

Data driven modeling to reduce fossil fuel consumption in a lime kiln integrated with biomass gasifier

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ABSTRACT: Biomass gasification, although already known and applied, is currently being consolidated as a sustainable alternative in the pulp industry, contributing to the reduction of fossil carbon dioxide (CO₂) emissions and to the utilization of forest residues. In this context, pulp mills are beginning to adopt biomass gasification within their chemical recovery cycles by integrating the technology with lime kilns. However, further process studies are still needed to support and optimize this application.

Thus, the present study aimed to analyze lime mud feed temperature by applying an artificial neural network model to a gasification system integrated with a lime kiln. For this evaluation, 10 periods of system stability throughout 2024 were selected under different operational conditions. Data from 28 potential predictive variables were collected, a total of 348 observations. This dataset was then processed using R software, where data treatment and model dimensionality reduction were performed, resulting in 10 predictive variables between gasifier and kiln. Next, the dataset was randomly divided into training (70% of the observations) and testing data. The established neural network model (using “neuralnet” package) was optimized, resulting in a configuration containing one hidden layer with three neurons. This setup enabled optimal estimation of the flue gas kiln outlet temperature, with mean absolute error (MAE) = 3.0°C and root mean square error (RMSE) = 4.1°C, applying the resilient backpropagation algorithm with backtracking — both below the thermocouple’s measurement error ($\pm 5.0^\circ\text{C}$) for the evaluated average temperature range (668.2°C). When the same dataset was modeled using the resilient backpropagation algorithm without backtracking, even better results were achieved: MAE = 2.5°C and RMSE = 3.7°C. Thus, after evaluating these and other configurations, it was concluded that the best model required 10 predictive variables and the backpropagation algorithm without backtracking to determine flue gas kiln outlet temperature. These results provide a better understanding of how gasifier and kiln variables influence the temperature in the lime kiln, which is essential to improve control and optimize the calcination process, avoiding supplementary fossil fuel consumption.

Application: This study is designed for those looking to better understand how to assess two systems, such as gasification and lime kiln, using data driven modeling methods.

Sustainability is currently one of the most widely discussed global issues, and reducing dependence on fossil fuels for energy generation is a major theme within this broader subject [1]. According to the International Energy Agency [2], in the last accounted numbers (2021), less than 20% of energy sources on the global generation matrix were renewable. Facing this scenario, biomass use for energy generation is a possible pathway for substitution of fossil carbon sources that can be exploited in various ways. As a raw material, its versatility (either dedicated crops growth or forestry residue utilization) is an important feature that has advantages over other energy generation types. Regarding the obtained products from biomass, different processes can produce several energy carriers, such as solids (i.e., biochar), liquids (i.e., bio-oils), gases (i.e., syngas), or even direct combustion for thermal energy generation. These different approaches for biomass use were summarized and grouped by Pascoli et al. [3], as shown at **Fig. 1**. This figure simplifies the various lignocellulosic biomass conversion routes and their

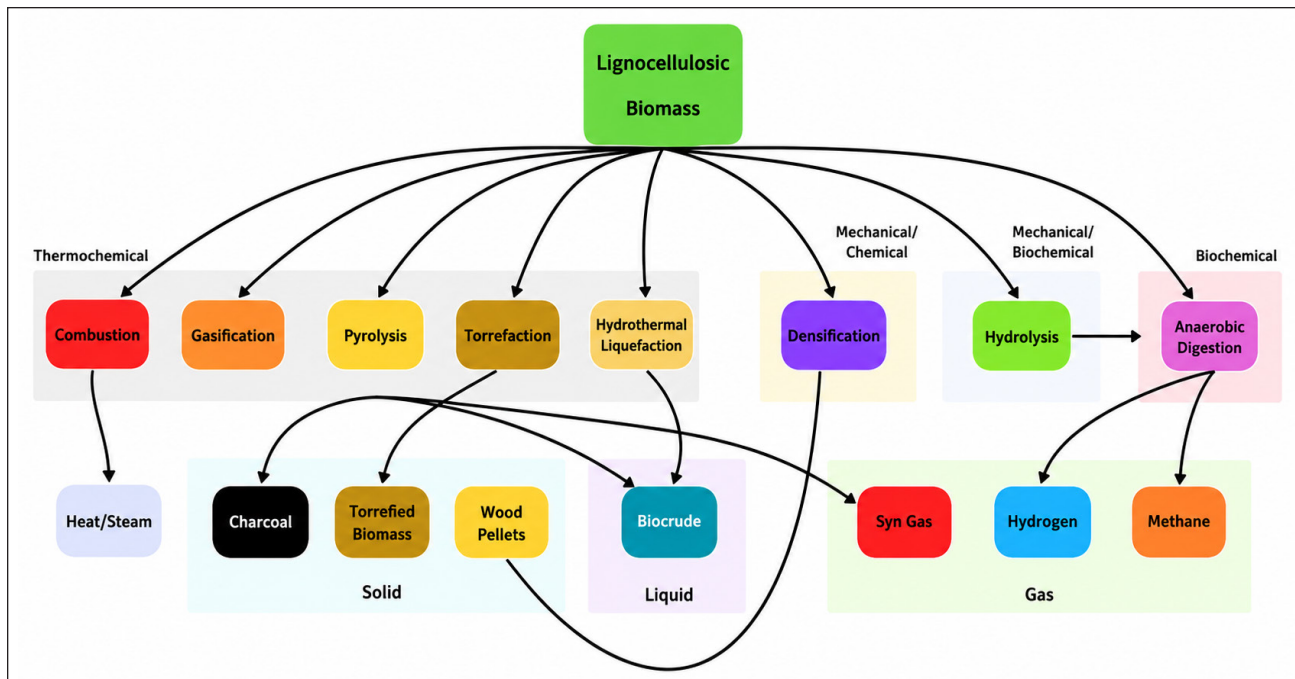
primary resulting products in solid, liquid, and gaseous forms.

