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Neural Network Based Modeling and Operational Optimization of Biomass Gasification Processes

Maurício Bezerra de Souza Jr., Leonardo Couceiro Nemer,
Amaro Gomes Barreto Jr. and Cristina Pontes B. Quitete

Additional information is available at the end of the chapter

1. Introduction

Gasification processes are rather complex and difficult to model as they include gas-solid two-phase flow, mass and heat transfer, pyrolysis, homogeneous gas phase reactions and heterogeneous gas-solid reactions. Modeling of these phenomena based on basic principles of conservation is still at an incipient stage of development [1]. Additionally, most of the works have focused on coal gasification (for example, see [2-3]). Consequently, the development of a mechanistic model demands that many idealizations and suppositions are made [4], resulting in a very simplified model with little predictive capability.

Artificial neural networks (ANNs) are universal approximators [5] and have received numerous applications [6]. The literature, as indicated by [7], points out their ability to recognize highly nonlinear relations and to organize disperse data in a nonlinear mode in the context of empirical or hybrid modeling. These characteristics of the ANNs are very interesting and useful, motivating their use in the modeling of biomass gasification processes.

Hence, the present work aims to investigate – through the use of artificial neural networks (ANNs) and literature data – the correlation between the composition of the produced gas and the characteristics of different biomass for several operating conditions employed in fluidized bed gasifiers. Additionally, the neural network based developed model is employed to find conditions that maximize the yield of a given component of the produced gas.

This work is structured as follows. In section 2, fundamental aspects concerning biomass gasification and the modeling of the process are briefly reviewed. Section 3 focus on the modeling based on ANNs, while section 4 presents the optimization investigations using the developed models. Finally, the main conclusions are presented in section 5.

2. Biomass gasification

2.1. Fundamental aspects

Gasification is a process in which a solid or liquid fuel is converted into a gaseous fuel with contact with a gasifying agent. Coal, biomass, petroleum coke and other materials can be used in the process. The produced gas is mostly composed of hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2) methane (CH_4), traces of heavier hydrocarbons (as ethane and ethylene), water, nitrogen (when air is used as gasifying agent) and some contaminants. Besides the gaseous products, there are also subproducts as tar and solid non-converted residual carbon (char) [8].

The gas composition and the production of subproducts depend on several factors as: energy delivered to the process, type of gasifier, operating conditions and type of biomass employed. The gas produced can be used in different applications such as: gas turbines or internal combustion enginees, production of syngas and, after an adequate cleaning up and reforming, production of hydrogen or direct use on fuel cells [9-10]. The reactions inside the gasifier can be divided in four stages according to the temperature [8]: drying (> 150°C); pyrolysis (150 -700°C); combustion (700 - 1500°C) and reduction (800 -1100°C).

Some characteristics of the biomass have a significative effect on the performance of the gasifier. For this reason, proximate and ultimate analyses are used in order to characterize the biomass [7].

Because of their flexibility for use with different types of biomass [8], only fluidized bed (bubbling and circulating) gasifiers were studied in the present work. Different gasification agents can be considered, such as: air, oxygen, steam or a combination of them. In the case of use of air or oxygen, the heat released by the exothermic reactions between the oxygen and the fuel is used to keep the gasifier in the operating temperature and as heat source for the endothermic reactions. When steam is employed, it is necessary to use an external heat source [8].

2.2. Modeling of the process

The availability of accurate biomass gasification process models would help the operation and optimization of these processes. However, as noted by reference [11], the majority of the works have been developed for coal. In comparison with coal, biomass is made up not only of lignin, but also of cellullose and hemicellulose, each one having its own thermal behavior, what makes the biomass gasification even more difficult [11].

Reference [12] commented the difficulties of developing a model based on the kinetic equations of the different reactions, together with the mass and energy balances and hydrodynamic considerations for a circulating fluidized bed biomass gasifier. In this work, the authors cite the objective of developing a model "as good as possible".

