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Biomass Briquettes for Sustainable Steam Production in Industries: Experiments, Thermodynamics Simulation and Explainable AI

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Abstract

Growing trends in sustainable production of energy in industries have fuelled the need for sustainable alternatives for the conventional sources of energy in industries. The current study investigates the use of briquette fuel made from agricultural and industrial waste material as an alternate fuel for the production of steam in industrial boilers through experimental analysis, thermodynamic simulation using Python and Machine Learning (ML) techniques. It was found that the tested biomass briquette fuel possesses good characteristics such as low moisture content (8-12%) and increased calorific value (3500-4800 kcal kg^{-1}). The economic analysis results showed a saving of Rs. 7,333 per day and Rs. 26.76 lakhs annually when biomass briquettes were used in place of firewood. Based on the Python program code developed, the maximum furnace temperature was estimated to be 1678 K, average furnace temperature was estimated to be 1320 K, rate of steam generation at 2120 kg h^{-1}, boiler efficiency at 81.6%, carbon dioxide emissions at 512 kg h^{-1} and NOx at 182 ppm. The performance of the machine learning algorithms such as XGBoost, LightGBM and CatBoost was outstanding, where XGBoost yielded the highest accuracy level (R^2 = 0.98). From SHAP analysis, it was clear that furnace temperature and fuel feed rate were key parameters for controlling boiler efficiency.

Keywords: *Sustainable energy; Biomass briquettes; Industrial boiler; Thermodynamic simulation; Machine learning; XGBoost; SHAP analysis*

1. Introduction

Biomass briquettes (BBs) have become popular renewable energy sources due to the high efficiency with which they can be used in converting agricultural wastes, forestry waste and industrial wastes into energy-rich solid fuels with better properties than traditional biomass fuels, especially as regards transportation, handling and storage while reducing reliance on fossil fuels and preventing pollution [1]. However, one major limitation associated with briquettes is their low energy output as a result of high moisture content, high ash content and slugging tendency. Pretreatment aimed at enhancing the combustion process of biomass briquettes, especially those made from lignocellulosic material like rice husk, groundnut shells, corn cobs and sugarcane bagasse [2]. Thermal treatment involving torrefaction followed by densification recognized as an efficient process for improving energy content, hydrophobicity, grindability and combustion properties of briquettes [3]. Besides thermal processes, chemical modifications have also been effective in improving briquette quality. Acid pretreatment of biomass mixtures has proved to be effective in decreasing non-combustible components while increasing energy yield in briquettes, especially those that contain rice husk and sawdust [4]. In addition to the enhancement of fuel characteristics, commercialization and economic benefits of producing biomass briquettes from abundant agricultural wastes that offer economical solid biofuel sources with profitability and potential for application in decentralized and industrial energy generation [5]. Moreover, production of biochar briquettes using tapioca sago wastes after their alkaline pretreatment and carbonization has been shown to result in enhanced fuel properties, suggesting that solid biofuels can be effectively produced from agricultural waste streams [6, 7].

The role of the quality of the fuel used and boiler operation parameters in influencing boiler performance of briquettes made using sawdust, cocoa shells, corn cobs, palm kernel shells and coconut husks, whose properties with suitable fuels for sustainable boiler use while facilitating the shift towards cleaner industrial heat generation [8]. In order to ensure optimal boiler operation and environmental performance due to the variation of combustion characteristics according to fuel type, monitoring and control techniques have become essential and a technique that involves using intelligent detection technology based on deep learning algorithms to detect the fuel type of briquettes for use in boilers has been suggested [9]. The numerical simulations of biomass fuel combustion in large-scale thermal systems showed how properties of the fuel, methods of delivery and combustion, among others, impact energy conversion efficiency, carbon

emissions and boiler stability [10]. With the aim of improving boiler performance, prediction and optimization techniques integrating data analysis, knowledge, uncertainties and multi-criteria decision making have been devised to satisfy energy efficiency and low pollutant emission objectives of biomass combustion [11]. Predictive capabilities of emission products and carbon dioxide emissions is still a difficult problem owing to the complicated internal combustion environment in the boilers used in industries and sophisticated AI model can estimate the spatial pattern of parameters related to combustion and help low carbon burning in the boilers by monitoring and predicting [12]. Apart from optimizing the process of combustion, another issue that needs to be considered is that of the durability of materials at high temperatures, whereby studies on fireside corrosion mechanisms have offered valuable information on this matter [13, 14].

Conversion of agricultural waste into briquettes provides an efficient approach towards mitigating the adverse impact of biomass burning in open fields, an important source of atmospheric contamination and carbon emissions, while at the same time making the fuel more manageable, improving combustion efficiency and energy utilization [15]. Emissions of briquettes are known to be affected by the type of biomass utilized, the quantity of ash, heterogeneity of the biomass and densification process parameters, influencing the combustion efficiency, emissions and overall thermal behavior [16]. Recent research has indicated that variations in the composition of biomass used can greatly influence calorific value, combustion efficiency, ash generation and emission of gases, underscoring the need for proper selection of biomass to enhance efficiency [17]. It has been shown in field experiments that utilization of specially formulated briquettes can help minimize emissions and material losses while ensuring adequate heat generation under practical conditions [18]. Moreover, advanced thermochemical treatments of biomass prior to conversion into briquettes including torrefaction have yielded positive results regarding their energy efficiency, lower moisture content and reduced emissions when utilized thermally [19, 20].

BB obtained from biodegradable wastes and biochar have desirable fuel properties, thus providing a green approach in improving energy production without relying on traditional sources of energy [21]. During the densification process, the amount of compaction pressure is crucial in determining the fuel quality, thermal conversion, alkali metals emission, among other parameters and hence the efficiency of the boiler system [22]. Several types of biomass wastes

were processed and made into briquettes with an enhanced calorific value and energy yield, thus demonstrating their ability to provide heat energy through combustion processes [23]. Several studies carried out with regards to emissions revealed that the proper optimization of the burning process could greatly lower NOx emission levels while still maintaining stable heat energy supply and hence biomass briquettes make a viable alternative fuel source for boilers [24]. Optimization of briquette preparation process has also been found to considerably influence several physical parameters such as density, fixed carbon content and calorific value [25]. Another method that has been noted as an effective approach to minimize GHG emissions while optimizing the efficiency of fuel burning is the inclusion of biomass as fuel in the industrial steam production process [26]. Mathematical studies have also proven the need for combustion optimization and heat transfer enhancement to increase efficiency and minimize pollution emissions from the boiler [27,28].