The thermochemical process to convert solid biomass into syngas is called gasification. This process occurs at elevated temperatures, typically between 600°C and 1000°C, under substoichiometric oxygen conditions, resulting in the partial oxidation of biomass components. The obtained gaseous product is composed of hydrogen gas, carbon monoxide, carbon dioxide, methane, nitrogen, and other substances of low molecular weight [4].

Depending on the utilization purpose, the produced gas must be purified, passing through a sequence of other processes to remove particles, adjust composition, and upgrade for conversion into value-added chemicals. Direct consumption for thermal energy generation by combustion is also a possible application, since biomass syngas has a significant heating value, varying between 3.0 to 6.0 MJ/Nm³ [5].

One major benefit from biomass gasification is the possibility for reducing carbon dioxide (CO₂) emissions when

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1. Different lignocellulosic biomass conversion routes.

compared to fossil fuels. A life-cycle analysis done by Volta and Yusi [6] in the pulp industry showed this positive effect; when a gasification plant operated using wood handling residues (barks and rejects from wood chipping classifiers), carbon dioxide equivalent (CO_2eq) emissions were approximately 1.6% lower than those of fuel oil used in a lime kiln.

To better understand the gasification process, mathematical modeling is an important technique that has been increasingly applied since the 2000s, especially due to the availability of new computing tools [7]. Phenomenological models (thermodynamic equilibrium, kinetic models, and computational fluid dynamics [CFD]-based modeling) and data-driven models (such as artificial neural networks) can be applied [8].

Phenomenological, or so-called “white-box,” models are based on fundamental principles of chemistry and physics and can be used to estimate process parameters, such as syngas composition, lower heating value, and tar production. Their main advantage is that the effect of each parameter on the model output can be directly understood and related to the resulting response [9].

In contrast, data-driven and machine learning models, so-called “black box” models, do not employ a theoretical description of the reaction mechanisms occurring in a gasification system. Instead, they predict important process outputs by learning relationships between input variables using mathematical and statistical methods. Although these models can provide accurate predictions within the range of input conditions provided, their performance may decrease when applied to conditions outside that range or when new inputs are introduced, limiting their agreement with reality [10].

The most common type of machine learning model is

the artificial neural network (ANN), which is highly capable of modeling complex nonlinear systems [11]. This feature allows application of ANNs in gasification applications such as biomass feedstock classification, prediction of syngas composition and heating value, and estimation of atmospheric emissions [12].

Although recent developments have expanded ANN applications in new studies, these models have been extensively studied since the 1980s. Inspired by the transmission of signals between biological neurons, they process data through an input layer, one or more hidden layers, and an output layer. During this process, the input data are propagated through interconnected neurons using weights and activation functions, ultimately producing the model output [13].

One predominant type of ANN, the feedforward multi-layer neural network, is composed of an input layer for data, an output layer that provides the results, at least one hidden layer, and connections between each layer (each having its own weight), which are subject to the restriction that neurons within the same layer do not form connections with each other [14].

In addition to the definition of a neural network’s structure, an essential part of its function is the training and validation phase. In this phase, input data is provided to the input layer, and the weights are adjusted in order to minimize the error between the value generated by the network and the known actual value. After the network has been trained, it is necessary to validate it using another dataset, which will demonstrate whether the neural network was effective in predicting the data [15].

A critical point in the training process for ANNs is the so-called overfitting effect, which can occur if there are too

many parameters to be determined from the input data. This leads to an over parameterization of the neural network, resulting in an output that correctly includes the trained points (as expected), but generates intermediate regions with inadequate values. To avoid this issue, a smaller number of neurons in the hidden layer can be employed, as well as the use of network regularization techniques or the application of Bayesian methods [16].

Among the applications of neural networks in gasification processes, Puig-Arnavat et al. [17] developed a study focused on fluidized bed gasifiers, in which good correlations between predicted and actual values were obtained for all modeled cases, along with low root mean square error (RMSE) values. The authors built neural network models for circulating fluidized bed (CFB) and bubbling fluidized bed (BFB) gasifiers separately, using the same input parameters except for the steam-to-dry biomass ratio, which was used only in the BFB gasifier models. For each type of gasifier, five separate neural network models were developed, each with one hidden layer and two neurons and a single output variable: gas production or the concentration of hydrogen gas (H_2), methane (CH_4), carbon dioxide (CO_2), and carbon monoxide (CO).

Another successful approach was developed by George, Arun, and Muraleedharan [18], which achieved a mean square error (MSE) of 0.71 and a correlation coefficient (R^2) of 0.987. In this study, a topology with multiple neurons in the output layer was employed, each providing a value calculated by the neural network. The conditions used were: four neurons in the network output (representing the composition of H_2 , CO_2 , CH_4 , and CO) and, in the input layer, the elemental composi-

tion of moisture content, ash content, temperature, and equivalence ratio. Regarding the hidden layer, in this case only one layer was used, which is the most commonly found structure for this type of application, according to the authors [18].

This study aimed to analyze and model an industrial gasification and lime kiln system at a pulp mill in Brazil using ANNs. This work provides a basis for further process analysis and may support future optimization and cost reduction, as no known application has been identified to date for improving process control between the gasifier and the lime kiln. The system was modeled using mathematical and computational tools to identify a suitable ANN architecture for predicting the flue gas kiln outlet temperature. The modeling approach involved evaluating different numbers of neurons in the hidden layer and comparing the use and absence of back-propagation during the determination of network weights and biases.