Previous literature papers employed neural networks to predict characteristics of combustion, pyrolisys or gasification processes. In reference [3], a hybrid gasification model

using ANNs was developed to estimate reactivity parameters of different types of coal with relative success. Reference [13] used ANNs to predict the emission of pollutant gases in the combustion process of a mixture of coal and urban solid residuals with a good agreement between experimental and predicted data.

In 2001, reference [1] developed a hybrid model for the gasification of biomass in a fluidized reactor that employed steam as gasification agent. The authors used multilayer ANNs to estimate parameters of a phenomenological model. The hybrid model was used to determine the production rate of the gas and its composition in terms of H_2, CO, CO_2 e CH_4. However, the neural networks were trained for each biomass separately.

In 2009, reference [7] used ANNs to predict LHV (lower heating values) of the gas and of the gas with tar and char and gas yields using the following input variables: type of residual (paper, wood, kitchen garbage, plastic and textile materials), gasification temperature and equivalence ratio. The results indicate that ANNs are a viable alternative for the modeling of the studied process.

3. Modeling using ANNs

3.1. Fundamental aspects

ANNs (Artificial Neural Networks) area a computational paradigm in which a dense distribution of simple processing elements is used to provide a representation of complex processes (and/or ill-defined and/or nonlinear).

ANNs are nowadays a standard modeling tool, being the feedforward paradigm named MLP (Multilayer Perceptron) the most popular one. Their fundamentals will not be discussed here as they can be found in several references [5, 14-16], only main aspects concerning topology and training of MLPs will be briefly commented in the following, as these ANNs were the ones chosen here.

The MLP paradigm is usually composed of an input, a hidden and an output layer of neurons. The neurons in the input layer are typically linear, while the ones in the hidden layer have nonlinear (often sigmoidal) activation functions. The neurons in the output layer may be linear or nonlinear. Each interconnection between two layers of neurons has a parameter associated with it that weights the feedforwardly passing signal. Additionally, each neuron in the hidden and output layers has a threshold parameter, also known as bias.

Typically, the neurons in the input layer simply forward the signals to the hidden neurons. The behavior of the neurons in the other layers will be explained using Figure 1.

Figure 1 exhibits the j-th neuron of the (k+1) layer of a multilayered neural network. This j-th neuron of the (k+1) layer receives a set of information $s_{pi,\,k}$ (i = 1, ..., n_k) – corresponding to the outputs (also called activations) of the n_k neurons of the previous layer – weighted, each one, by the weight $w_{j\,i\,k}$ corresponding to its connection. The neuron sums up these weighted inputs and the resulting value is added to a internal limit, a bias that can be represented by $\theta_{j,k+1}$. The neuron 'j' produces a response for the set of signals, according to an activation function f( ) [5, 14-16]:
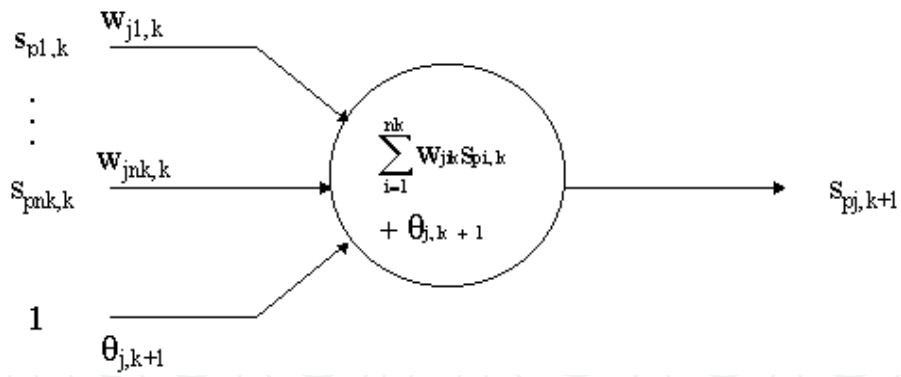
Figure 1. j-th neuron of layer (k+1).