The incorporation of Machine Learning (ML) technology into biomass energy processes has provided promising ways to improve fuel quality prediction, combustion processes and process automation. In this regard, the application of recent developments proves that ML techniques can be effectively applied to enhance manufacturing processes through intelligent prediction, optimization and decision-making in sophisticated engineering tasks, thus contributing to the creation of data-driven and sustainable production processes [29]. In relation to biomass briquetting processes, it is possible to state that ensemble ML techniques have been applied successfully to predict the quality of briquette based on its physico-mechanical parameters, minimizing the necessity for expensive and lengthy experiments [30]. Also, ML classifiers used to discriminate between various feedstocks that are optimal for biomass briquette production [31]. Prediction of combustion properties, physical parameters and emissions of biomass briquettes using ML technologies [32].

However, the significant improvements have been made in the use of biomass for energy production, most of the current literature mainly deals with predictions of briquette quality, feedstock categorization, or optimization of combustion variables. Little emphasis has been paid on the development of an integrative method involving assessment of biomass briquettes in industrial boilers by integrating fuel characteristics, boiler efficiency, emissions, Python programming and explainable ML models. Thus, the novelty of the current work is the development of an integrated approach that integrates experimental testing of boiler efficiency

and performance with ML and SHapley Additive exPlanations (SHAP). The major research gap identified in the current literature is lack of comprehensive assessments of the effects of biomass briquettes on boilers, fuel efficiency, emissions and modeling of the relationship between them using artificial intelligence methods. This research aims at assessing BB as an alternative fuel for boilers by fuel characterization, efficiency testing, emissions assessment, Python-assisted simulation of combustion, prediction using ML and Explainable Artificial Intelligence (XAI). The flowchart shown in Figure 1 shows the process flow employed in this study. Biomass residues from agriculture and industries are subjected to drying, sizing, briquetting, cooling and storage operations for the production of biomass briquettes. Fuel characterization and performance testing of biomass briquettes in boilers are performed, which include calorific value, moisture content, ash content, combustion rate and emission testing.

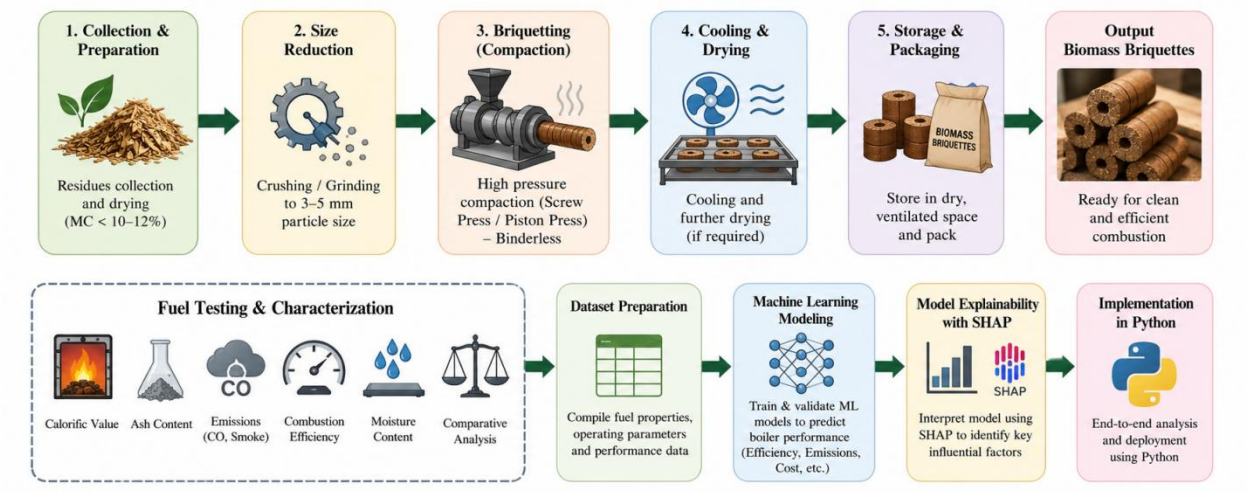


Fig. 1 Integrated Workflow for BB Boiler Performance and ML-SHAP Analysis

2. Materials and Methods

In this research, a comprehensive system of assessment of biomass briquettes as a green renewable fuel resource for steam production in industry is proposed. This methodology includes processes of biomass briquettes production, characterization, experimental assessment of boiler performance, emissions and fuel comparisons, followed by modeling. In the first stage, agricultural and industrial biomass waste was treated using dehydration, size reduction, compaction, cooling and storage operations.

2.1 Biomass Briquette Preparation and Characterization

Biomass briquettes were fabricated through a sequential densification process using agricultural and industrial biomass residues as feed stocks to generate a consistent and energy-rich solid fuel product suitable for use in boilers for industrial operations.

First, readily available agricultural and industrial biomass residue samples were collected and underwent preliminary cleaning processes to remove any undesirable impurities like stones, dust and other extraneous substances. The collected biomass was dried under controlled drying conditions to lower the moisture level to less than 10-12 wt.% which was considered ideal for effective briquetting and burning of biomass material. Moisture control is very important because excess moisture decreases the calorific value of biomass briquettes and hence reduces their energy efficiency. It also negatively impacts briquette durability and storability.

After proper drying, the collected biomass was size-reduced to produce relatively uniform particle sizes through crushing and grinding processes. Particle size was kept within the range of about 3-5 mm so that the biomass could be homogeneously mixed and smoothly fed into the briquetting machine.

After this, the processed biomass particles were then used for making the briquettes using a high-pressure briquetting machine with a screw press or piston press type. Briquetting process involved binder-free technology where the natural lignin in the biomass served as an intrinsic binder due to high temperature and pressure. During the process of compaction, the mechanical interlocking and thermoplastic behavior of the lignin were exploited to obtain cylindrical briquettes without using additional binders or any chemicals. The use of binder-free process increases fuel purity, reduces costs and is environmentally sustainable. Once the briquetting process was completed, the newly formed briquettes were left to cool down at room temperature. The cooling step enables the solidification of softened lignin and mechanical stabilization of briquettes. Additional drying was done, whenever needed, in order to ensure removal of moisture and increase durability. After being cooled and dried, the briquettes were then stored under dry and ventilated conditions to avoid moisture intake and deterioration of briquette quality before its usage. Proper packaging was employed for transportation purposes and storage of the briquettes.

