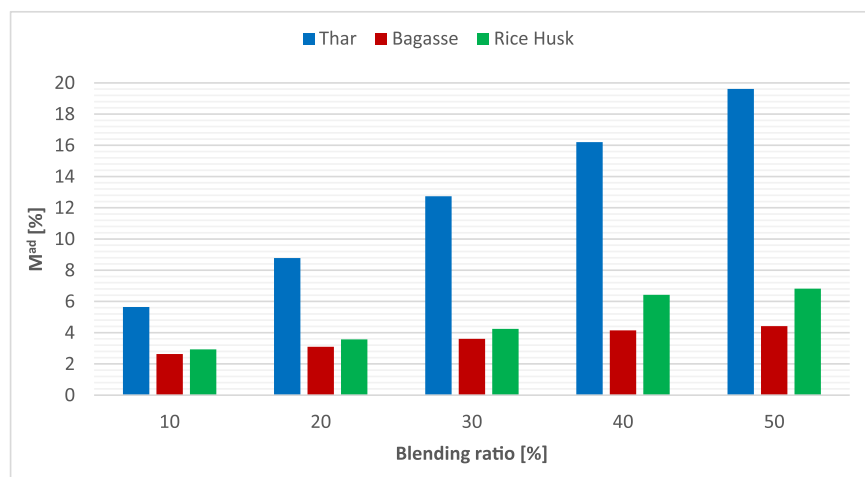The elemental analysis depicted that the parent bituminous coal has the lowest hydrogen content among

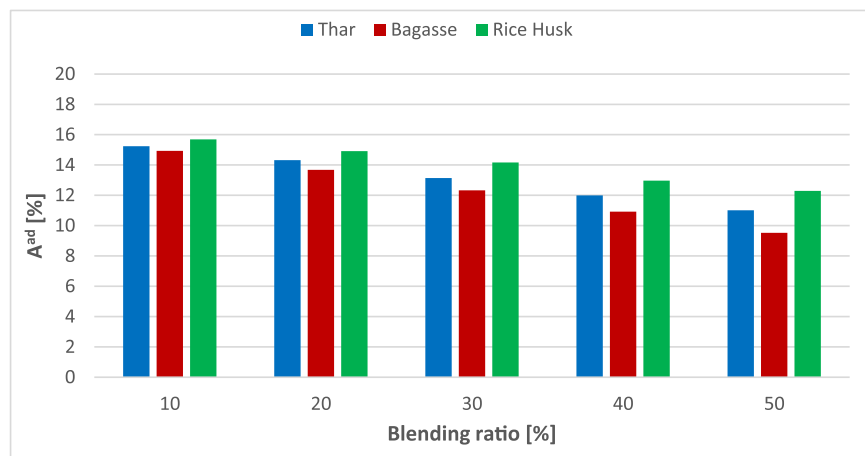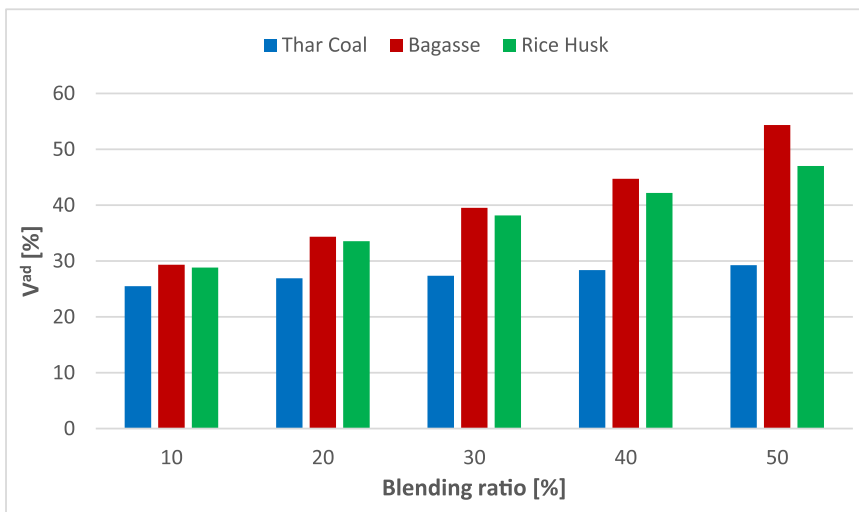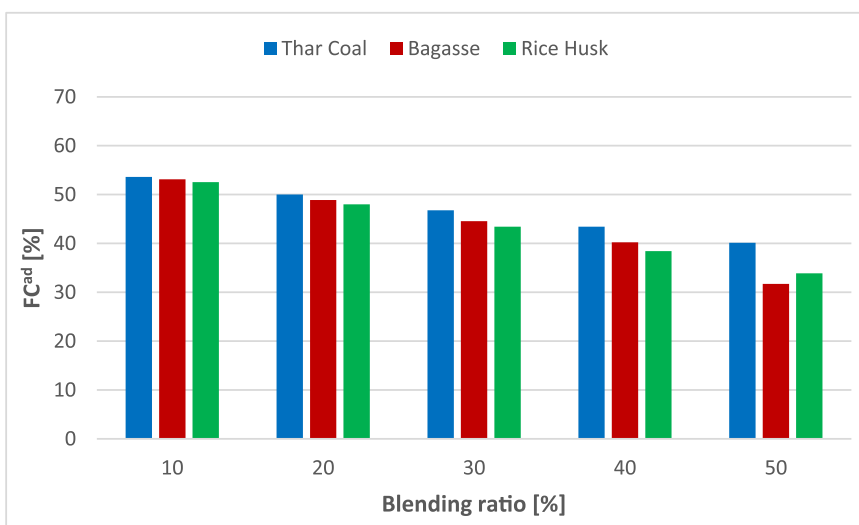FIGURE 2 The moisture content of blended fuel samples.