The behavior of a neuron can be mathematically expressed by:

$$\lambda_{pj,k+1} = \left[\sum_{i=1}^{n_k} w_{jik} s_{pi,k} \right] + \theta_{j,k+1} \tag{1}$$

Some examples of activation functions are given below:

Linear function:

$$f\left(\lambda_{pj,k+1}\right) = \lambda_{pj,k+1} \tag{2}$$

Sigmoidal function:

$$f\left(\lambda_{pj,k+1}\right) = \left[1 + \exp\left(-\lambda_{pj,k+1}\right) \right]^{-1} \tag{3}$$

Hyperbolic tangent function:

$$f\left(\lambda_{pj,k+1}\right) = \tanh\left(\lambda_{pj,k+1}\right) \tag{4}$$

The training of an ANN is the determination of its parameters (weights and biases) using input-output data patterns. Typically, a function that gives the error of the network for the training patterns is minimized using multidimensional indirect optimization techniques. For MLP networks, an efficient approach is to start the optmization iterations using the backpropagation technique (which employs gradient descent search) and then proceed to a conjugate gradient search until a sufficiently small error function is obtained [17].

In order to guarantee the ability of the neural network to generalize when presented to new data, the available input-output patterns are randomly divided into two sets: one for training (usually 2/3 of the available set) and the other for validation (the remaining 1/3).

3.2. Methodology

First, a literature search was carried out for experimental biomass gasification data. Data from several references for gasification of different biomass were collected [4, 7, 9-10, 18-34].

The data search had three main information focuses: the gasification system (technical and operating aspects), type of biomass and the characteristics of the produced gas, as described in the following:

- Gasification system: type of gasifier as well as the dimensions of the reactor, the operating conditions and the gasification agent employed.
- Biomass: proximate and ultimate analysis data were collected. Additionally, when the heating value was not provided, its value was estimated based on the ultimate analysis data.
- Produced gas: the main information collected was the composition in terms of H_2, CO, CH_4 and CO_2.

Some characteristics of the gasification system (as the type of bed and the operation pressure) were restricted in the search for building the database that would be further used to train the neural networks. So, the ANNs were trained for fluidized bed gasifiers, using sand as bed and operated at atmospheric pressure. Only laboratory and pilot dimensions were used in this study. Initially, data for all the gasification agents were included in the training of the ANNs.

The complete database built had 181 input-output experimental patterns taken from references [4, 7, 9-10, 18-34] and can be obtained from the corresponding author under request. In the following, some observations are presented regarding the collected data:

- The contents of ashes, volatile components and fixed carbon were determined on a dry matter basis.
- The variable S/B indicates the ratio between the values of steam and biomass feed mass flows.
- The variables C, H, N, O and S indicate the mass percentage of carbon, hydrogen, nitrogen, oxygen and sulfur, respectively in the biomass fuel.
- The composition of the produced gas is given in volumetric percentage.
- The variable C_2H_n indicates the sum of the hydrocarbons with two atom of carbon that are formed in the process (mostly, ethylene and ethane).

At first, the choice of the input variables for the ANNs model was made heuristically, considering the analysis of the studied problem and the influence of the input variables in the prediction of the composition of the produced gas. Later, a sensitivity analysis was also implemented in order to help in that task.

In this work, the Statistica Neural Networks – SNN (Statsoft®) software was used in order to train and validate the neural networks. The ANNs that presented the best performance were of the kind MLP (Multilayer Perceptron). MLPs are feedforward, multilayered neural networks that typically present one input, at least one hidden layer and one output layer of computational nodes (the neurons). Details can be found in several references, including [5]. The MLPs employed in this work had one hidden layer of hyperbolic tangent neurons.