Characterization of the produced biomass briquettes was undertaken to ascertain their capability as a fuel source in high-pressure steam boilers. A proximate analysis of the briquettes was done based on ASTM D3172 to measure moisture, volatile matter, ash and fixed carbon. These tests

provide important information about the combustion characteristics, ignition characteristics, formation of ash residues and general fuel quality. An ultimate analysis was undertaken based on ASTM D5373 to measure the elemental composition of Carbon (C), Hydrogen (H), Nitrogen (N), Sulfur (S) and Oxygen (O). This test is crucial in understanding the combustion processes involved, as well as the emissions that can be formed from the process. Higher heating value or the calorific value was measured based on ASTM E711 using a bomb calorimeter. The results obtained from the proximate analysis, ultimate analysis and calorific value of the briquettes were used in comparative fuel evaluation, boiler performance evaluation, emissions analysis and ML modeling for performance prediction.

2.2 Experimental Study of Boiler Performance and Emissions

Biomass briquettes (BB) were investigated as an alternate fuel by conducting experiments on a high-pressure industrial steam boiler under normal production operations. The main purpose of the investigation is to analyze the performance, fuel consumption, efficiency, emission characteristics and economic viability of the use of BB as fuel compared to regular fuels. The experimental boiler test rig includes the combustion chamber, fuel feeding system, steam generation, pressure measuring device, temperature measuring equipment and exhaust gas release device.

Figure 2 shows the manufactured biomass briquettes that result from the compaction of biomass residues from both agriculture and industries without the use of binders. The briquettes have a compact cylindrical structure, which suggests that the briquettes have appropriate mechanical strength that would allow for convenient handling and storage, as well as transport, for use in boilers.



Fig. 2 Manufactured biomass briquettes

Figure 3 shows the apparatus used for testing combustion efficiency of the biomass briquettes within an experimental boiler system. The boiler testing apparatus comprises biomass briquette

fuel hopper, screw feeder, combustion chamber, steam boiler, pressure gauge, safety valve, temperature gauge, water level gauge, feed water inlet, Forced Draft (FD) blower, ash pit, steam outlet and data acquisition system.

Before conducting the experiment, the boiler was checked for its stable operations and then started for testing. The manufactured BB was introduced into the boiler at a controlled rate for its stable operations. During the running period of the boiler, parameters such as fuel consumption rate, steam generation rate, pressure and furnace temperature and exhaust gas were recorded. Based on the recorded data, thermal efficiency was calculated.

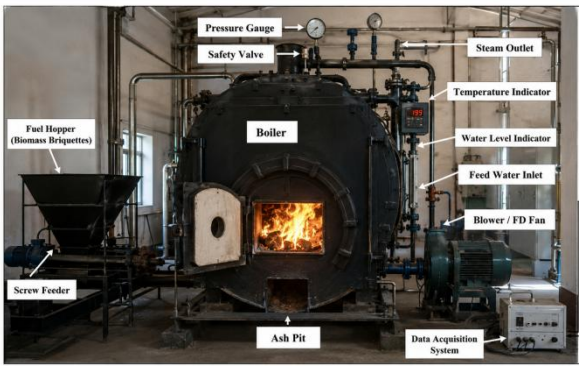


Fig. 3 Experimental Setup for BB Boiler Performance Evaluation

Boiler efficiency was calculated according to the standards outlined in the ASME Performance Test Code 4 (ASME PTC 4). The calculation was based on the ratio between the useful heat produced for steam production and the total amount of heat energy that resulted from the burning of fuel. The total energy consumption was calculated using the steam produced the fuel flow rate and the fuel calorific value. It is worth noting that the above methodology facilitated the comparison of energy usage performance of BB relative to that of firewood, coal and furnace oil. Effective energy output was calculated using the fuel's calorific value and thermal efficiency. The amount of biomass briquettes, firewood, coal and furnace oil needed to produce the desired energy output was then calculated. Furthermore, an analysis of the daily, monthly and yearly cost of burning biomass briquettes, firewood, coal and furnace oil was done based on the market prices of the fuels mentioned.

Measurement of emissions was done to assess the environmental efficiency of burning biomass briquettes. The emissions produced during the burning process of biomass briquettes in the boiler were tested in accordance with the method provided by the United States Environmental Protection Agency (EPA) emission testing approach. The assessment of emissions was done

based on major pollutants which were Carbon Monoxide (CO), Carbon Dioxide (CO_2) and the visibility of the smoke. These pollutants are considered as a criterion, which related directly to the combustion process, environmental effects and efficiency of the combustion process. The results of the experiments conducted for the measurement of fuel properties, boiler performance tests and emissions have been recorded comprehensively.

2.3 Python-Based Simulation, Machine Learning and SHAP Analysis

From the measurements, the properties of experimental fuels, the operation parameters of boilers, the performance of fuels compared to each other and parametric simulations have been used. In total, there were 120 observations made from realistic operating conditions considering the experimentally designed biomass briquettes. In addition to these, there were input and output variables, where the input variables included moisture, ash, fixed carbon, volatiles, carbon, hydrogen, oxygen, nitrogen, sulphur, fuel flow rate, air/fuel ratio, percent excess air, boiler pressure and furnace temperature. Output variables included heat input, steam production rate, boiler efficiency, specific fuel consumption, CO, CO_2, NOx, SO_2 and particulate matter (PM), cost of steam production per ton and carbon footprint reduction.

Table 1. Input and Output Variables for Python-Based Simulation, ML & SHAP Analysis

Variable Type	Category	Variables
Input Variables	Proximate Analysis	Moisture Content (%), Ash Content (%), Fixed Carbon (%), Volatile Matter (%)
	Ultimate Analysis	Carbon (%), Hydrogen (%), Oxygen (%), Nitrogen (%), Sulfur (%)
	Operating Conditions	Fuel Feed Rate (kg/h), Air-Fuel Ratio, Excess Air (%)
	Boiler Parameters	Boiler Pressure (bar), Furnace Temperature (°C)
	Thermal Performance	Heat Input (kW), Steam Generation Rate (kg/h), Boiler Efficiency (%)
	Fuel Performance	Specific Fuel Consumption (kg/kWh)
Output Variables	Emissions	Carbon Monoxide (CO, ppm), Carbon Dioxide (CO_2, %), Nitrogen Oxides (NOx, ppm), Sulfur Dioxide (SO_2, ppm), Particulate Matter (PM, mg/m^3)
	Economic Performance	Cost per Ton Steam (Rs./ton)
	Sustainability Performance	Carbon Footprint Reduction (%)

All the variables used as inputs and outputs in the simulation, modeling process and SHAP analysis using Python as displayed, Table 1. The variables include fuel properties, boiler

operation, thermal efficiency, emissions, economics and sustainability to evaluate the viability of biomass briquettes for use in industrial boilers.

