APPROACH TO PREDICT CHEMICAL EXERGY AND SYNGAS YIELD IN BRAZILIAN BIOMASS WASTE GASIFICATION USING AN ARTIFICIAL NEURAL NETWORK

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ABSTRACT

In this paper, multi-layer feed forward neural networks are used to predict the chemical exergy, hydrogen mole fraction, carbon monoxide mole fraction, and methane mole fraction during gasification of Brazilian wastes biomasses during gasification in a bubbling fluidized bed reactor. These artificial neural networks (ANNs) with different architectures are trained using the Adam back-propagation algorithm and a cross validation is also performed to ensure that the results generalize to other unseen datasets. A rigorous study is carried out on optimally choosing the number of hidden layers, number of neurons in the hidden layer and activation function in a network. Ten input and four output parameters are used to train and test various neural network architectures in single output prediction paradigms using the available experimental datasets. The model selection procedure is carried out to ascertain the best network architecture in terms of predictive accuracy. The simulation results show that the ANN based methodology is a viable alternative which can be used to predict the performance of a bubbling fluidized bed gasifier.

1 INTRODUCTION

Biomass is a significant source of sustainable energy, holding the potential to reduce dependence on fossil fuels and cut down CO_2 emissions. In Brazil, biomass plays a vital role, contributing 25.5% to the nation's internal energy supply (Thraen and Shaubach, 2017; Habib *et al.*, 2023). The abundant biomass resources in Brazil provide an opportunity to convert biomass wastes into valuable energy commodities like hydrogen, ammonia, and power, offering a way to decrease greenhouse gas emissions, energy consumption, waste disposal costs, and environmental impacts. Diverse materials such as sugarcane bagasse, orange bagasse, corn, and coffee residues are available for bioenergy production. Thermochemical routes, particularly the synergy between air separation and biomass gasification techniques, have been explored to harness biomass conversion and valorization technologies (Sapali S, 2013).

Vargas, Flórez-Orrego and de Oliveira Junior, 2023 argue the shift towards renewable energies in chemical sectors to reduce fossil fuel dependency. This paper emphasizes the potential of residual biomass, like sugar cane and sewage sludge, for environmentally friendly fuel production. The study optimizes biomass-based biochemical routes, aiming for negative emissions and increased circular economy efficiency. Achieving an overall negative emission balance, the hydrogen and ammonia production routes remove substantial CO_2 from the atmosphere.

Recent developments have explored alternative modeling techniques to optimize biomass conversion processes, with ANNs being widely employed. ANNs offer shorter processing times for system output prediction and optimization, effectively capturing non-linear relationships between input and output parameters. Several studies have utilized ANNs to predict gasification parameters, such as Mikulandric et al. (Mikulandrić *et al.*, 2014) and Serrano et al. (Serrano, Golpour and Sánchez-Delgado, 2020), showcasing robust correlations with experimental studies.

Vargas and Oliveira Jr, 2023 developed an ANN prediction model for a green electric energy generation process through the gasification of Brazilian biomass residues. Utilizing various biomass sources, including sugarcane and orange bagasse, sewage sludge, corn residues, coffee residues, eucalyptus

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residues, and municipal waste. The three-layer feed-forward neural network demonstrated high accuracy ($R^2 > 0.993$).

In light of this information, the objective of this study is to use Brazilian waste biomass for prediction of chemical exergy and H_2, CO, and CH_4 mole fractions, particularly in gasification plants. Aspen Plus® simulator (ASPENTECH, 2011) replicated the bubbling fluidized bed gasifier, providing data on gasification. This information was used to formulate a comprehensive ANN model, introducing an innovative approach to evaluating properties through machine learning techniques on simulation data and computing pivotal parameters as performance indicators. In this research, computational frameworks originating from methods of artificial intelligence are utilized to comprehend the non-linear mapping challenge. These varieties of frameworks have the capability to forecast the efficiency of intricate systems (encompassing gasification). As a result, this investigation is concentrated on leveraging the potential of the ANN methodology to assess the performance of Brazilian biomass waste gasification in a fluidized bed reactor.

2 Material and Methods

2.1 Biomass characterization

Evaluating biomass samples significantly improves gasification system efficiency and enhances synthesis gas quality. Biomass characteristics, including fixed carbon (FC), ash content, volatile matter (VM), and moisture (M), are determined through Proximate and Ultimate analyses measuring carbon (C), hydrogen (H), oxygen (O), nitrogen (N), and sulfur (S) levels. In this study, ten biomass samples from existing literature (see Table 1) were chosen as primary raw materials, with results summarized in Table 1.