FIGURE 3 The ash content of blended fuels samples.

FIGURE 4 The volatile matter content of blended fuel samples.

FIGURE 5 The fixed carbon content of blended fuel samples.

all the considered fuels. Therefore the increase in the blending ratio leads to an increase in the hydrogen content of fuel blends (Figure 6).

Finally, the elemental analysis shows that lignite coal has the highest S content of all the considered fuels. On the other hand, the sulfur content of biomass is lower than that of the parent bituminous coal. That is why the sulfur content of a fuel blend increases with thar and decreases with the biomass fuels blending ratio (Figure 7).

The coal heating value test on the bomb calorimeter indicated that imported coal (bituminous coal) has the highest LHV. At the same time, the other three fuels are close in heating value lower than that of bituminous coal (Table 2). Consequently, the increase in the blending ratio leads to a decrease in blended fuels (Figure 8).

Blending 10%–20% thar coal with imported coal keeps us within the prescribed limits of boiler design with a small decrease in calorific fuel value and ash content, which decreases the ash loading in the fuel gas, but an increase in hydrogen content (almost 5%) and volatile matter. When a fuel with high volatile matter is blended with a fuel with moderate volatile matter, care must be practiced while dealing with coal mill outlet temperatures as such fuels are vulnerable to catching fire on their own.[1] With this much blending, a considerable decrease in coal imports will be observed, eventually decreasing coal shipping and transportation.