Boiler simulation based on Python language was designed in order to assess the influence of different parameters on the performance and emission properties of the boiler system. This simulation included data on the characteristics of the fuel used and thermodynamic relations that govern the process of energy conversion and water vapor generation. All numerical and statistical computations were done using NumPy and Pandas. Thermodynamics computations were done with the help of SciPy library. Visualization of results was done by means of Matplotlib and Plotly software. The simulation allowed for the estimation of heat input, steam generation rate, efficiency and emission properties depending on different fuel characteristics.

After the simulation process was completed, several ML models were constructed in order to derive dependencies between the independent and dependent variables in the dataset. Before constructing predictive models, all available data was preprocessed to ensure data validation and normalization as well as some feature scaling if necessary. Then the dataset was split into training and testing subsets. Algorithms that are known for their effectiveness in prediction of nonlinear relationships and multi-dimensional variables in technical applications include ensemble learning techniques, namely Extreme Gradient Boosting, Light Gradient Boosting Machine and CatBoost.

The performance of the proposed models was analyzed using statistical measures such as Coefficient of Determination (R^2), Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). These measures were used to evaluate the performance of prediction and determine the better machine learning algorithms used in the study. The selected machine learning algorithm based on the prediction measure was used to analyze features for its performance.

In order to provide greater model interpretability, SHAP were used to interpret the optimized machine learning model. SHAP is a game-theoretic-based approach for XAI. It provides an understanding of how the input attributes contribute towards the model output by providing a contribution value to each attribute. This measure helps in determining the key parameters affecting the boiler system regarding efficiency, fuel, emissions and sustainable performance. The use of integrated simulations with ML and SHAP analysis, as proposed in this work, is a very powerful tool for the evaluation of biomass briquette utilization as industrial boiler fuel.

3. Result and Discussion

The physicochemical characteristics of the prepared biomass briquettes are investigated to ascertain whether they are suitable for use as fuel for generating power. The performance of the high-pressure steam boiler is further assessed on the basis of its characteristics such as consumption of fuel, production of steam, efficiency of the boiler and energy use efficiency. The environmental impact of the biomass briquettes is then assessed by contrasting emission profiles of different energy sources.

3.1 Fuel Properties Analysis and Boiler Performance Evaluation

The properties of biomass briquettes have been analyzed and compared to other types of fuels in order to ascertain the applicability of the fuel for industrial steam production.



Fig. 4 Comparative Fuel Property Analysis

The importance of fuel properties cannot be understated in relation to combustion efficiency, heat transfer performance, rate of fuel consumption, formation of emissions and general boiler performance. The characterization of the fuel indicates that biomass briquettes are advantageous when compared to firewood and offer comparable thermal properties to commercial solid fuels.

The analysis of the relative fuel properties is illustrated in Figure 4. This shows that BBs contain lower moisture content (8-12%) compared to firewood (20-60%), which enhances their burning capacity and energy efficiency. The reduction in moisture content increases the amount of heat produced for steam production since less heat is lost through the process of vaporizing water from the fuel. Biomass briquettes also have higher calorific value between 3500 and 4800 kcal/kg when compared to firewood. Furthermore, BBs were less prone to generating excessive amounts of ash compared to firewood. This improvement in fuel qualities has affected the performance of the boiler positively. The greater calorific value and low water contents of the briquettes led to more stable burning and better flame and thermal efficiencies than the traditional firewood used. Moreover, the briquette being solid in form is easy to handle, transport and store, thus eliminating some problems that come with bulk fuels like biomass. Another benefit of using briquettes was cleaner combustion that translated to reduced smoke and carbon monoxide emissions, thereby promoting environmental performance.