Table 1: Proximate (%) and Ultimate (%) analysis results of selected biomass samples for training of the ANN model.

Biomass	M	FC_{db}	VM_{db}	Ash_{db}	C	H	N	S	Cl	O	*REF.*
Sugar cane bagasse	50.00	14.32	83.54	2.14	46.70	6.02	0.17	0.02	0	44.95	(Ardila *et al.*, 2012)
Sewage sludge	18.40	7.60	64.90	27.50	33.90	6.30	5.88	0.67	0.21	25.50	(Languer *et al.*, 2020)
Sugar cane straw waste	31.30	12.80	20.60	13.00	49.00	5.60	0.80	0.30	0	44.00	(Franco Jacome, 2014)
Coffee waste	8.88	14.48	75.85	0.79	49.33	5.86	0.66	0.04	0	43.24	(Manrique *et al.*, 2020)
Eucalyptus waste	7.73	16.38	74.91	0.98	48.65	6.16	0.28	0	0	44.91	(Guerrero *et al.*, 2005)
Urban municipal waste	49.16	13.94	71.83	14.23	42.04	5.90	0.66	0.10	0	29.87	(Gutierrez-Gomez *et al.*, 2021)
Orange bagasse	9.23	13.20	30.60	6.20	46.40	5.54	1.70	0	0	40.15	(Alves *et al.*, 2020)
Corn waste	60.29	12.62	84.22	0	47.54	6.33	1.32	0.08	0	42.22	(Pan-In and Sukasem, 2017)
Banana stem	12.56	9.96	80.27	8.00	39.00	7.30	0.82	0	0	54.84	(Rambo, Schmidt and Ferreira, 2015)
Coconut shell	15.98	19.40	72.90	0.80	46.60	7.10	0.32	0	0	41.80	(Akogun and Waheed, 2019)

M, moisture content; VM, volatile matter content; FC, fixed carbon content; db, dry basis.

2.2 Modeling and simulation of the gasification systems

Figure 1 presents the configurations for biomass waste gasification, as based on (Flórez-Orrego, Maréchal and de Oliveira Junior, 2019; Domingos *et al.*, 2021; Vargas, Flórez-Orrego and de Oliveira Junior, 2023). The simulations are conducted using Aspen Plus® software (ASPENTECH, 2011), with the equation of state being the Peng-Robinson EoS with Boston-Mathias modifications. The model for

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waste biomass gasification employs the Battelle Columbus Laboratory (BCL) indirect gasifier, which operates at atmospheric pressure with steam serving as the gasification medium. This arrangement prevents nitrogen dilution in the produced syngas by using a separate double-column system for the combustion and gasification processes (Kinchin and Bain, 2009). Subsequent to the gasifier, thermal catalytic cracking of the produced tar takes place. For more detailed information on the model and simulation see (Vargas, Flórez-Orrego and de Oliveira Junior, 2023).

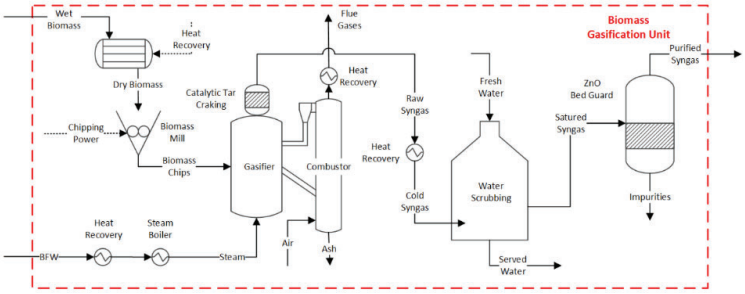

Figure 1: Syngas production from biomass gasification—process modeling approach for ANN analysis.

2.3 Artificial neural network design

The ANN mimics biological processes, simulating the human brain's behavior and learning. As universal approximators, ANNs make predictions based on existing data, finding use in data-driven research where predictive accuracy is vital. Despite widespread application, there is limited literature on using ANNs for Brazilian biomass gasification modeling. The multilayer feed-forward neural network in Figure 1 illustrates its structure with multiple inputs and one output variable. It uses non-linear transfer functions and the Adam enhancement algorithm for optimization (Kingma and Ba, 2014). This algorithm combines RMSProp and Momentum, managing both adaptable learning rates and momentum effectively. Adam is computationally efficient, requiring minimal memory, crucial for extensive-scale scenarios. It remains unaffected by diagonal rescaling of gradients, addressing challenges like saddle points or meager gradients. Adam has shown commendable outcomes in diverse neural network scenarios. The ANN model incorporates ten process parameters: carbon, hydrogen, nitrogen, sulfur, oxygen, moisture content, ash, fixed carbon, volatile materials, and gasifier temperature. To manipulate the data it was used the library Pandas (Team, 2020), and the TensorFlow package available within the Python environment was employed (Abadi *et al.*, 2022). This package facilitates the training of an Artificial Neural Network by estimating the weights between neurons in consecutive layers, effectively simulating synapses.