METHODS

The process to be modeled is the integration between a biomass gasifier and a lime kiln, which are part of the recovery cycle. Biomass gasification is supplied by wood chips and forestry residues (such as barks and fines), which are mixed before gasification. The resulting syngas is consumed at the lime kiln to generate heat for the calcination reaction, which is an important reaction for lime recovery, as well as for production of white liquor.

For the data-driven modeling development using a feedforward ANN, a dataset containing 348 observations was used. These included the 28 predictor variables listed in **Table I** plus flue gas kiln outlet temperature (lime mud

Gasification Variables	Lime Kiln Variables
Biomass temperature	Lime kiln production rate
Biomass feed screw 1 rate	Primary air flow rate
Biomass feed screw 2 rate	Primary air temperature
Gasification temperature bed	Primary air pressure
Gasification temperature reactor top	Secondary air flow rate
Ashes recirculation temperature	Secondary air pressure 1
Sealing air flow rate 1	Secondary air pressure 2
Sealing air flow rate 2	Secondary air pressure 3
Fluidization air flow rate	Secondary air pressure 4
Fluidization air pressure	Lime mud temperature
Gasification temperature outlet	Burned lime temperature outlet
Gasifier pressure	Lime mud solids content
	Burned lime residual carbonate
	O ₂ residual at ESP
	CO residual at ESP

I. Variables selected as potential predictors in the feedforward artificial neural network (ANN) model (ESP: electrostatic precipitator).

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feed into kiln), considering a 3-min interval between each observation across different periods during 2024 from the gasification–lime kiln system. The observations were acquired during stable conditions when supplementary fuel was not used.

The data was first pre-processed by removing empty values or any entries that showed errors. Subsequently, outlier removal was applied, using the criterion of excluding all values that were more than 50% above or below the interquartile range of the data.

Next, time scale adjustment was applied; the gasifier data was lagged by 3 min relative to the lime kiln data (the average residence time observed between the two parts of the equipment). Finally, data was standardized based on the variance of each variable in order to proceed with dimensionality reduction through principal component analysis (PCA), restricting the number of variables used to those that explained at least 90% of the variance of the original data.

With the processed data, 70% of the observations were randomly selected for training and 30% for later validation. The “neuralnet” package in R software [20] was used to formulate the ANN, testing a different number of neurons with one hidden layer until reaching an optimal condition where the error parameters stabilized with the smallest number of layers and neurons to predict flue gas kiln outlet temperature. This location is displayed in **Fig. 2**, along with the main parts of a rotary lime kiln.

Another parameter for determining the best ANN con-

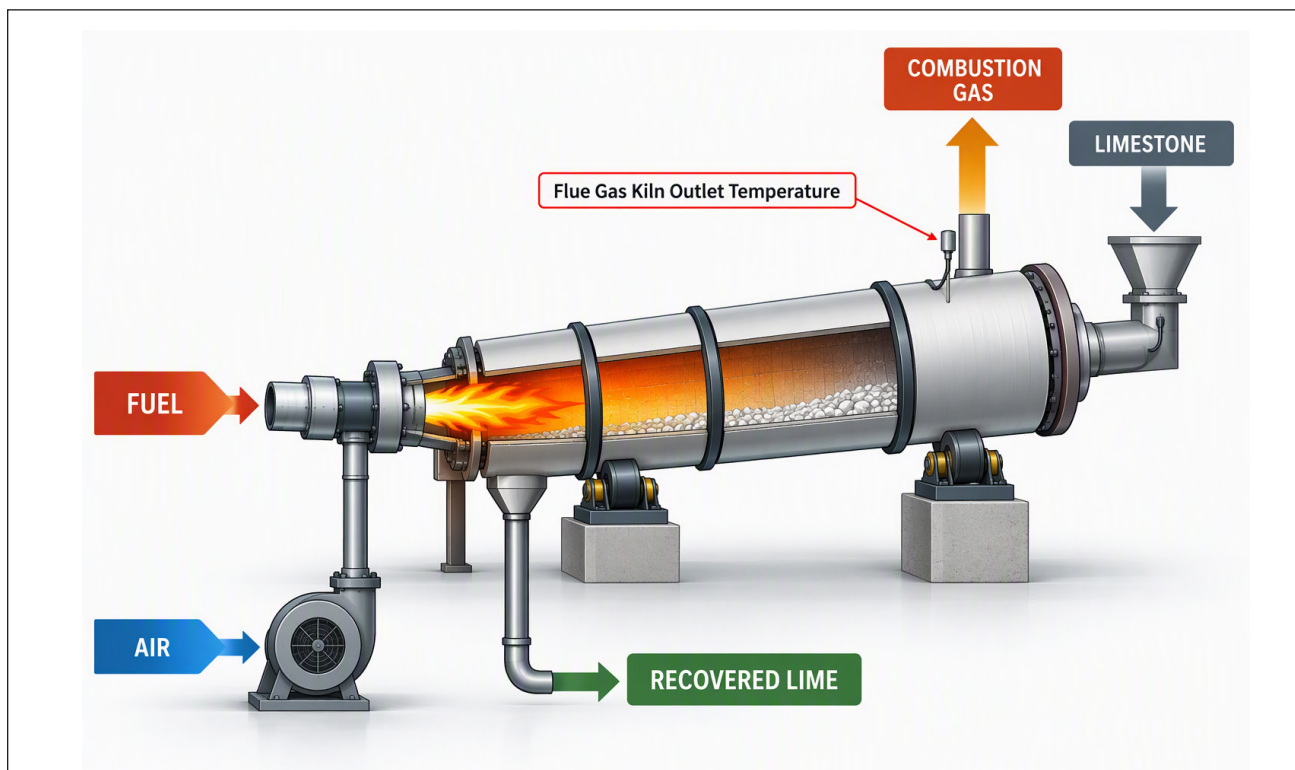
figuration was the use or not of backtracking on the resilient backpropagation algorithm applied, with the aim of error minimization. Backtracking is a correction mechanism used during ANN training. When a change in the gradient direction indicates that a weight update may have overshoot a minimum of the error function, the previous adjustment is reversed and the update step is reduced.