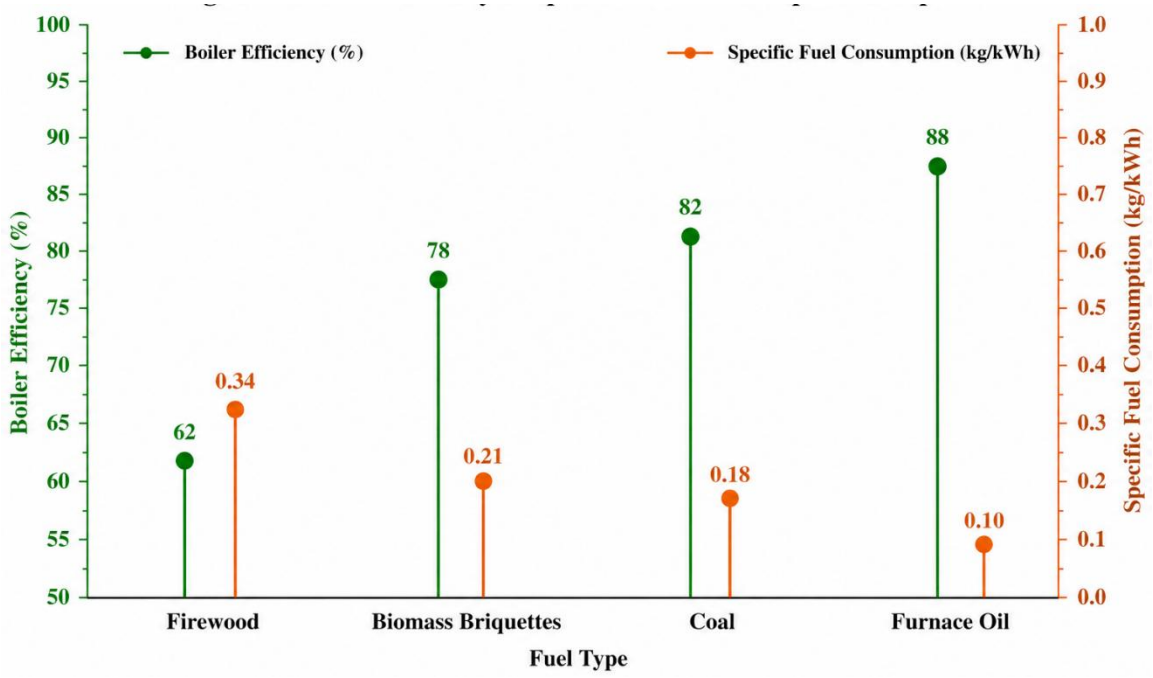


Fig. 5 Boiler Efficiency & Specific Fuel Consumption

Effect of fuel type on boiler efficiency and Specific Fuel Consumption (SFC) has been demonstrated in figure 5 below. There is clear evidence of an inverse relation between the two for the analyzed types of fuels. Firewood was noted to have low boiler efficiency (62%) and high SFC of 0.34 kg/kWh, which was mainly attributed to its high moisture content and poor calorific value. On the other hand, biomass briquettes were seen to have high boiler efficiency (78%), with their specific fuel consumption being reduced to 0.21 kg/kWh. This was possible since biomass briquettes have better fuel quality in terms of moisture content, calorific value and energy density. Both coal and furnace oil showed a high rate of efficiency based on their calorific values, but on the downside, both fuel types generate significant carbon emissions. It was thus concluded that biomass briquettes show favourable results in regards to thermal efficiency, fuel consumption, environmental issues and cost effectiveness.

Table 2. Boiler Performance, Emission and Economic Comparison of Different Fuels

Parameter	Firewood	Biomass Briquettes	Coal	Furnace Oil
Moisture Content (%)	20–60	8–12	10–15	<1
Calorific Value (kcal/kg)	2500–3500	3500–4800	5500	9500
Boiler Efficiency	Low	High	High	High
Ash Content	High and Variable	Low and Consistent	Moderate	Negligible
Emissions	High Smoke and CO	Low Smoke and Cleaner Combustion	High CO_2 and SO_2	High CO_2
Fuel Requirement (ton/day)	13.51	8.46	7.90	4.53
Cost per Ton (Rs.)	4300	6000	7000	18000
Total Cost per Day (Rs.)	58,093	50,760	55,300	81,540
Environmental Impact	Deforestation Risk	Renewable and Eco-friendly	High Carbon Emissions	Fossil Fuel Based
Industrial Suitability	Moderate	Excellent	Excellent	Excellent

Comparison in terms of performance and economic analysis of boilers fueled by different types of fuels has been illustrated in Table 2. For example, using the assumption of a daily requirement of 40 MWhs of energy and a boiler efficiency of 80%, the amount of biomass briquettes required was 8.46 tons while the firewood required would be around 13.51 tons. There would obviously be a huge saving of about 5 tons of fuel due to the high energy content of biomass briquettes.

However, coal and furnace oil needed lower amounts of fuel since their calorific values are very high.

From an economic point of view, biomass briquettes proved more feasible than other sources of fuel. BBs were found to have a daily operation cost of Rs. 50,760 which was less than the daily cost of firewood (Rs. 58,093), coal (Rs. 55,300) and especially furnace oil (Rs. 81,540). The use of biomass briquettes helped save Rs. 7,333 every day which amounted to an annual saving of Rs. 26.76 Lakhs. This shows that there was a 12.62% cost saving in using BBs.With regard to the environment, it is evident that the biomass briquettes produced relatively clean burn patterns with low levels of smoke formation and lower carbon monoxide production than wood. The environmental benefit of using a renewable fuel source is also a factor that helps minimize the carbon footprint involved in producing heat through the use of renewable bioenergy. In consideration of the above factors, it is evident that biomass briquettes provide a practical alternative to boiler fuels.

3.2 Python Thermodynamic Boiler Simulation

The development of the thermodynamic simulation for the combustion of biomass briquettes in the industrial steam boiler was done using Python programming. The simulation is designed for the prediction of various performance metrics in biomass briquette combustion in an industrial steam boiler. Experimental data from the experiments were used in establishing the input parameters of the simulation. The computation of numerical values was done using NumPy and Pandas packages in Python, whereas calculations of thermodynamics and energy balance were done using SciPy. The purpose of developing the simulation software is to determine heat input, temperature distribution in the furnace, steam generation rate, efficiency of the boiler and emissions. The input parameters that have been considered in designing the thermodynamic simulation include moisture content (10%), ash content (6%), fixed carbon (18%), volatile matter (66%), fuel feed rate (500 kg h^{-1}), air-fuel ratio (2.2) and excess air (20%). Such parameters were considered due to their experimental values of biomass briquettes, which were obtained during tests in boiler trials. In addition, the calorific value of the biomass briquettes has been estimated to be 4386 kcal kg^{-1} (18.36 MJ kg^{-1}). This is the average value obtained in biomass characterization analysis.

The temperature profile inside the furnace was modeled based on heat transfer relations and combustion energy balance equations. The results of the heat simulation performed using the

developed computer codes in Python are shown below in Figure 6. The region with the maximum temperature values was found inside the zone of primary combustion next to the burner, where temperatures reached 1678 K. These temperature values indicate that the maximum region is located in the zone of maximum volatile emissions and oxidation of fixed carbon.Based on the conducted simulation, the average value of the temperature inside the furnace was about 1320 K. According to the results available in literature, the average temperature values in biomass-fired industrial boilers range between 1143 K and 1346 K. The temperature in the superheater region was higher due to radiation from the combustion chamber, whereas in the economizer region, temperature values were lower due to heat absorption from the flue gases.