Coal transportation in the world from dock to the power station is majorly done by railway network because of the advantages over road transportation.[2] Still, this transportation leads to a rise in air pollution comprising particulate matter and trace metals, which pose a significant threat to the health of people lodging in the vicinity of these rail tracks. Fuel blending will lessen the transportation of coal, eventually leading to a reduction in the pollutants emitted.
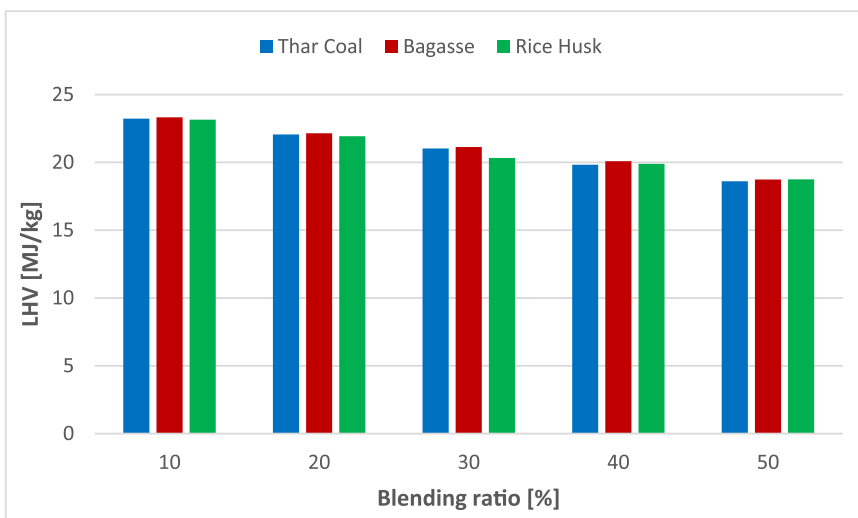
Biomass has a big advantage of very little sulfur content and less ash content in bagasse than coal. The
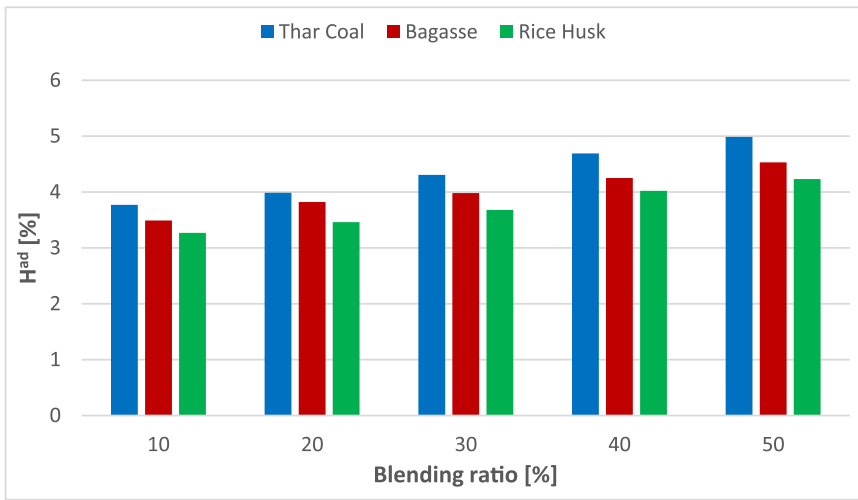
FIGURE 6 The hydrogen content of blended fuel samples.
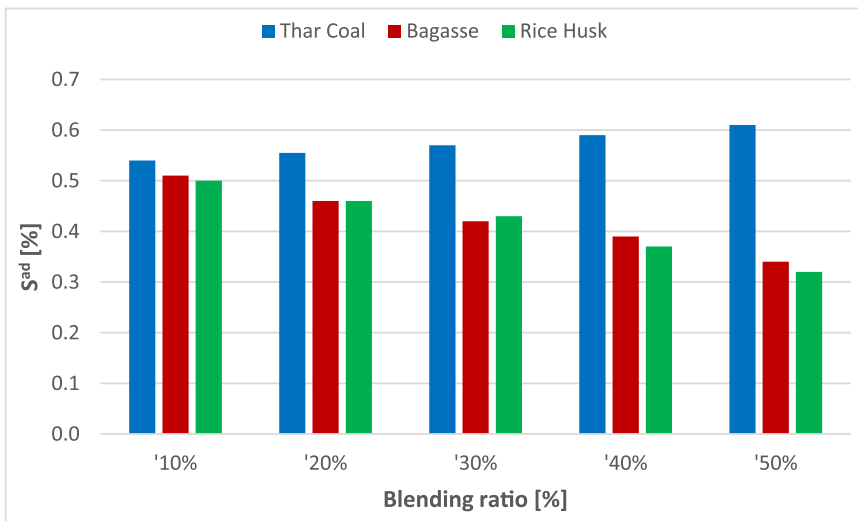
FIGURE 7 The sulfur content of blended fuel samples.