Lastly, half of initial number of predictors was put to the test in several ANN configurations, varying the number of neurons in each hidden layer and number of layers until a stable error was achieved.

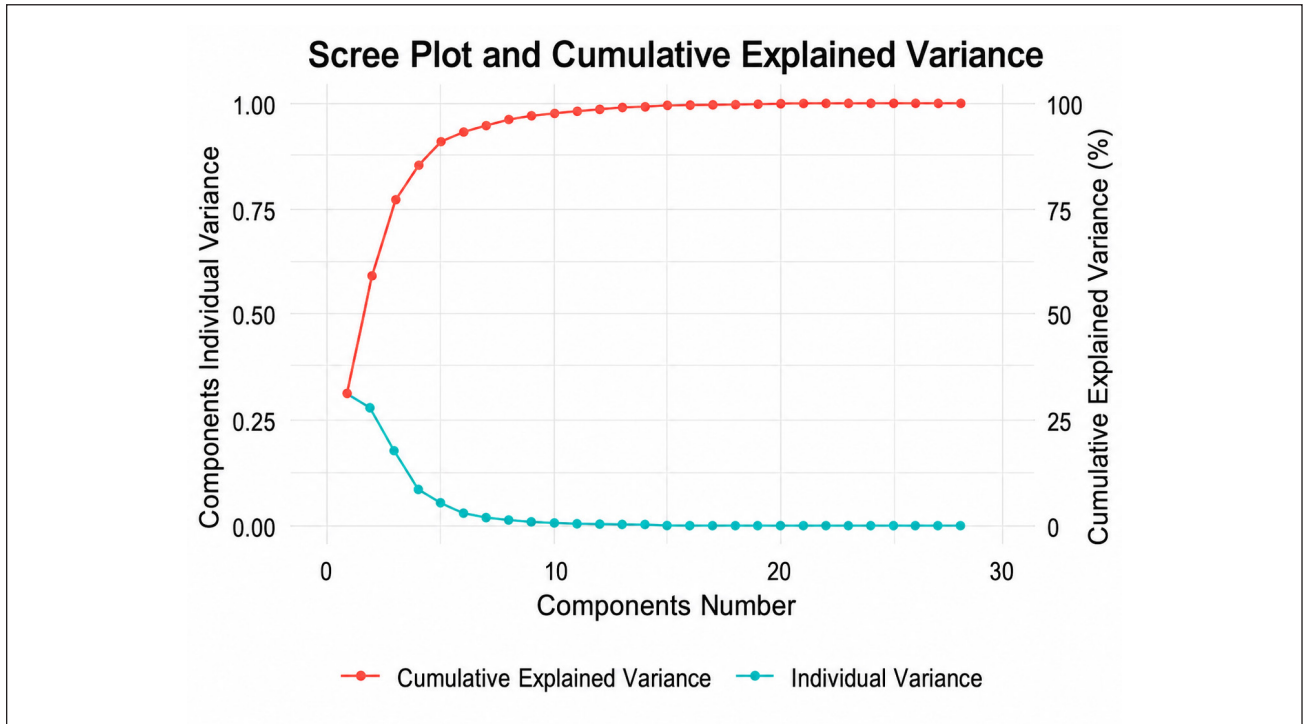
The resulting models were evaluated based on the mean absolute error (MAE) and root mean square error (RMSE). Finally, the developed models were compared against the tolerance limits of the temperature measurement instruments (type K thermocouples) for positive temperatures, according to ASTM E230/E230M-11 “Standard specification and temperature-electromotive force (emf) tables for standardized thermocouples.”

RESULTS AND DISCUSSION

After the data pretreatment described in the Methods section, PCA was performed, reducing the initial 28 variables to only 10, since the target cumulative variance was reached and the additional variables contributed less than 0.5%, as shown in the scree plot graph in **Fig. 3**. A scree plot helps determine how many principal components to retain by identifying the point where additional components explain little extra variance (stabilization point).



2. Lime kiln schematic identifying flue gas kiln outlet temperature. Image from [19].



3. Scree plot variances.

Under these conditions, 97.7% of the system's variance was covered, which provided greater robustness in prediction and allowed the inclusion of biomass feeding and lime kiln production rate variables in the model. These are important for the parameterization of the gasification and calcination processes.

The ten predictor variables, ordered from highest to lowest variance, are:

1. Primary air temperature
2. Primary air flow rate
3. Fluidization air temperature
4. Gasifier pressure
5. Primary air pressure
6. Lime mud temperature
7. Biomass temperature
8. Lime kiln production rate
9. Sealing air flow rate 2
10. Biomass feed screw 2 rate

Next, using 70% of the standardized data for training, several neural network combinations were tested applying the resilient backpropagation algorithm, starting with one hidden layer containing five neurons. After successive attempts, the best configuration based on the test data (i.e., the lowest errors with the fewest neurons) was found to be a single hidden layer with three neurons, using backtracking to adjust weights and bias.