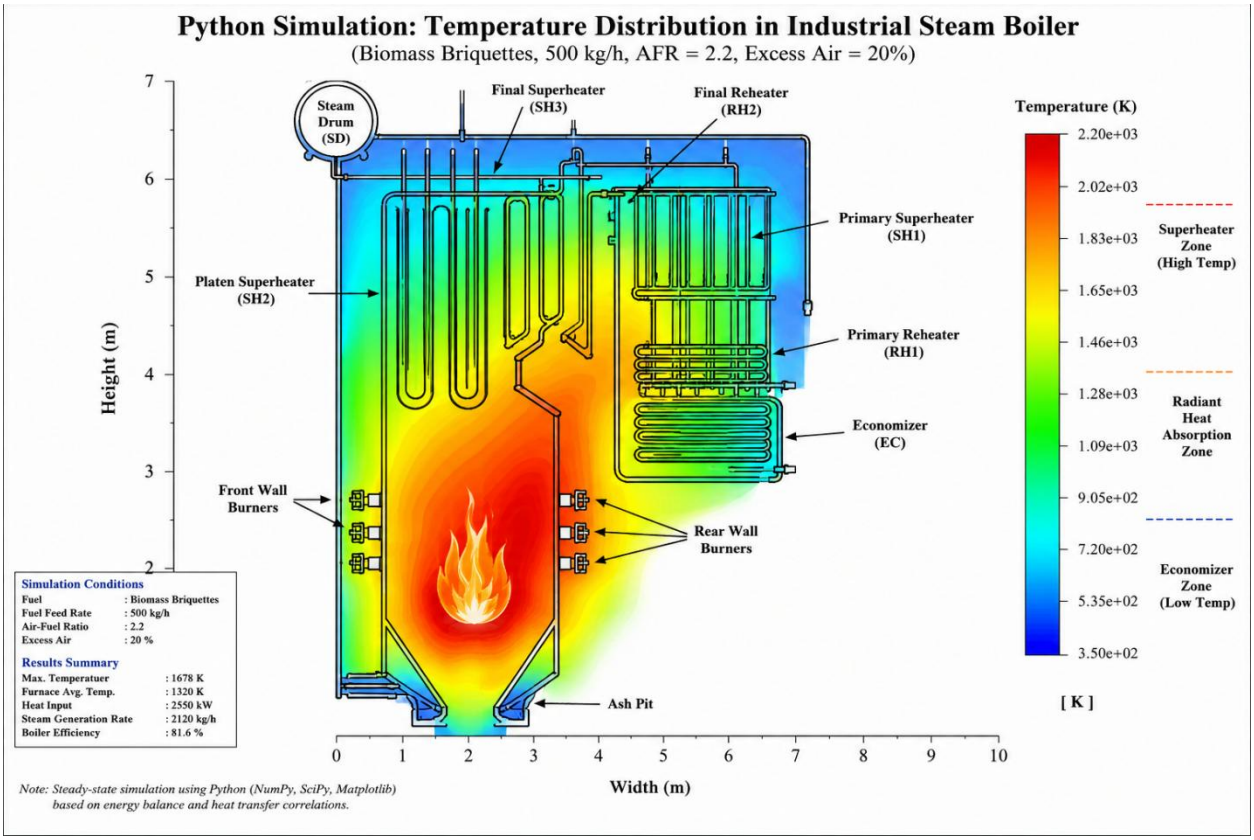


Fig. 6 Python-based thermodynamic simulation for temperature distribution

Furthermore, it is important to note that the simulated efficiency of the proposed boiler design using the given parameters was about 81.6%, which correlates with high-efficiency combustion behaviour of biomass briquettes. This increase in efficiency may be explained by reduced latent losses due to low moisture content, increased calorific value and stability of combustion process compared to common firewood. In addition, the developed simulation approach was used to

predict emissions from a given system based on some empirical equations. Thus, for the specified operational conditions, the emission rate for carbon dioxide (CO_2) was calculated as approximately 512 kg h^{-1}, while nitrogen oxides (NOx) were expected to be at an approximate level of 182 ppm. The moderate level of NOx emissions was mainly determined by controlled furnace temperatures and usage of excess air for burning purposes. Overall, the estimated emissions are notably lower compared to coal-based plants.

According to the results of the simulation in Figure 7 (a), the relationship between fuel feed rate and heat input into the system shows an almost linear increase. As the rate of feed was increased from 100 to 800 kg h^{-1}, the heat input showed proportional increase from around 510 kW to 4080 kW. With an experimental operation point of 500 kg h^{-1} feed rate, the simulated heat input was found to be 2550 kW. This result supports the effect of fuel feed rate on the heat input in the system.

In Figure 7 (b), the effect of moisture content on boiler efficiency is shown. In accordance with the simulation results, the efficiency decreases with increasing fuel moisture content. Boiler efficiency was seen to decrease from 90.8% at 5% fuel moisture content to 65.1% at 35% fuel moisture content. With an experimentally chosen moisture content of around 10%, the predicted boiler efficiency was found to be 81.6%. This is because moisture in the fuels requires additional latent heat in order to be evaporated. The findings confirm the necessity of keeping the moisture content in biomass briquettes to a minimum in order to achieve efficient boiler performance.