FIGURE 8 The lower heating value (LHV) of blended fuel samples.

blend of biomass with imported coal will not only lessen the sulfur dioxide emissions but also decrease the load on the sulfur desulphurization unit of the power plant. The blending proportion of 20% biomass with coal will be deemed appropriate for the boiler requirements without affecting the power generation. The fuel ratio, which is the ratio of fixed carbon to volatile matter, is an indication of flame stability, the lower the value higher will be the combustion efficiency. The fuel ratio of 20% bagasse blended with coal is 1.42, which is much lower than the pure coal fuel ratio of 2.32, indicating high combustion efficiency when biomass is mixed with coal.

3.2 | Development of a ML model

In this work, three data-driven modeling algorithms, namely Ridge Regressor, Nystroem Kernel SVM Regressor, and Linear Regressor, are deployed for modeling the lower heat value of the fuel blends against their characterized properties, for example, air-dried moisture (%), ash (%), volatile matter (%), fixed carbon (%) and hydrogen (%). The algorithms have demonstrated excellent performance in modeling lab-scale and enterprise-level systems.[25] Furthermore, the comparative performance analysis would enable the selection of the better-working model for the present study.[26]

Ridge Regressor is a high-level end-to-end procedure. It is an elastic net model based on block coordinate descent—a common form of derivative-free optimization. ElasticNet is a linear regression model trained with L1 and L2 as regularisers. This combination allows for learning a sparse model where few of the weights are nonzero like Lasso while still maintaining the regularization properties of Ridge. The model is named either Elastic-Net, Ridge or Lasso Regressor, depending on the value of the alpha parameter. ElasticNet is useful when there are multiple correlated features. While Lasso is likely to pick one feature randomly, ElasticNet is likely to pick both.[26]

Nystroem Kernel SVM Regressor and Linear Regressor are other interesting models considered in the study. Support vector machines are a class of "maximum margin" classifiers as they seek to maximize the separation they find between classes and can optionally include a penalty function that allows them to misclassify some observations for the sake of wider margins between the classes for the rest of the observations. Such an approach makes support vector machines a very robust class of ML models. SVMs are very efficient in high-dimensional spaces, and it also includes cases where the number of dimensions exceeds the number of observations. The model approximates the feature mappings,

which can significantly reduce learning costs with large data sets.[26]

The generalized linear model (GLM) is a flexible generalization of ordinary linear regression, and it allows for response variables with error distribution models other than a normal distribution. The GLM generalizes linear regression by permitting the linear model to be related to the response variable via a link function and by allowing the magnitude of the variance of each measurement to be a function of its predicted value.[26]

Among the dozen artificial intelligence modeling approaches,[24] AutoML or AML appears to be the most promising as it offers the ability to explore optimal hyper-parameters during the training process, known as hyper-parameter optimization (HPO), feature engineering and architecture search as the response to the traditional deep learning models, which performance highly depends on the neural networks topology.[22,27,28] To this end, we utilized the DataRobot platform (https://www.datarobot.com/), which employs an AutoML approach.[26]

DataRobot uses AutoML to build models that solve real-world problems across domains and industries. DataRobot takes the data you provide, generates multiple ML models, and recommends the best model to put into use. You do not need to be a data scientist to build ML models using DataRobot, but an understanding of the basics will help you build better models. DataRobot supports many different approaches to ML modeling—supervised learning, unsupervised learning, time series modeling, segmented modeling, multimodal modeling, and more.

This paper deals with supervised learning providing inputs and output data. In a regression project, the output, that is, the target is a numeric value. A regression model estimates a continuous dependent variable given a list of input variables (also referred to as features or columns).