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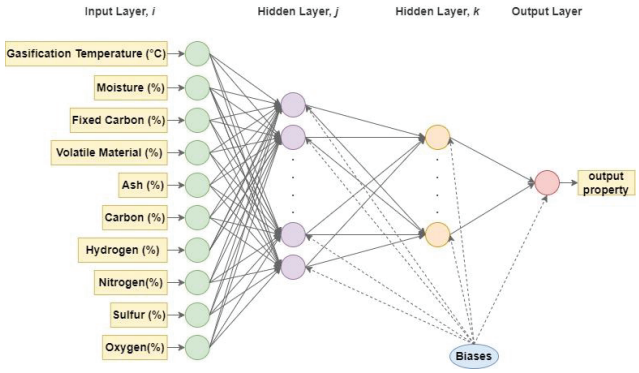

Figure 2: Architecture of Feedforward Neural Network employed in this work.

2.4 Proposed approach of ANN based methodology and optimization of the model parameters

The methodology in Figure 3 proposes an optimal neural network architecture by varying hidden layers, transfer functions, neuron quantities, and learning rates. Each configuration undergoes 50 runs to minimize training error and avoid local minima during weight/bias tuning. Model performance is assessed using metrics like mean absolute error (MAE) and root mean squared error (RMSE). Mean squared error (MSE), a common metric for training ANNs, represents the average squared difference between predicted and experimental values.

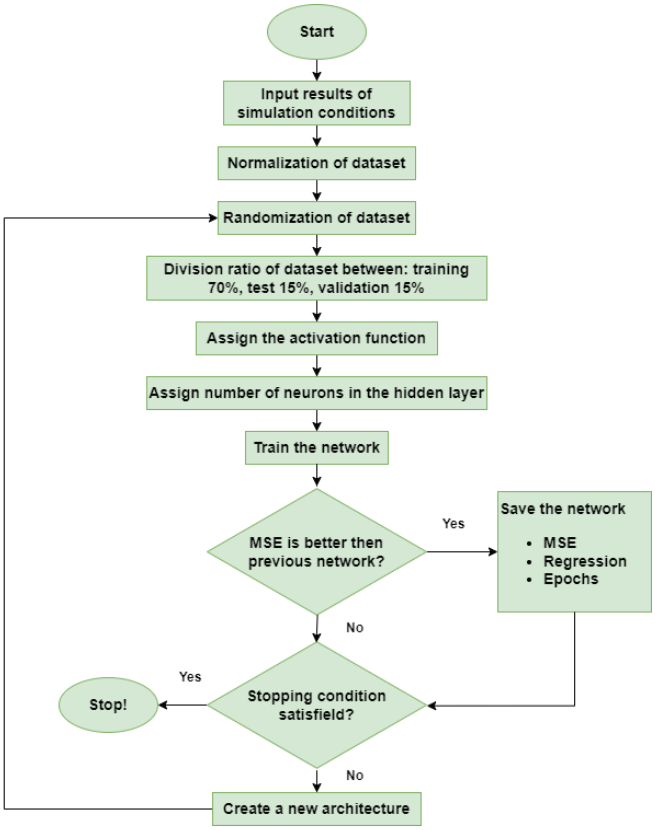

Figure 3: Flowchart of the proposed methodology.

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In the scenario, four ANNs cater to chemical exergy, and the mole fractions of H_2, CO, and CH_4. An exploration of internal network parameters, including hidden layer characteristics, neuron quantity, and transfer function, is conducted. Determining the optimal number of neurons in the hidden layer is crucial, impacting the balance between predictive accuracy on training data and generalization to untrained data. This study challenges the traditional trial-and-error method, employing a rigorous cross-validated accuracy check. Addressing inconsistencies and premature convergence during weight and bias optimization, the study adopts multiple randomizations of the optimizer and data shuffling in training, validation, and testing sets. This ensures accurate error estimates and aids in determining the best-suited ANN architecture. The balance challenge between predictive accuracy and generalization capability is carefully considered.