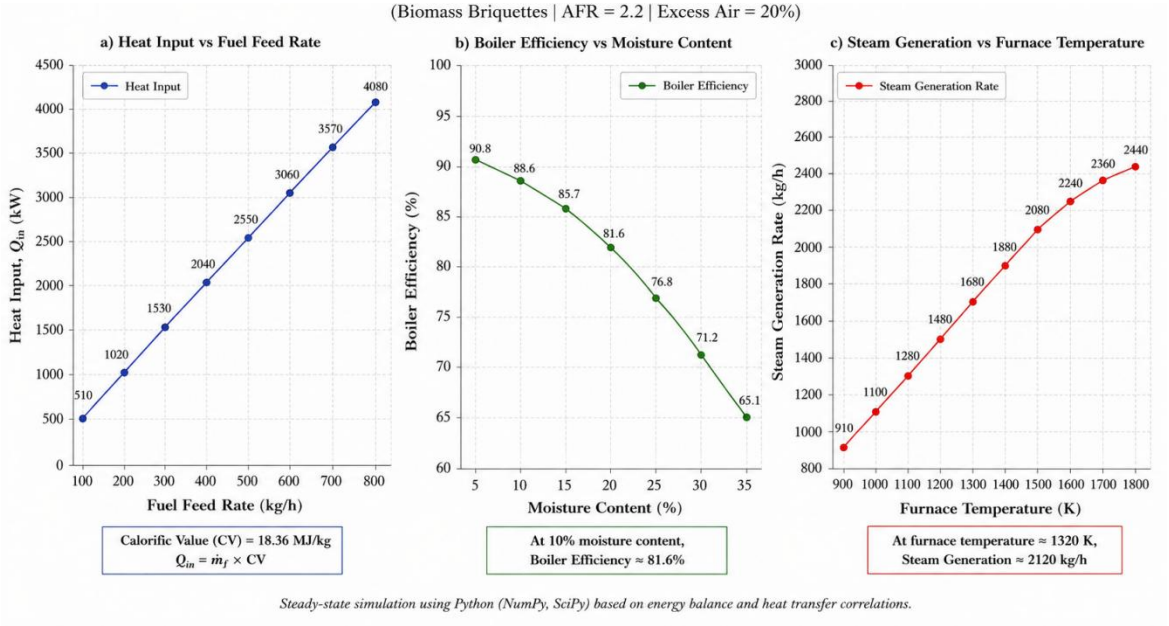


Fig. 7 (a – c) Boiler Simulation Results

The effect of furnace temperature on the rate of steam generation is illustrated in Figure 7 (c). According to the model's predictions, there will be a marked increase in steam generation as the furnace temperature increases due to the higher heat transfer rates inside the boiler. The generation rate of steam rose from 910 kg h^{-1} at 900 K to 2440 kg h^{-1} at 1800 K. At the calculated average furnace temperature of 1320 K, the steam generation rate would be 2120 kg h^{-1}. These results suggest that steam generation rate could be significantly improved by using biomass briquettes to maintain steady high-temperature combustion. The modeling results indicate that the use of biomass briquettes offers favorable thermodynamic performance owing to their low moisture content and high calorific value. The obtained values of boiler efficiency and steam generation rate of 81.6% and 2120 kg h^{-1} respectively corroborate the experimentally established performance of combustion.

3.3 Prediction using ML Models and Interpretation by SHAP

In order to build an intelligent predictive framework for biomass briquette-based boiler systems, three advanced ML ensemble models, such as XGBoost, LightGBM and CatBoost were applied for predicting the relevant performance parameters and emissions. The machine learning dataset was created based on the experimentally observed values of fuel properties, operating conditions, thermodynamic simulations' results and emissions generated due to biomass briquettes combustion. Features of the machine learning dataset included moisture content, ash content, fixed carbon, volatile matter, fuel feeding rate, air-to-fuel ratio, excess air, boiler pressure, furnace temperature, heat input and steam generation rate. Target variables included boiler efficiency, CO_2 emission and NOx emission. Before building any machine learning model, the dataset was first preprocessed for removing any potential inaccuracies. Numerical features were normalized. All data samples from the dataset were randomly split into three subsets - training (70%), validation (15%) and testing (15%). The training dataset was used during model training, whereas the validation set was used for tuning model hyperparameters and avoiding overfitting. Optimization of the hyperparameters of each model was done via grid search with cross-validation to optimize the learning rate, maximum depth, the number of estimators, subsampling rate and regularization factors.

The predictive performance of the built models was analyzed based on the R^2, RMSE and MAE. The performance comparison metrics are presented in Table 3. In terms of predicting boiler efficiency, the best-performing models were XGBoost and CatBoost models with an R^2 of 0.98,

followed by LightGBM with a lower R^2 value of 0.97. The model with the least prediction error was XGBoost with RMSE and MAE values of 0.25 and 0.18, respectively. XGBoost also showed the best performance when predicting CO_2 and NOx emission levels. This can be explained by the fact that XGBoost is a gradient boosting framework and has effective regularization.

Table 3. Performance evaluation metrics of ML models for boiler performance and emission prediction

Target Variable	Model	R^2	RMSE	MAE
	XGBoost	0.98	0.25	0.18
Boiler Efficiency (%)	LightGBM	0.97	0.31	0.22
	CatBoost	0.98	0.27	0.20
	XGBoost	0.95	0.05	0.03
CO_2 Emission (%)	LightGBM	0.93	0.07	0.05
	CatBoost	0.94	0.06	0.04
	XGBoost	0.96	2.84	2.10
NOx Emission (ppm)	LightGBM	0.94	3.42	2.54
	CatBoost	0.95	3.06	2.31

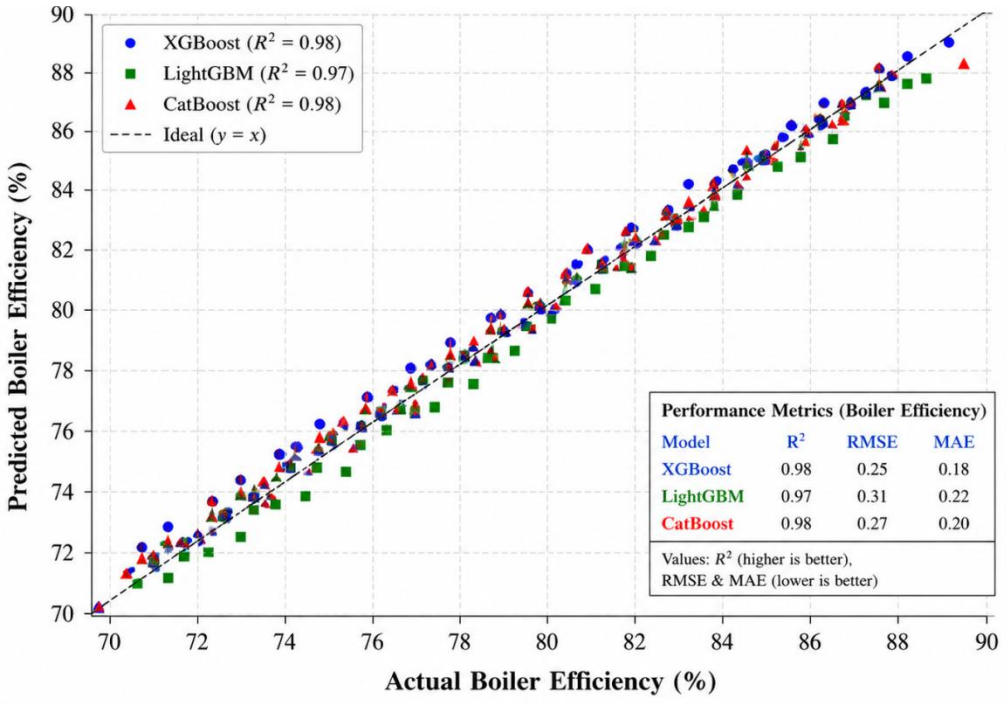


Fig. 8 Actual vs Predicted Boiler Efficiency

The plot showing the actual-versus-predicted relationship of boiler efficiency through the application of the proposed optimized XGBoost model is shown in Figure 8. The closeness of the data points to the 45-degree line signifies a very good agreement between the actual and predicted values. This implies that the developed model can perform excellently well in predicting the target variables. The good prediction performance of the developed model suggests that the experimental and simulated parameters chosen are good representations of the physical phenomena taking place inside the system. Of all the applied ML techniques, XGBoost showed excellent predictive performance, with the highest accuracy rate and minimum prediction errors for all the target variables considered. Hence, the XGBoost algorithm was utilized for SHAP analysis. SHAP allows for quantitative analysis of the contribution of individual features to the ML model prediction results.