DataRobot can simultaneously run numerous state-of-the-art open-source algorithms and deploy the best models in real-time. The system searches through various combinations of modeling approaches and selects the top models for implementation. A unique sequence of data processing, feature engineering, algorithm training, and algorithm tuning is termed a blueprint, which defines the selected modeling approach.[26] The software is capable of running multiple predictive models concurrently, thereby automating time-consuming model building and enabling the selection of high-quality, highly scalable models.[27,29–31]

The DataRobot software (https://www.datarobot.com/) belonging to the AutoML platform is used in the study.[26] The building process of predictive models covers several versions of each algorithm and loads of possible
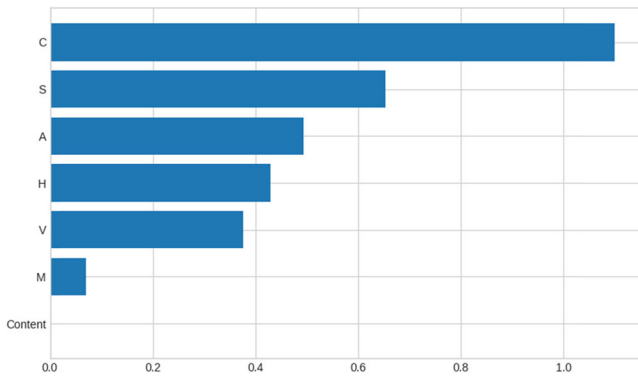
FIGURE 9 Mutual information scores for the input data sets.

data settings and preprocessing combinations. As a result, a Ridge Regressor was developed as a high-level end-to-end procedure for fitting the model. It stands for the elastic model using block coordinate descent—a common form of derivative-free optimization.[26]

Since better features make better models, feature engineering is one of the most critical steps in building a great ML model. The procedure allows for determining the essential features with mutual information (MI).[32] Consequently, feature engineering permits improving a model's predictive performance, reducing computational or/and data demands, and improving the results' interpretability.

During the first step, we construct a ranking of features with a feature utility metric. It is a general-purpose metric, that is, a function measuring associations between a feature and the target. This procedure allows us to choose a smaller set of the most valuable features to develop initially and lower computing time. The "MI" metric is more than a correlation as it can detect any relationship, while correlation only detects linear relationships. It is also easy to use and interpret, computationally efficient, theoretically well-founded, resistant to overfitting, and able to detect any relationship.[32] Roughly speaking, MI expresses how many questions one expects the feature to answer about the target. To be more precise, MI describes relationships between a feature and the target in terms of uncertainty. It is considered to measure the extent to which knowledge of one quantity reduces uncertainty about the other. This uncertainty is here measured using a quantity from information theory known as "entropy," where the entropy of a variable means roughly: "how many yes-or-no questions one would need to describe an occurrence of a variable, on average"; in other words, the more questions one has to ask, the more uncertain one must be about the variable.[32] Since the target is the real-valued function, we use the mutual_info_regression metric in the feature selection module of the Scikit-learn library to compute the MI

scores, in contrast to the mutual info_classif metric dedicated to categorical targets. The results, given in Figure 9, reveal that C (fixed carbon [%]) and S (sulfur [%]) content are the most important features, followed by A (ash [%]), H (hydrogen [%]), V (volatile matter [%]), M (air-dried moisture [%]). All six features exhibit a strong relationship with LHV and are selected for developing ML models.

The performance matrix is built on three parameters, namely, coefficient of determination (R^2), root mean squared error (RMSE) and mean absolute error (MAE). The performance indicators are introduced to evaluate the effectiveness of the models in modeling the LHV against the different combinations of the fuel blends, thereby selecting a better-performing model. The mathematical expression of the performance indices is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2}, \qquad (1)$$

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

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|, \qquad (3)$$

here, y_i and $\hat{y}_i$ are the actual and model predicted values for $i = 1, 2, 3, ..., N$. Similarly, $\bar{y}_i$ is the average of the actual value of the output variable. R^2 varies from zero to one, which signifies the no-correlation or perfect correlation among the actual and model-predicted responses. Similarly, RSME and MAE are the error terms calculated to estimate the error present in the model's responses.