In summary, the study explores training ANNs for biomass gasification modeling complexities and advances the traditional supervised learning data analysis workflow. The approach in Figure 3 serves as a guideline for deciding optimal hidden layers, neuron quantities, and activation functions in ANN-based models. Multiple runs and robust error estimation contribute to the reliability and accuracy, marking a significant advancement in this field.

3 RESULTS AND DISCUSSIONS

The models were trained and tested using a combination of the non-linear sigmoid and linear ReLu activation functions in the hidden layer. The dataset used to develop the ANN model contains 12,000 records of which 70% are used for training, 15% for testing, and 15% for validating the ANN model. Additionally, the input datasets are normalized by maximum and minimum values, and they are randomized for each iteration, meaning that for each step of the optimization of the hidden layer, 10-fold cross-validation was employed.

The networks are trained with various numbers of hidden neurons in a hidden layer with different combinations of transfer functions. The performance of the network is evaluated based on MSE. The ANN architecture with the lowest MSE indicates a better model (the best model is represented in the figures below by a red 'x' for different by-products and properties) in terms of predictive accuracy.

The graphs in Figure 4 provide a three-dimensional view of the best prediction accuracy for the double-layer model. These graphs are useful for identifying optimal combinations when tuning an ANN regression model. They serve as a graphical visualization as the number of neurons in the layers varies. The color of the point, determined by MSE, is presented on the side scale axis, where the x and y axes represent the number of neurons in hidden layer (HL) 1 and 2, respectively, while the z axis presents the model's learning rate (LR). The optimal number of neurons in the hidden layers for the models is shown in Table 2 based on the reported minimum MSE, in percent.

Thus, the models that exhibit better predictive accuracy when the sigmoid transfer function are used in both layers. However, it is noteworthy that the model for predicting the mass fraction of carbon monoxide showed very close MSE values for the combination of sigmoid/sigmoid activation functions (HL_1 = 19 and HL_2 = 6 with LR = 0.01) and ReLu/sigmoid (HL_1 = 19 and HL_2 = 9 with LR = 0.001) with MSE equal to 0.0124% and 0.0128%, respectively.

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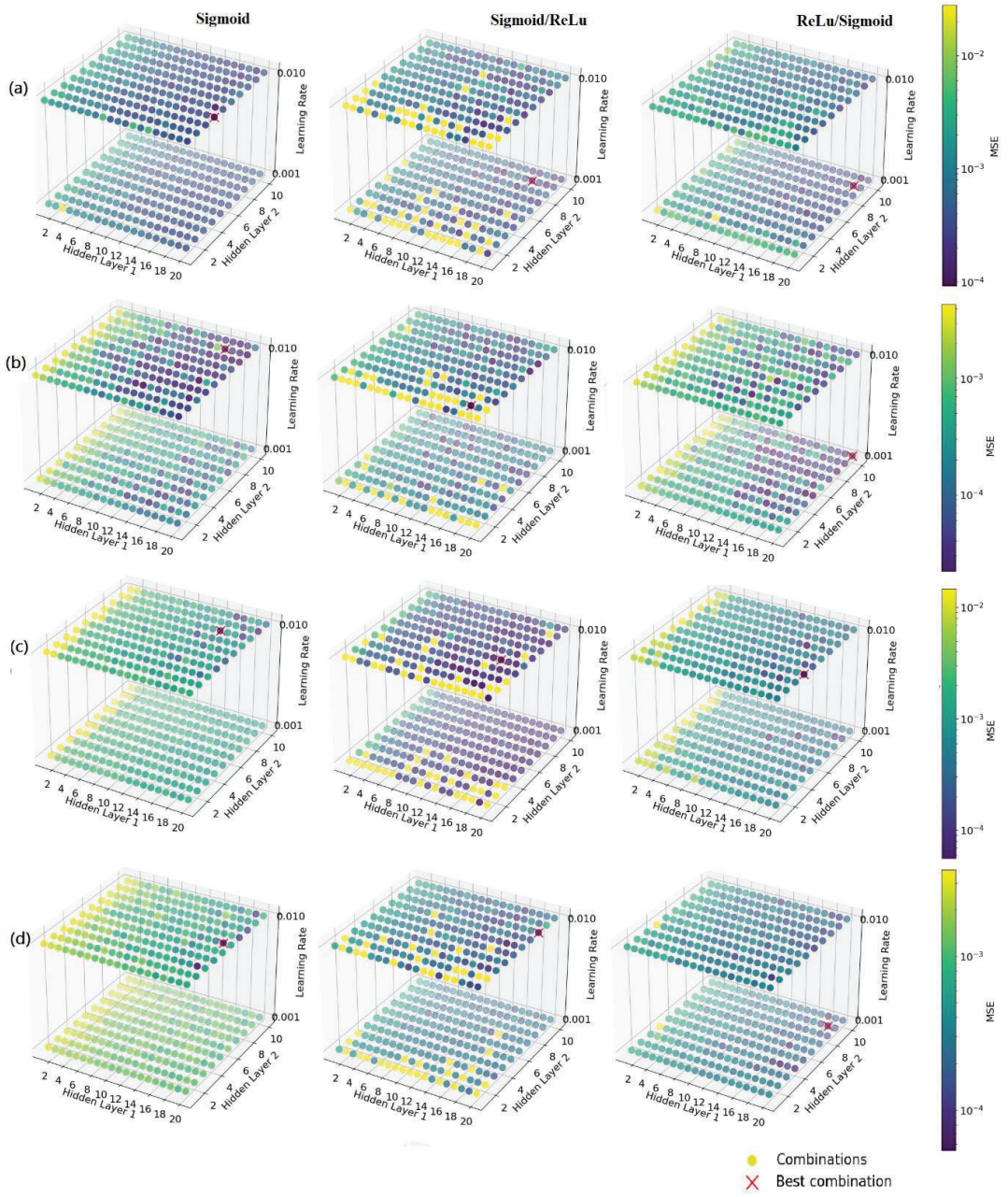