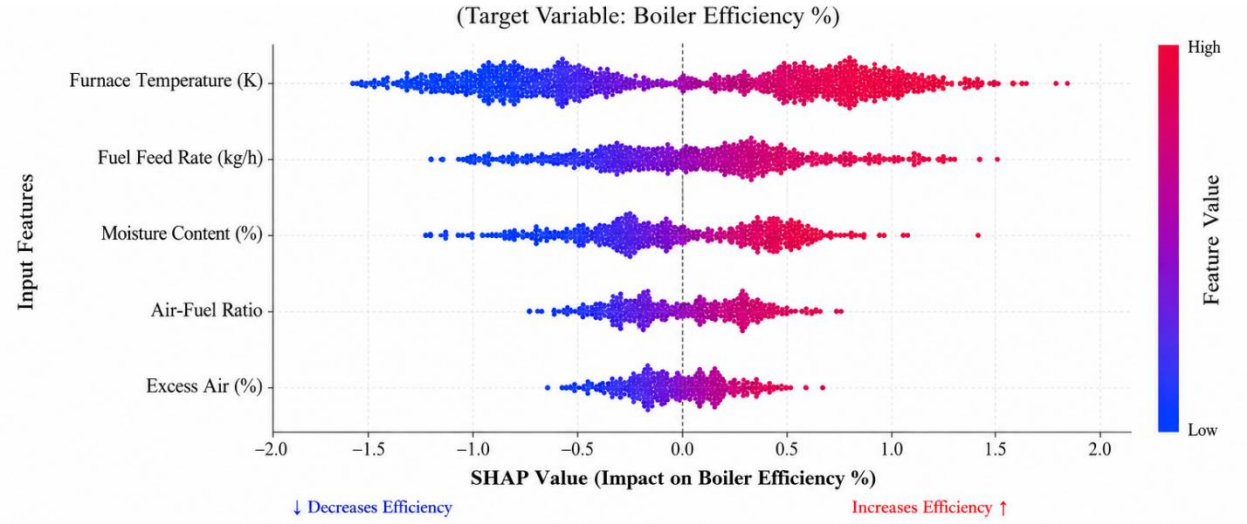


Fig. 9 SHAP Summary Analysis for Boiler Efficiency Prediction

Figure 9 shows the SHAP summary analysis for boiler efficiency prediction, while the overall feature ranking is presented in Table 4. The analysis indicated that furnace temperature was the main factor influencing boiler efficiency. High furnace temperature positively influenced boiler efficiency prediction since it facilitated the processes of combustion completeness, volatility formation, fixed carbon combustion and effective heat transfer. The dominance of furnace temperature is explained by basic laws of combustion and thermodynamics, since thermal energy availability is directly responsible for steam generation in boilers. The feed rate of fuel was identified as the second most impactful feature. High fuel feed rate meant higher heat input into the boiler, which led to increased thermal energy availability and steam generation. Nevertheless,

extremely high fuel feed rates could negatively influence combustion processes, causing heat losses.

The moisture content was the third-most influential variable with a mostly negative SHAP contribution for efficient prediction. Higher moisture contents decreased the boiler efficiency since the energy generated was used for evaporating water rather than forming steam. The findings were supported by the experimental fuel characterization, where the use of biomass briquettes was more effective due to their relatively lower moisture content. Air-fuel ratio was the fourth-ranked variable. The SHAP value suggested that an optimal air-fuel ratio improved the combustion process efficiency and enhanced thermal efficiency. Low air led to inefficient combustion, while too high air increased stack heat losses and decreased flame temperatures. Therefore, the air-fuel ratio should be maintained at an optimal level to ensure efficient operation of the boiler. Excess air was found to be the fifth-most influential variable in predicting thermal efficiency. Adequate excess air promoted stable combustion and decreased emissions, although excessive excess air cooled the furnace and decreased thermal efficiency.

Table 4 SHAP ranking of influential parameters for boiler efficiency

Rank	Variable	Influence on Prediction
1	Furnace Temperature	Very High
2	Fuel Feed Rate	High
3	Moisture Content	Moderate–High
4	Air-Fuel Ratio	Moderate
5	Excess Air	Moderate

A highly accurate relationship between fuel properties, operation parameters and boiler performance parameters could be achieved using ML model. Integration of XGBoost-based predictions along with interpretability using SHAP is a great example of both high prediction accuracy and physical transparency of the combustion process. All those findings show great potential for combining machine learning and explainable artificial intelligence in the field of biomass boilers' operation.

4. Conclusion

Biomass briquettes were assessed as an environmentally friendly and sustainable fuel to replace traditional firewood used in industrial steam boilers via a combined approach consisting of experimental analysis, thermodynamic simulations, machine learning predictions and SHAP

interpretability analysis. It was identified from the fuel characterizations that the new fuel has relatively low moisture content, high calorific value, increased stability in the combustion process and cleaner combustion properties than the current wood fuels. The performance of the steam boiler with biomass briquettes resulted in high energy performance with decreased fuel use and lower emissions.

Based on the simulation using a Python model, there is a relatively accurate estimation of the combustion characteristics and heat transfer process in the steam boiler. The thermodynamic simulation yielded estimates of furnace maximum temperature of 1678 K, average furnace temperature of 1320 K, steam production of 2120 kg h^{-1}, boiler efficiency of 81.6%, carbon dioxide emissions of 512 kg h^{-1} and nitrous oxides of 182 ppm.

The ML models performed extremely well in predicting the performance and emissions from the boiler. Of all the tested algorithms, XGBoost provided the best prediction performance with an R^2 value of 0.98, 0.95 and 0.96 for efficiency, CO_2 emission and NOx emission, respectively. The SHAP technique helped in giving the physical explanation to the developed model and showed furnace temperature, fuel feed rate, moisture content, AF ratio and excess air as the main factors impacting the performance of the boiler.

In summary, it can be said that biomass briquette is indeed a promising fuel for steam production from boilers. The coupling of thermodynamic simulation, machine learning and explainable artificial intelligence can be considered an effective approach for achieving intelligent boiler monitoring, prediction and energy optimization. The future research direction may include digital twin creation using the data acquired through real-time sensors, advanced CFD combustion simulation, multi-criteria optimization of the operating parameters, industrial validation considering different compositions of the fuels and hybrid AI framework combining deep learning and reinforcement learning.

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