The calculation and model development procedure generated 91 different AI models. The above-described metrics, that is, R^2, RMSE, and MAE measured for the Linear Regressor, Nystroem Kernel SVM, and Ridge Regressor models under the validation, cross-validation, and holdout are computed and presented in Figure 10A–C, respectively. The data-distribution curves are also constructed along the axes of Figure 10A–C depicting the modeling performance and learning the distribution profiles of the target variable by the models.

The true and model-based responses to predict the LHVs of the fuel blends are presented in Figure 10A–C. Closely observing the performance metrics of the three models, it is found that the Ridge Regressor model has presented better performance than the Linear Regressor and Nystroem Kernel SVM. The R^2 value for validation
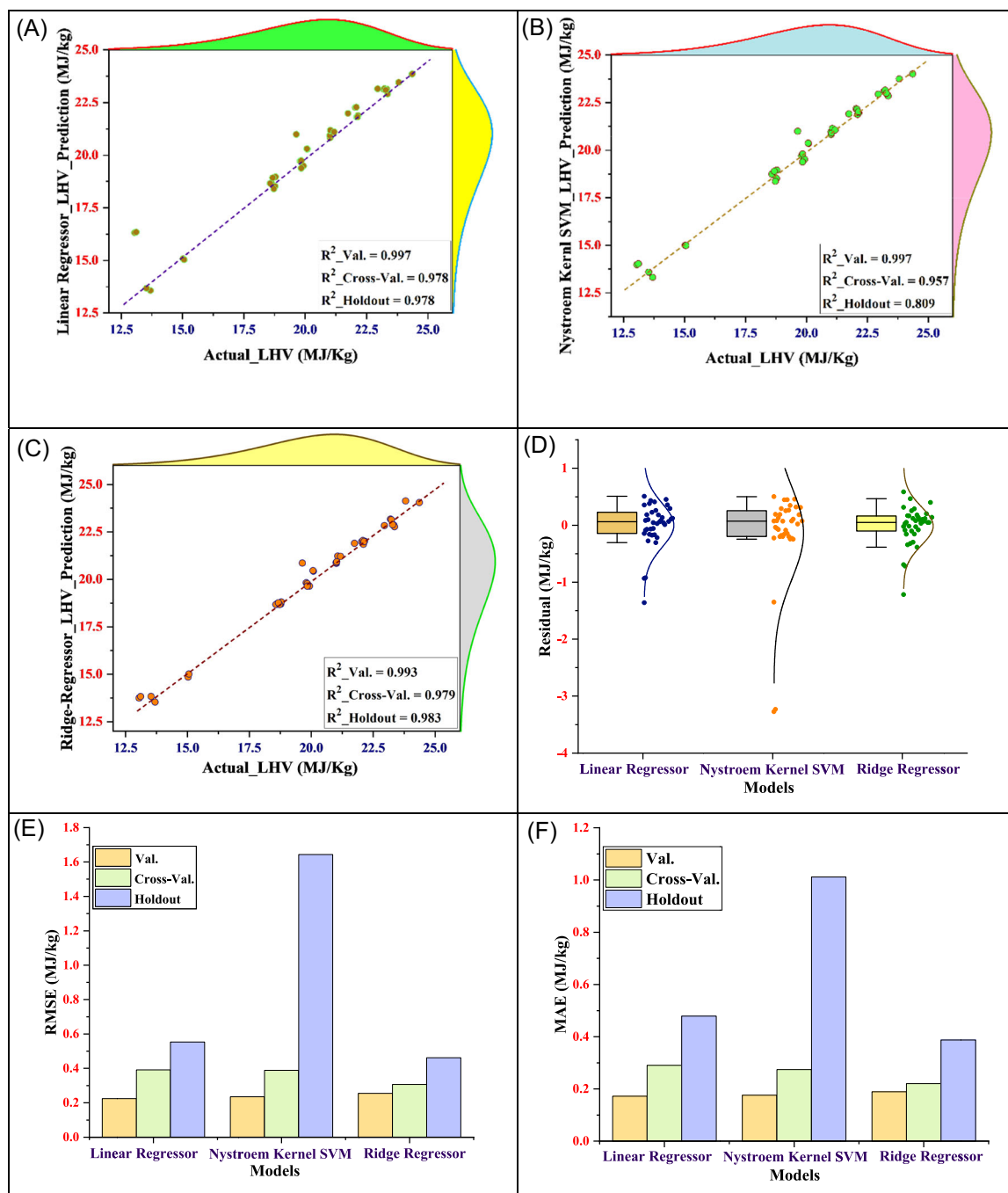
FIGURE 10 Modeling performance comparison of Linear Regressor, Nystroem Kernel SVM, and Ridge Regressor. The modeling performance is measured for three different data sets, that is, Validation, Cross Validation and Holdout. The coefficient of determination (R^2) is measured between the actual and model simulated responses and presented for (A) Linear Regressor, (B) Nystroem Kernel SVM, and (C) Ridge Regressor. The residual measured for the model-predicted responses are shown in (D). Similarly, RMSE and MAE calculated for the three models' responses are presented in (E) and (F), respectively.