Figure 4: Combination plot of MSE for double layer models (a) Chemical Exergy, (b) y_CH_4, (c) y_CO and (d) y_H_2.

Figure 5 displays training graphs for different products. The ANN model's accuracy for chemical exergy conversion in the training set has a high R^2 value of 99.81%, indicating a great match. The mean square error (MSE) is low, 0.0112%, attributing to the effective ANN weight estimation using 70% of the dataset for training. The residues histogram in Figure 5b supports the agreement between observed and predicted values, displaying an average near zero. For carbon monoxide modeling (Figure 5e), the R^2 value is lower at 99.12%, but still considered excellent. The corresponding histogram (Figure 5f) shows values close to zero, reinforcing the model's reliability.

2023 https://doi.org/10.52202/077185-0173

Table 2: Training performance of the best ANN configuration.

Property	Activator	MSE (%)	Hidden Layer 1	Hidden Layer 2	Learning Rate
Exergy	**Sigmoid/Sigmoid**[a]	**0.0112**	**20**	**4**	**0.01**
Exergy	Relu/Sigmoid	0.0320	19	9	0.001
Exergy	Sigmoid/Relu	0.0408	17	9	0.001
y_CH_4	**Sigmoid/Sigmoid**[a]	**0.0436**	**16**	**8**	**0.01**
y_CH_4	Relu/Sigmoid	0.1036	20	4	0.01
y_CH_4	Sigmoid/Relu	0.6953	17	5	0.01
y_CO	**Sigmoid/Sigmoid**[a]	**0.0124**	**19**	**6**	**0.01**
y_CO	Relu/Sigmoid	0.0128	19	9	0.001
y_CO	Sigmoid/Relu	0.0287	20	8	0.01
y_H_2	**Sigmoid/Sigmoid**[a]	**0.0268**	**17**	**9**	**0.01**
y_H_2	Relu/Sigmoid	0.0850	20	10	0.001
y_H_2	Sigmoid/Relu	0.3187	18	2	0.01

[a]Corresponds to the optimum NN model for the prediction of gasifier performance.
y: molar fraction

On the other hand, Figure 6 illustrates testing graphs, with Figure 6c showcasing the ANN model's accuracy for hydrogen mole fraction prediction on the training set, displaying a remarkable fit with a high R^2 of 99.31% and a low MSE of 0.0256%. The testing set, representing 15% of the dataset, was used for ANN weight estimation. The residual histogram in Figure 6b supports the strong agreement between observed and predicted values, with an average close to zero. Again, despite the lowest R^2 at 98.92% for carbon monoxide (Figure 6e), the model is still considered excellent, confirmed by the close-to-zero values in its residual histogram (Figure 6f).