Under these conditions, calculated errors for MAE and RMSE were 3.0°C and 4.1°C, respectively. These results, when compared to thermocouple measurement error

($\pm 5.0^{\circ}\text{C}$ for the average data set temperature: 668.2°C), showed a well-adjusted prediction within the acceptable error range. **Figure 4** shows the plotted predicted and measured temperatures and the highlighted thermocouple error represented by the colored area around measured points.

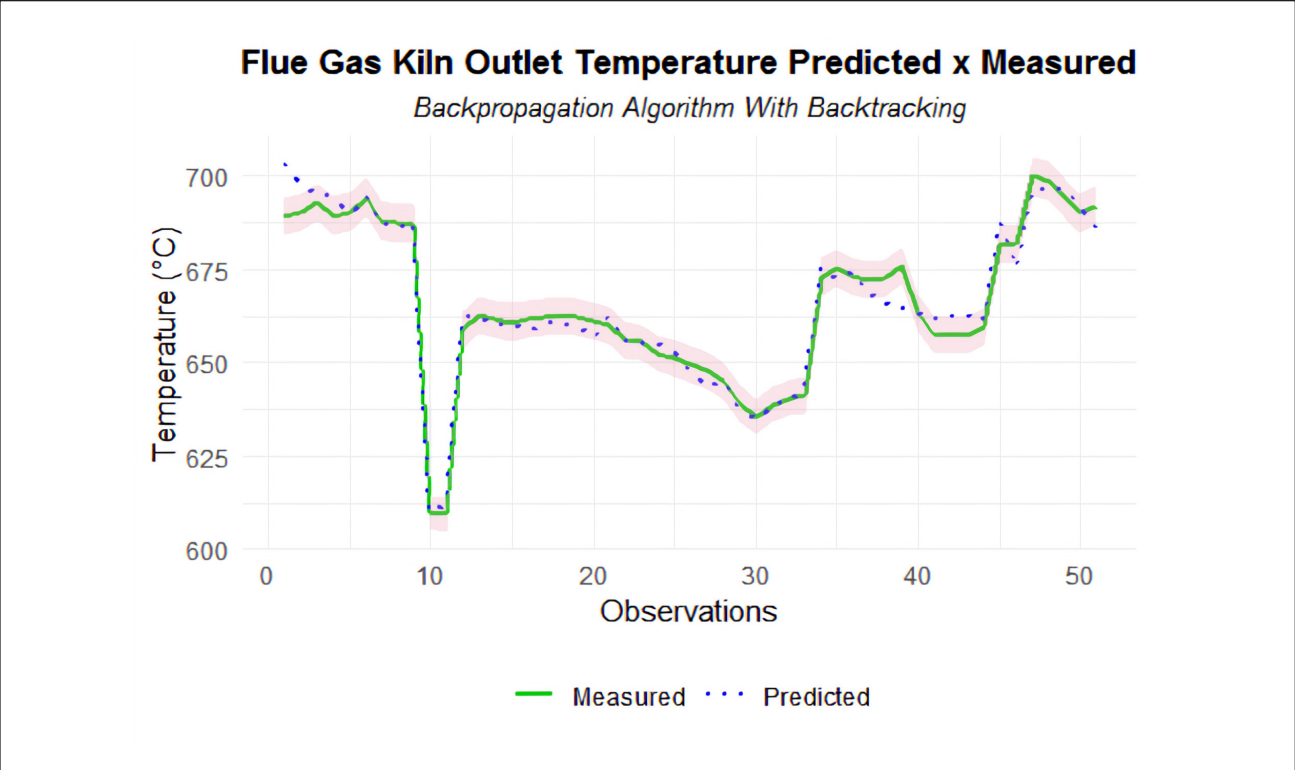
Backtracking use typically avoids overshoot on errors. However, depending on the dataset, minimum error sometimes is not easily achieved, which requires a modeling approach with less constraints. Thus, a second assessment was also done with the top 10 predictors, using the resilient back-propagation algorithm without backtracking and keeping the other assumptions. With this modeling configuration, weights were even better adjusted, reaching a minimum error for both parameters of MAE = 2.5°C and RMSE = 3.7°C using only two neurons at the hidden layer. Similar to Fig. 4, **Fig. 5** shows the results for the established ANN without backtracking.

In comparing Fig. 5 and Fig. 4, it is possible to observe a better fit for the backpropagation algorithm without backtracking for temperatures above 675°C , considering the thermocouple error. Nonetheless, both models show a good correspondence between measured and predicted temperatures that is acceptable for industrial application.