(R2_Val.), cross-validation (R2_Cross-Val.) and holdout (R2_Holdout) are 0.993, 0.979, and 0.983, respectively which is quite close to those of the Linear Regressor and Nystroem Kernel SVM. Similarly, the residuals for the three model-based predictions are also calculated and presented in Figure 10D. The residuals are the highest for

the Nystroem Kernel SVM model. In contrast, linear and Ridge Regressor-based models have nearly the same distribution of residuals around zero depicting the good predictive performance of the models. To compute the error among the model simulated responses and the actual values, RMSE and MAE are calculated and

presented in Figure 10E,F, respectively. Comparing the RMSE and MAE of the three models for validation, cross-validation, and holdout data sets, it is found that Ridge Regressor has presented the superior performance in terms of comparatively the lower errors measured for its predictions. The errors computed for the Ridge Regressor, that is, RMSE and MAE under validation, cross-validation, and holdout data sets are 0.2550, 0.3067, 0.4618, and 0.1893, 0.2203, 0.3870 MJ/kg, respectively which are comparatively lower than those of Linear Regressor and Nystroem Kernel SVM. The superior modeling performance of Ridge Regressor to predict the LHV of the fuel blends in demonstrated, and the model can be applied to conduct the model-based simulation and optimization analysis for the design of optimum fuel blends to support the zero emissions optimization of the power plant. Thus, in future work, comprehensive model-based optimization analysis using mechanistic and evolutionary optimization techniques would be conducted to select an optimum fuel blend that can support the power generation as demanded from the grid and reduces the emissions discharge as well.

4 | CONCLUSIONS

In the paper, we employ ML models to predict the LHV of bituminous fuel blends with lignite and biomass of different shares. The South African imported bituminous coal, lignite thar coal extracted from the Thar Coal Block-2 mine, sugarcane bagasse and rice husk are analyzed in the paper. The results show that models generated using the AutoML platform exhibited acceptable performance levels in predicting LHV. However, the best model is the Ridge Regressor with the R^2 value for validation, cross-validation and holdout equal to 0.993, 0.979, and 0.983, respectively. The model can be easily applied to predict the LHV of the considered fuel blends.

Using biomass, we can quickly deal with evolving anthropogenic issues, that is, greenhouse gases and organic pollutants emissions.[33–35] It will also be advantageous for the environment as it is a green waste which will replace fossil fuels. Its abundance near the power plant will resolve the availability issues, and its storage in the fuel yard can also offset the seasonal changes. Furthermore, model-based optimization analysis would be conducted to design the optimum fuel blends supporting the power generation and emissions discharge from the plant.

NOMENCLATURE

A   ash content (wt.%)
FC   fixed carbon content (wt.%)
H   hydrogen content (wt.%)
M   moisture content (wt.%)
S   Sulfur content (wt.%)
V   volatile matter content (wt.%)

SUPERSCRIPTS

ad   air-dried basis

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