4. Results

### 4.1. Modeling results using ANNs

ANNs were trained using partial information about the gasification system and the biomasses in order to make predictions about the produced gas (composition in terms of H_2, CO, CH_4, CO_2, C_2H_n). The following information concerning the operating conditions of the gasifier was used as input variables to the neural network: equivalence ratio, steam/biomass ratio (S/B), temperature of the gasifier (T) and gasification agent used (the categories: air, steam, air/steam, steam/oxygen). Additionally the following information about the biomass was also used as input variables to the neural network: proximate (specifically, moisture, ash and volatile contents) and ultimate (specifically, C, H and O percentages) analysis data.

It must be emphasized that only partial information was used in order to avoid a large number of input variables to the neural network and, consequently, a large number of neurons and of parameters, that could lead to an overdimensioned neural network, with little predictive capability [5], considering the limited amount of literature data used for training.

A very detailed study was carried out, concerning the design and comparison of multilayered (MLP) neural network models models. ANNs with multiple and individual outputs were trained. The inclusion of an input categorical variable that classified the gasifier as 'bubbling' or 'circulating fluidized bed' was also investigated. Comparison with multi-regression linear models was performed and the MLP outperformed the linear models in all the cases studied here, due to the nonlinear nature of the data. This study is fully described in reference [35]. Here, due to space reasons, selected results are shown. The selection aimed to provide illustrative results of the application of ANNs in the modeling and optimization of gasification of different type of biomass in fluidized gasifiers.

In the following, preliminary results considering both bubbling and circulating fluidized bed gasifiers are presented. For the choice of this 'universal' neural network, three hundred ANNs were compared employing 2/3 of the patterns in the built database for training and 1/3 for validation. A total of 131 patterns were available for the prediction of the output variables (H_2, CO, CH_4, CO_2 and C_2H_n). The data for the continuous input variables were between the following limits: *7.5 < Moisture < 9.4; 71.02 < Volatiles < 82; 0.32< Ash < 26.4; 36.57 < C < 48; 4.91 < H < 6.04; 39 < O < 45.43; 0 < Equivalence ratio < 0.9; 0.113 < S/B < 4.7 and 650 < T < 900.* The gasification agent was considered as a categorical input variable for this 'universal' neural network.

A total of 300 MLPs, with different topologies, was trained using the Statistica Neural Networks. The ANN selected was the one that presented the smallest error for validation. It presented a topology consisting of 13 neurons in the input layer (4 for the categorical variable and 9 for the continuous input variable), 13 in the hidden layer and 5 in the output layer. This configuration can be seen in Figure 2.
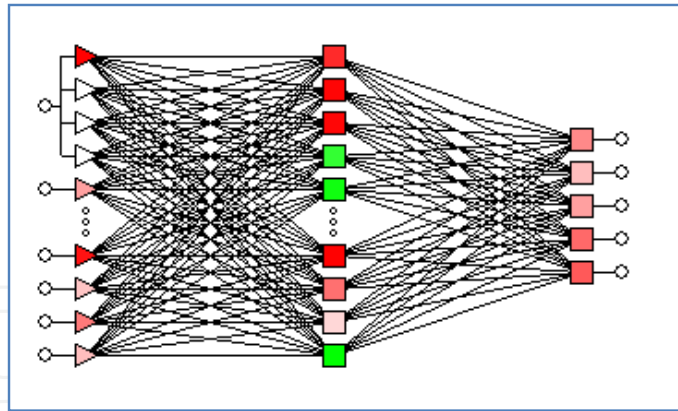
Figure 2. Topology of the multiple output neural network 13:13:5 MLP

Table 1 presents an analysis of the performance of the neural network. One statistical parameter used in the analysis was the SD-ratio parameter, which calculates the ratio between the standard-deviation of the ANN model and the standard-deviation of the training and validation (or selection) data. If the SD-Ratio is 1.0, then the network does no better than a simple average. A low (lower than 0.25) SD-ratio for the validation (or selection data) is indicative of a very good generalization capability of the ANN. This criterium (named here Select Performance) was used to select the best neural network during the training phase. It can be seen that the values of the SD-Ratio are between 0.13 and 0.18, with the exception of the result for C_2H_n, which was a bit higher (0.34).