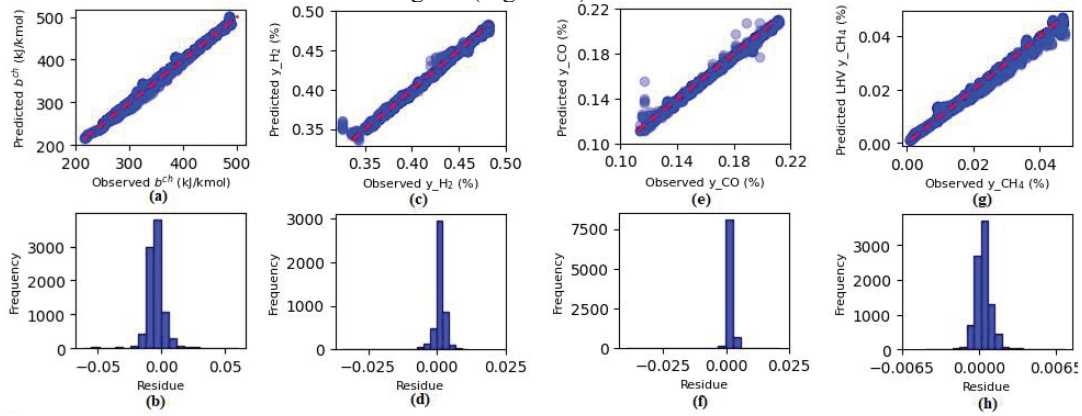

Figure 5: Comparison between training set for: (a) predicted and observed chemical exergy (b), histogram of residues for the chemical exergy, (c) predicted and observed hydrogen mole fraction (d), histogram of residues for the hydrogen mole fraction, (e) predicted and observed carbon monoxide mole fraction, (f) histogram of residues for the carbon monoxide mole fraction, (g) predicted and observed methane mole fraction and (h) histogram of residues for methane mole fraction.

Finally, Figure 7 presents graphs illustrating the validation phase of the ANN model. In Figure 7c, focusing on predicting hydrogen mole fraction, the model exhibits an exceptional fit with a high R^2 of 99.11% and a low MSE of 0.0476. This testing set, representing 15% of the dataset, played a crucial role in estimating ANN weights, providing insights into the model's generalization. The residual histogram (Figure 7b) supports robust agreement between observed and predicted values.

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The analysis extends to predicting carbon monoxide levels (Figure 7e), registering the lowest R^2 during testing at 98.58%, still within the excellent range. The residual histogram (Figure 7f) underscores the model's consistency in producing residuals close to zero, affirming its reliability in predicting carbon monoxide concentrations.

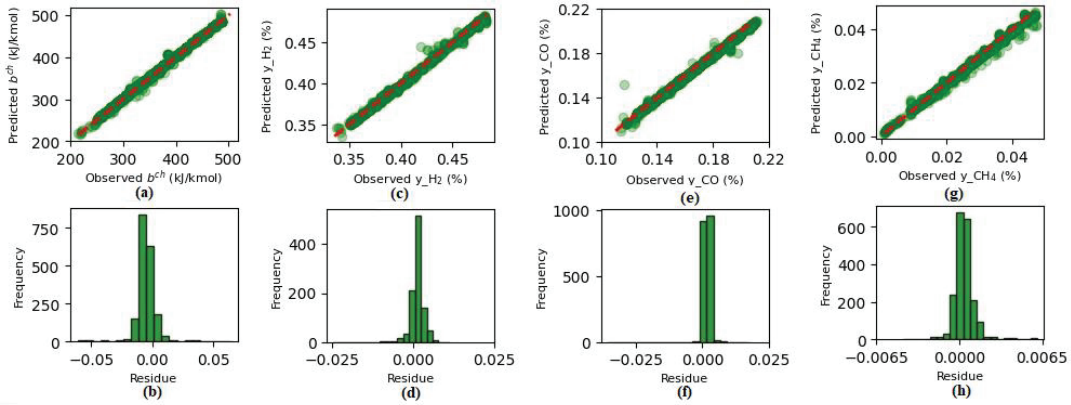

Figure 6: Comparison between tasting set for: (a) predicted and observed chemical exergy (b), histogram of residues for the chemical exergy, (c) predicted and observed hydrogen mole fraction (d), histogram of residues for the hydrogen mole fraction, (e) predicted and observed carbon monoxide mole fraction, (f) histogram of residues for the carbon monoxide mole fraction, (g) predicted and observed methane mole fraction and (h) histogram of residues for methane mole fraction.