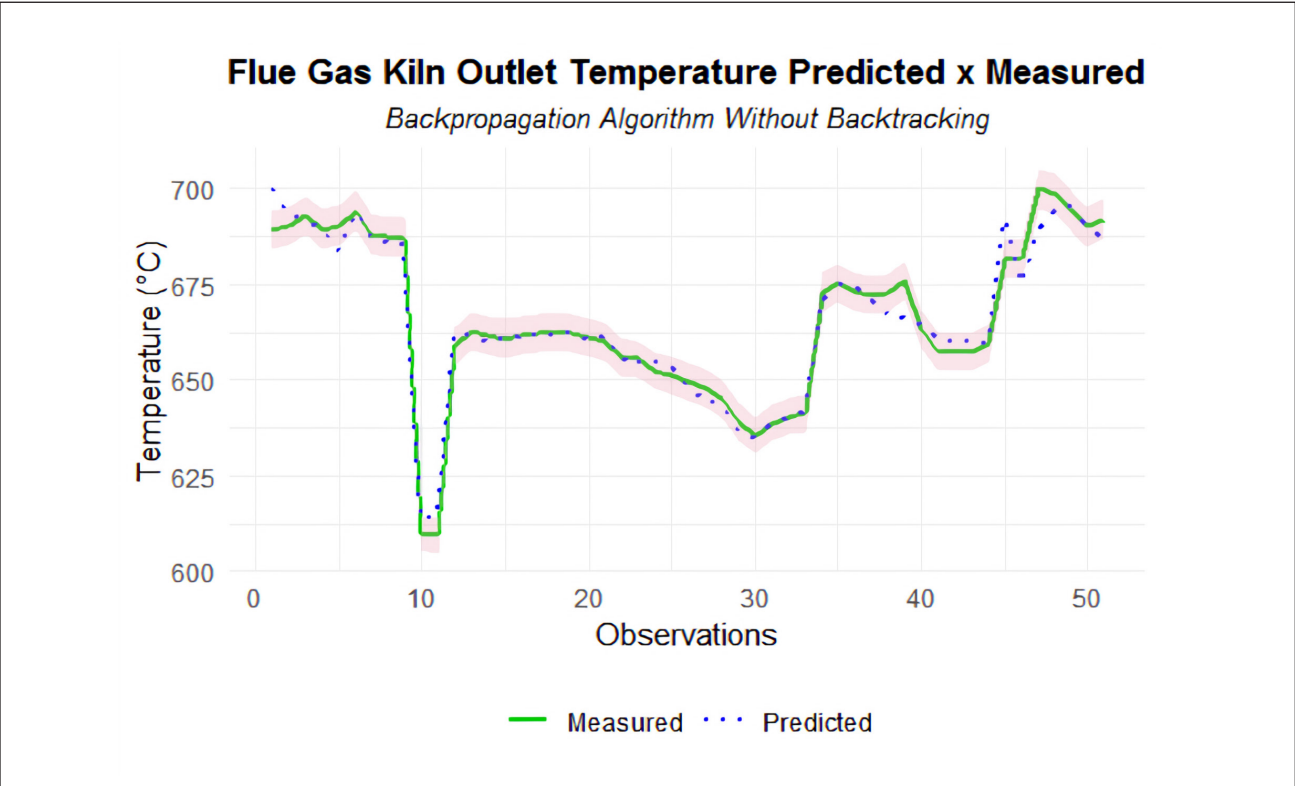
In addition, a simplified capability analysis was done by identifying the most frequent data in the original dataset as verified by quartiles, as **Fig. 6** shows. The difference between the 1st and 3rd quartiles is approximately 25°C , which can be easily differentiated by both models' precision.

Because the models predicted the kiln outlet flue-gas temperature with errors within the measurement uncer-

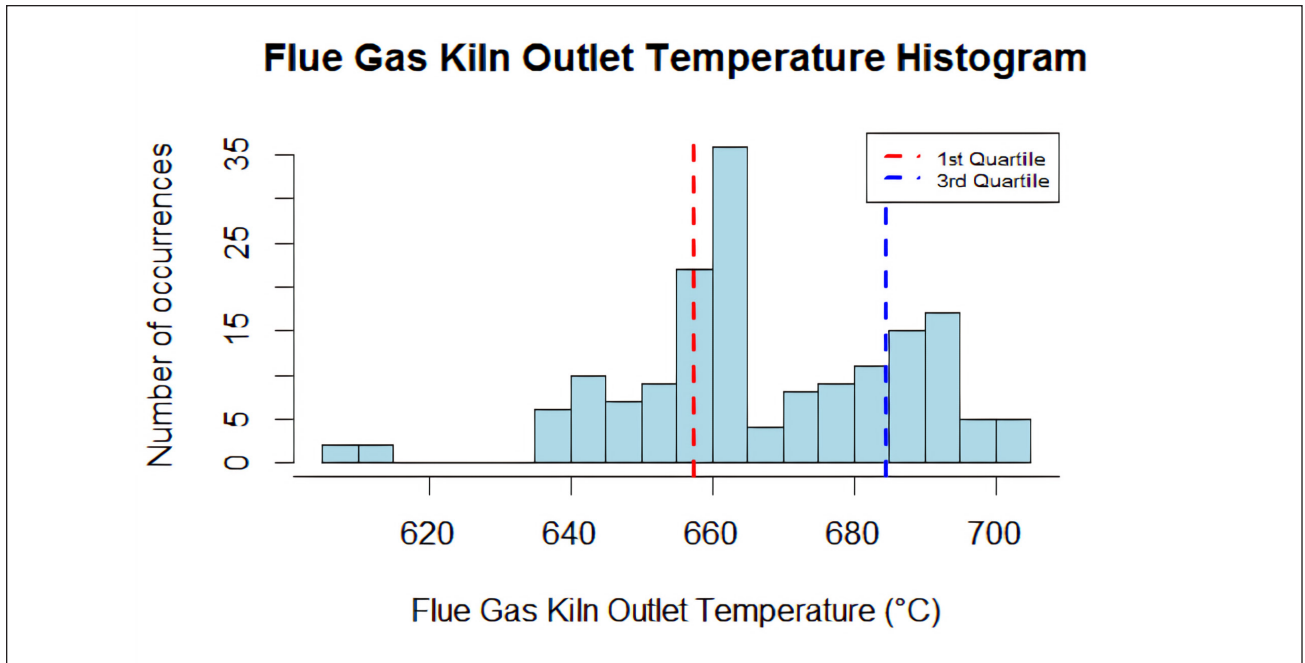
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4. Flue gas kiln outlet temperature, predicted vs. measured, with backtracking.