Table 1 also show that high standard Pearson-R correlation coefficient between the actual and predicted outputs for the five output variables. In order to have accurate predictions, this parameter should be as close to one as possible. The high correlation between the predicted concentrations and the observed ones can also be observed in Figures 3 to 7. The lowest value for the correlation coefficient was observed for the prediction of C_2H_n, which shows the highest dispersion. This was similar to what had been obtained for the SD-Ratio and can be explained by the fact that the concentration of these components is very small in the produced gas; for that reason, many authors do not take their presence into account.

	H_2	CO	CH_4	CO_2	C_2H_n
Data mean	38.62	27.71	4.84	27.20	1.46
Data S.D.	17.99	14.32	4.58	12.47	1.87
Error mean	-0.23	-0.16	-0.04	0.11	0.03
Error S.D.	2.29	2.13	0.82	2.15	0.63
Absolute Error mean	1.68	1.47	0.50	1.56	0.28
SD-Ratio	0.13	0.15	0.18	0.17	0.34
Correlation	0.99	0.99	0.98	0.99	0.92

Table 1. Analysis of the Performance of the Multiple Output 13:13:5 MLP

A correlation of 1 indicates only that a prediction is perfectly linearly correlated with the observed outputs. So, here, in order to judge the quality of the predictions, a high Pearson-R correlation coefficient will be required together with small SD-Ratio parameter.

A sensitivity analysis was also carried out in order to evaluate the importance of each input variable to the predictive performance of the neural network. In this analysis, if one specific variable is considered 'unavailable' (that is, only its means value is used) the performance of the network should deteriorate and its Error should increase. Based on this fact, the sensitivity analysis, calculates the ratio between the Error and the Baseline Error (i.e. the error of the network if all variables are 'available'). If the Ratio is one or lower, then making the variable 'unavailable' either has no effect on the performance of the network or enhances it. This way, the higher the Ratio, the most important is that particular input variable to the performance of the ANN.

Table 2 presents the results of the sensitivity test, where the Rank lists the variables in order of importance. The results in Table 2 indicate that all listed 10 input variables are important; thus, it can be concluded these variables are needed in order to perform accurate predictions, being the gasification agent the most important one.

Even though these first results were quite satisfactory, improved results were sought. In order to obtain more parsimonious (in terms of number of neurons) models, without harming the statistical parameters (SD-Ratios and correlation parameters), individual – one for the prediction of each component gas – MLPs, with only one output variable, were trained.

Again, for the sake of conciseness, the results will be summarized, being their complete description found in reference [35].