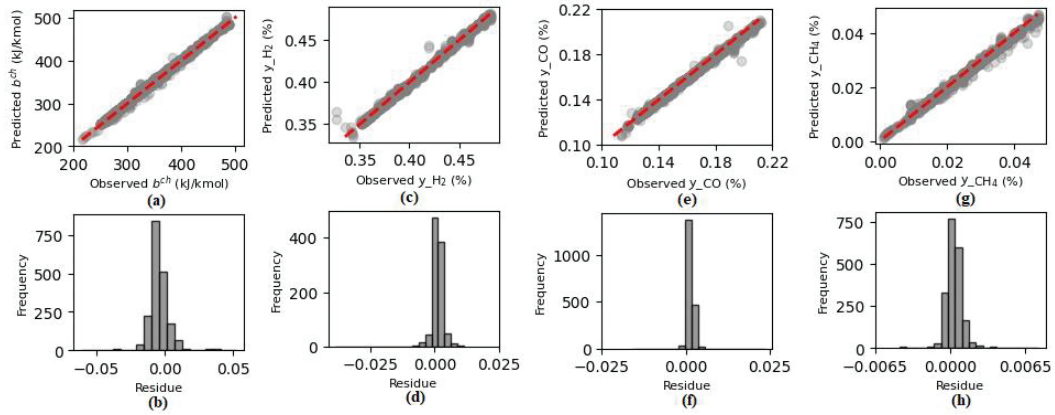

Figure 7: Comparison between validation set for: (a) predicted and observed chemical exergy (b), histogram of residues for the chemical exergy, (c) predicted and observed hydrogen mole fraction (d), histogram of residues for the hydrogen mole fraction, (e) predicted and observed carbon monoxide mole fraction, (f) histogram of residues for the carbon monoxide mole fraction, (g) predicted and observed methane mole fraction and (h) histogram of residues for methane mole fraction.

As illustrated in Figure 8, the training and validation curves exhibit consistent patterns, attaining their lowest error values at different epochs. The ANN model underwent specific iterations for each target variable, with chemical exergy reaching 100 epochs in Figure 8a, hydrogen at 110 epochs in Figure 8b, carbon monoxide at 200 epochs in Figure c, and methane at 290 epochs in Figure d. Throughout these iterations, the MSE consistently decreased, ultimately converging to a minimum plateau. This visual representation not only aligns with previous findings in literature (Yoru, Karakoc and Hepbasli, 2009;

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Ozonoh *et al.*, 2020) but also indicates the absence of overfitting in the well-trained model. Thus, the ANN model demonstrates robust generalization capabilities.
It is noteworthy that, during the validation phase, methane exhibited higher instability in MSE compared to other variables, signifying potential challenges in accurately predicting methane concentrations.

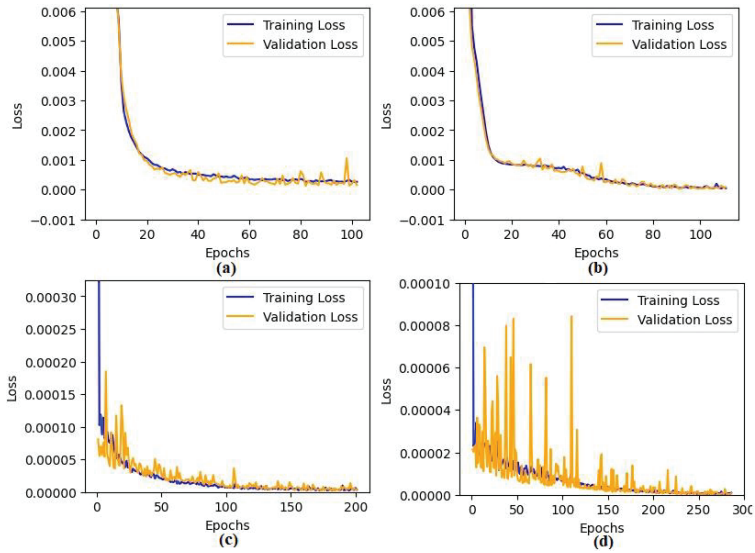

Figure 8. Mean square error value during the training and validation of ANN model: (a) chemical exergy model, (b) H_2 Model, (c) CO Model and (d) CH_4 Model.