5. Flue gas kiln outlet temperature, predicted vs. measured, without backtracking.



6. Flue gas kiln outlet temperature histogram.

Model	Number of Neurons at Hidden Layer	Number of Predictors	MAE, °C	RMSE, °C
ANN with backtracking	3	10	3.0	4.1
		5	3.0	4.4
ANN without backtracking	2	10	2.5	3.7
		5	3.0	3.8

MAE: mean absolute error; RMSE: root mean square error.

II. Summary of artificial neural network (ANN) models using different configurations and respective errors.

tainty, simplified ANN structures were evaluated to reduce their dependence on input predictors. Thus, a reduction from 10 to five predictors was accomplished for algorithms with and without backtracking. **Table II** summarizes the results, along with the previous results.

To properly evaluate the model's performance, a correlation analysis between measured and predicted results was also performed, as shown in **Fig. 7**.

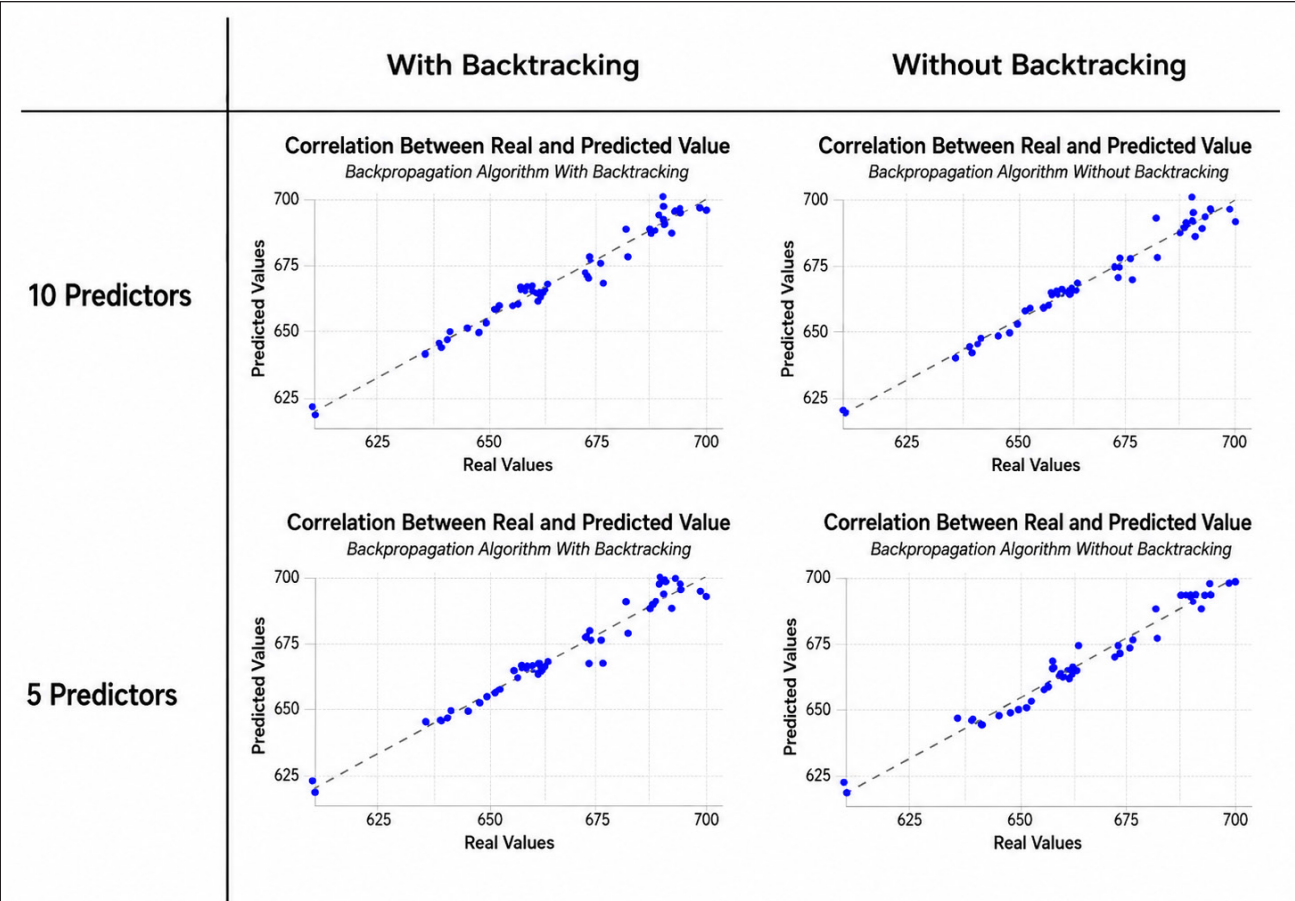
Analyzing differences between models with and without backtracking, a higher scattering from the $y = x$ line for models with backtracking at high values ($> 680^{\circ}\text{C}$) can be observed. The adjustment for models without backtracking shows better control at this range, which is positive for its application.

When the reduction of predictors is analyzed, a lower absolute accuracy occurs for both cases. Nonetheless, the ANN without backtracking was not drastically affected, sustaining the low deviation, especially at high temperatures. Thus, for analyzing mill data, this model was considered the most adequate.