A total of 300 MLPs with different topologies was trained for each individual output MLP. The best one for each case was considered as the one that presented the smallest SD-Ratio for the validation patterns. Table 3 presents the results of the individual output MLP against the multiple output MLP.
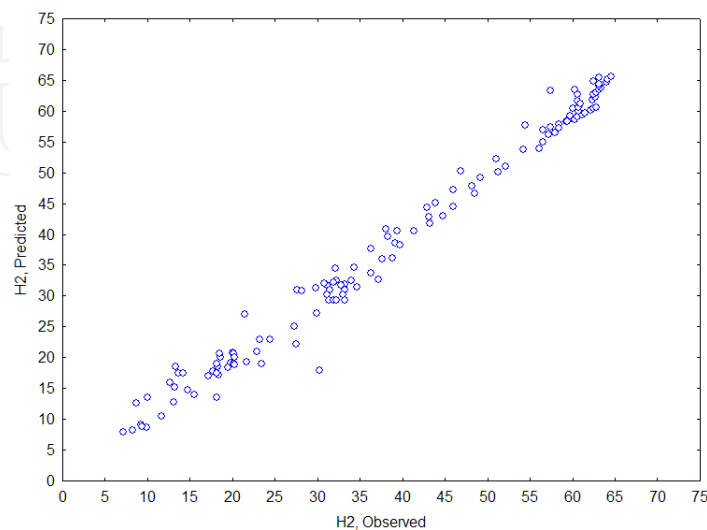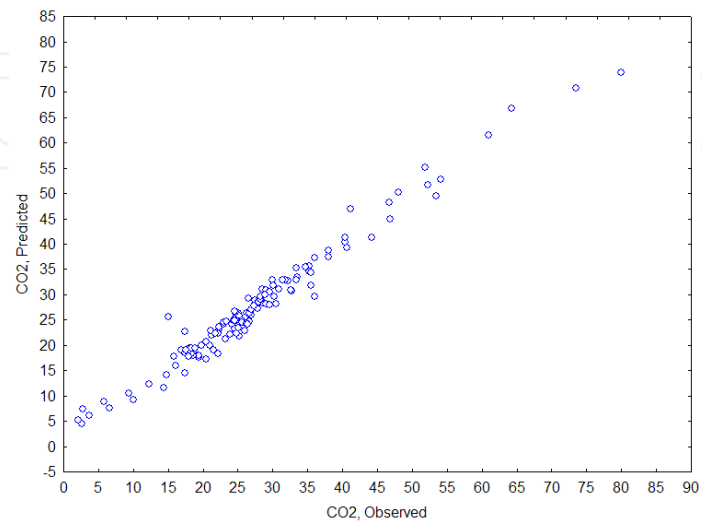

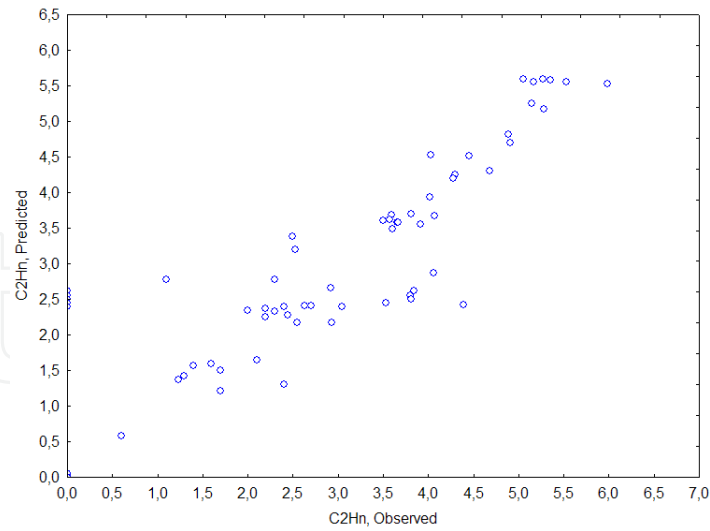**Figure 3.** Prediction of H2 concentration in the output gases for the Multiple Output 13:13:5 MLP
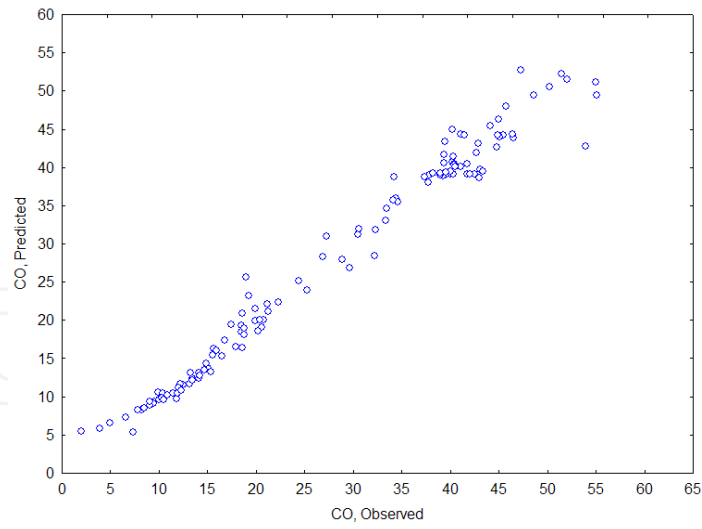
Figure 4. Prediction of CO concentration in the output gases for the Multiple Output 13:13:5 MLP
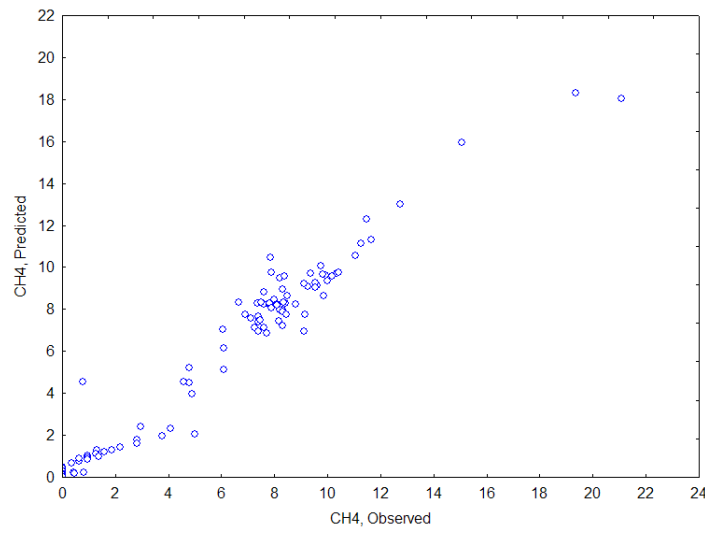
Figure 5. Prediction of CH4 concentration in the output gases for the Multiple Output 13:13:5 MLP