In Table 3, the predicted and calculated values of synthesis gas properties from gasification are listed with the relative error (%) for selected biomass samples used in the validation set.
As observed in Table 3, the developed ANN model in this study exhibited high proficiency in estimating the values of synthesis gas properties at the point with the best architectures suggested by the optimization process. The error values were found to be between 23% and 2.6% for biomass samples used in the training, testing, and validation sections of the ANN model.
The gasification temperature is another critical parameter influencing the composition of synthesis gas, particularly the H_2 content (AlNouss *et al.*, 2020). Due to the complex interplay of exothermic and endothermic reactions, the chemical equilibrium state is directly influenced by the gasification temperature. Higher temperatures favor the chemical equilibrium towards the reactant side for exothermic reactions, while endothermic reactions shift towards the product side following Le Chatelier's principle.
The error values indicate that the ANN model accurately predicted the values of properties in synthesis gas originating from gasification for biomass samples in both training and additional validation studies. Even for biomass with different physicochemical characteristics, such as orange bagasse and sugar cane bagasse, the error values are very small. These results support the validity of the model, emphasizing that there is no overfitting in the ANN model.

https://doi.org/10.52202/077185-0173

Table 3: The relative error value (%) in syngas and exergy for different gasification temperature (biomass samples for training).

Biomass	Gasification Temperature (°C)	b^{ch} Calc. (MJ/kg)	b^{ch} Pred. (MJ/kg)	Error (%)
Sugar cane bagasse	850	19.43	20.23	4.2
Sewage sludge	900	18.13	17.02	6.1
Coffee waste	870	15.46	17.21	10.1
Eucalyptus waste	850	15.76	16.35	3.7
Urban municipal waste	970	17.34	18.87	8.8
Orange bagasse	820	15.54	17.26	11.1
Banana stem	830	16.13	18.21	12.8
Biomass	**Gasification Temperature (°C)**	**y_CO Calc. (M.F)**	**y_CO Pred. (M.F)**	**Error (%)**
Sugar cane bagasse	850	0.2543	0.2343	7.8
Sewage sludge	900	0.2243	0.1743	22.2
Coffee waste	870	0.2165	0.2665	23.0
Eucalyptus waste	850	0.2398	0.2188	8.7
Urban municipal waste	970	0.2476	0.2616	5.6
Orange bagasse	820	0.2387	0.2044	14.3
Banana stem	830	0.2287	0.2687	17.4
Biomass	**Gasification Temperature (°C)**	**y_H_2 Calc. (M.F)**	**y_H_2 Pred. (M.F)**	**Error (%)**
Sugar cane bagasse	850	0.5598	0.5398	3.5
Sewage sludge	900	0.5972	0.5472	8.3
Coffee waste	870	0.5238	0.5738	9.5
Eucalyptus waste	950	0.5786	0.5576	3.6
Urban municipal waste	870	0.5196	0.5336	2.6
Orange bagasse	820	0.5458	0.5115	6.2
Banana stem	830	0.5519	0.6319	14.4
Biomass	**Gasification Temperature (°C)**	**y_CH_4 Calc. (M.F)**	**y_CH_4 Ped. (M.F)**	**Error (%)**
Sugar cane bagasse	850	0.0254	0.0234	7.8
Sewage sludge	900	0.0328	0.0278	15.2
Coffee waste	870	0.0298	0.0348	16.8
Eucalyptus waste	850	0.0197	0.0176	10.6
Urban municipal waste	970	0.0222	0.0236	6.2
Orange bagasse	820	0.0265	0.0231	12.9
Banana stem	830	0.0231	0.0271	17.2

b^{ch} : specific chemical exergy (MJ/kg)

4 CONCLUSIONS

This study presents a neural network (ANN) model trained using the Adam algorithm, incorporating a combination of activation functions such as Sigmoid and ReLU. This model was utilized to predict the exergy yield and molar fractions of H_2, CH_4, and CO. The input data comprised residues from Brazilian biomass utilized in a double-column BCL gasifier, encompassing process parameters and elemental composition. Furthermore, it introduces an optimization method for selecting the hyperparameters of

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the ANN. The obtained results demonstrate that the predictive performance of the explored ANN models aligns well with simulated datasets, suggesting that ANNs can serve as an alternative method for modeling complex thermochemical processes. The trained ANN models exhibited high precision and performance, achieving R^2 values above 98% in all cases, with the MSE considered sufficiently low. While the initial application of this new approach provided valuable insights into equilibrium modeling, it is advisable to calibrate the ANN model with more data due to its self-adaptive nature and reliance on data, without significant prior assumptions about the model's structure. The trained ANN model can effectively predict the performance of similar gasifiers operating under comparable experimental conditions. However, it is crucial to retrain the model if there are changes in the physical parameters at the input of the regression problem. Additionally, caution is warranted when applying the same ANN prediction model to heterogeneous data originating partially or entirely from different experimental protocols. This may necessitate dividing the prediction problem into smaller subproblems, sharing common points to enhance prediction accuracy.

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