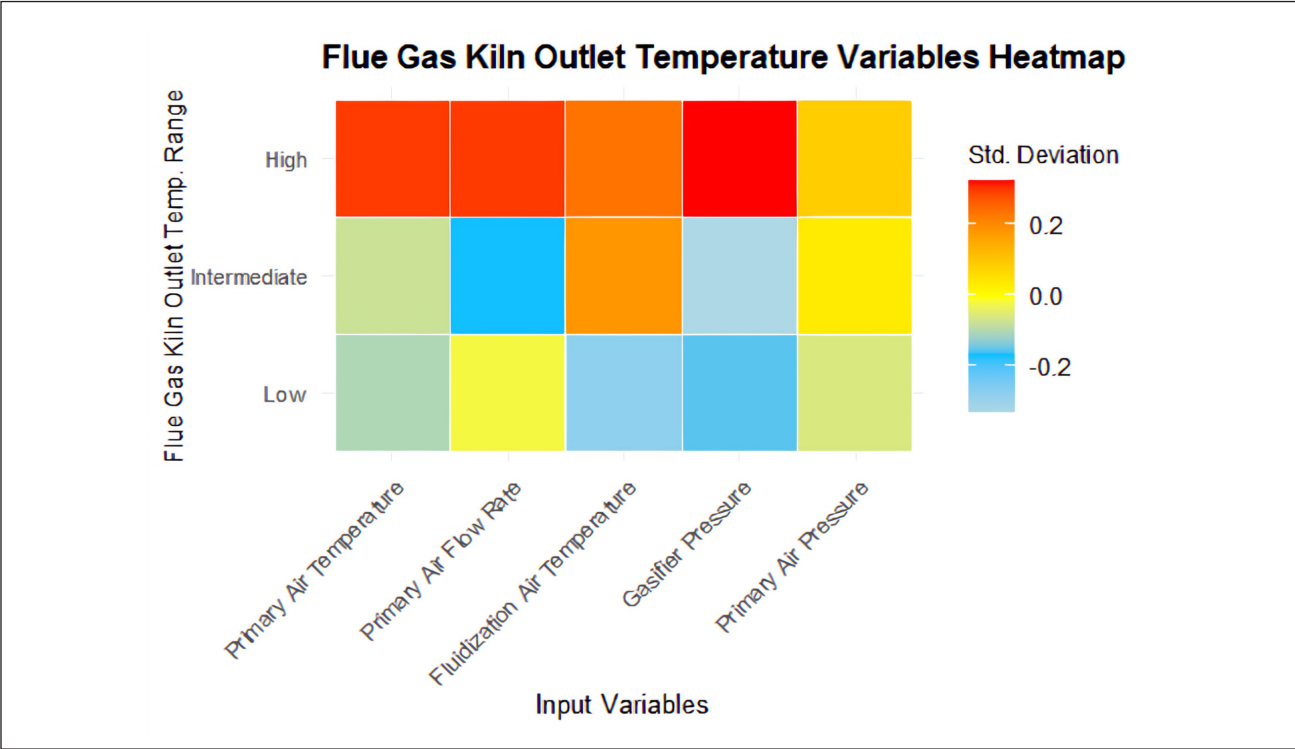
Once the best model was selected, the variables were analyzed to identify the conditions associated with the highest temperatures, which may indicate greater thermal efficiency, and the lowest temperatures, which may require supplemental natural gas to maintain the kiln's thermal profile.

Figure 8 shows a heatmap chart for better confirmation of variable combinations generating different ranges of flue gas kiln outlet temperatures (divided by low, intermediate, and high). In this assessment, the five input variables (predictors) were classified by color according to their standard deviation (positive or negative) from average, providing a qualitative indication of predictor levels across the different flue gas kiln outlet temperature ranges.

Analysis of the **Fig. 8** heatmap verifies that high flue gas outlet temperatures are obtained by combining the highest values of all 5 predictors, although primary air pressure should be slightly above average. Under low temperature conditions, most variables tended to be below average, ex-



7. Correlation between measured and predicted values



8. Variable heatmap for flue gas kiln outlet temperature.

cept primary air flow rate, which remained at average conditions for the dataset studied.

Intermediate flue gas kiln outlet temperatures resulted from a combination of higher, lower, and predictor values. Fluidization air temperature was the only input variable above average value.

CONCLUSIONS

In this study, data-driven models were able to describe and predict the integration of gasification and calcination parameters, particularly for flue gas kiln outlet temperature, which is an important operational parameter in achieving lime mud conversion efficiency.

Among the four tested configurations, the best results were achieved using the resilient backpropagation algorithm without backtracking. This configuration reached the lowest MAE and RMSE at 2.5°C and 3.7°C, respectively, when 10 predictors were used. After a reducing to five predictors, the error increased to MAE = 3.0°C and RMSE = 3.8°C; however, for all cases, this increase was below the $\pm 5.0^\circ\text{C}$ range of thermocouple error for the average temperature range used.

The predicted vs. measured data scatter plot showed satisfactory adjustments for all tested models. The model with five predictors and without backtracking showed the lowest scattering for high temperatures ($> 680^\circ\text{C}$), resulting in an optimum model performance for this range.

Finally, predictor assessment using a heatmap chart proved a valuable tool for parameter checking and monitoring, clustering different operational conditions to predict lime kiln flue gas outlet temperature.

ABOUT THIS PAPER

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ABOUT THE AUTHORS

This study occurred as a result of a development opportunity with the company where several of the authors work. To our knowledge, this research is the first of its kind. We found developing the knowledge to program R software the most difficult aspect of this study.

Through the study, we learned that sometimes the most sophisticated approach (such as using backtracking) does not yield the best result. So, it was particularly interesting to find a simple way to model a gasification and lime kiln system.

Mills can use this information for further development of machine learning models that integrate biomass gasification with lime kilns. Our next step is to expand the database and combine models to create a hybrid model for gasification and the lime kiln.



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