Figure 6. Prediction of CO2 concentration in the output gases for the Multiple Output 13:13:5 MLP

Figure 7. Prediction of C2Hn concentration in the output gases for the Multiple Output 13:13:5 MLP

	Gasification agent	Moisture	Ash	Volatiles	C	H	O	RE	S/B	T
Ratio	3.74	1.12	1.88	2.24	2.76	1.97	3.27	2.33	2.49	1.80
Rank	1	10	8	6	3	7	2	5	4	9

Table 2. Multiple output 13:13:5 MLP: sensitivity analysis

The analysis of the results presented in Table 3 show that it was possible to keep the predictive performance of the ANNs using individual output instead of multiple output models. The SD-Ratio and correlation parameters were of the same magnitude but the individual models had less neurons in the layers. It should be clarified here that for part of the models (as the ones for CO and CO_2) less variables were used in the input layer as sensitivity analysis showed that some variables were not necessary for an accurate prediction and were discarded as inputs [35].

	Multiple MLP			Individual MLP		
	SD-Ratio	Correlation	Topology	SD-Ratio	Correlation	Topology
H_2	0.13	0.99	13:13:5 MLP	0.13	0.99	11:9:1 MLP
CO	0.15	0.99	13:13:5 MLP	0.14	0.99	10:6:1 MLP
CH_4	0.18	0.98	13:13:5 MLP	0.13	0.99	13:9:1 MLP
CO_2	0.17	0.99	13:13:5 MLP	0.20	0.98	10:11:1 MLP

Table 3. Performance of the Individual Output MLP

Additionally, sensitivity tests – as the ones shown in Table 2 – revealed that the gasification agent was again the most important variable for the individual output MLPs as was the case for the multiple output ones. This motivated the development of 'specialized' MLPs for the prediction of the percentage composition of the four most important components (H_2, CO, CH_4, CO_2) in the output gas of bubbling, fluidized gasifiers.

High correlations values (ranging from 0.94 to 0.99) were obtained for these 'specialized' ANNs. In the following, results are shown for the neural network that predicts the hydrogen percentage in the produced gas of a bubbling fluidized gasifier, using steam as the gasification agent.

The obtained MLP presents 7 linear neurons in the input layer (for the input variables: 1. moisture (%wt); 2. volatile content (%wt); 3. C (%wt); 4. H (%wt); 5. O (%wt); 6. S/B; 7. T (^{o}C)); 10 hyperbolic neurons in the hidden layer and 1 linear neuron in the outtput layer. It was trained using the backpropagation method during the 100 initial epochs and the conjugate gradient during the 127 last ones [5, 35]. This ANN will be further cited here as 7:10:1 MLP.

Figure 8 illustrates the topology of the 7:10:1 MLP (a) and its results (b). A very high correlation (0.99) between predicted and observed value was obtained. Table 4 presents the results of the sensitivity test for the input variables. It can be seen that the mass percentage of hydrogen in the biomass fuel is the most important input variable for the prediction of hydrogen in the produced gas, as expected.

## 4.2. Preliminary results of operational optimization

A preliminary investigation was also conducted of the optimization of the operation of a particular gasifier using the gasification model provided by the neural network. The neural model described in the previous section for a bubbling gasifier using steam as the gasificant agent was employed. For this study, the biomass was fixed and the operating conditions (in terms of T and S/B) were varied, according to the data present in the built database [35] in order to maximize the yield of a given component in the produced gas.

The results for wood and straw biomasses and maximization of the production of hydrogen are described in the following to illustrate the procedure. Initially, the response surfaces using the neural model and the data for each biomass were plotted as shown in Figure 9 (a) and (b) for wood and straw, respectively. Analyzing these surfaces, the most adequate directions for changes in the operational variables can be chosen if the objective is to increase the production of hydrogen.

In Figure 9, the operating variables were varied considering the availability of data in that operating range. So, temperature was varied between 800 and 850 ^{o}C, for wood, and 650 and 900 ^{o}C, for straw. For the ratio S/B, the considered ranges were 1.1 < S/B < 4.7, for wood, and 0.4 < S/B < 0.9, for straw. It can be seen in Figure 9 that, if the operating values are restricted to those ranges, the maximization of H_2 in the produced gas demands higher S/B ratios and opposite directions for T (lower T for wood and higher T for straw). So, the model provided by the ANN provides information that could give the operator the right trends to maximize the production of a given product of interest.

Advancing a further step in the optimization, just for the sake of a preliminary investigation, the ability of the neural network to generalize (interpolating the training data) was also evaluated.

For the bubbling gasifier, with steam as the gasificant agent, the database training data included the operating variables in the range 650 < T < 900 ºC and 0.113 < S/B < 4.7 and three different biomasses (wood, straw and pine sawdust). A stochastic optimization method, the
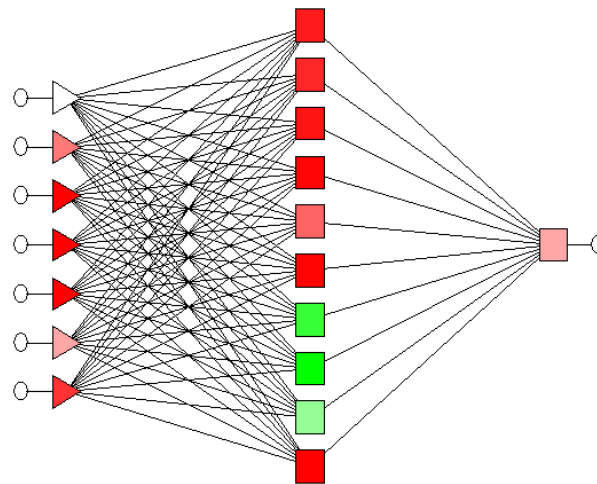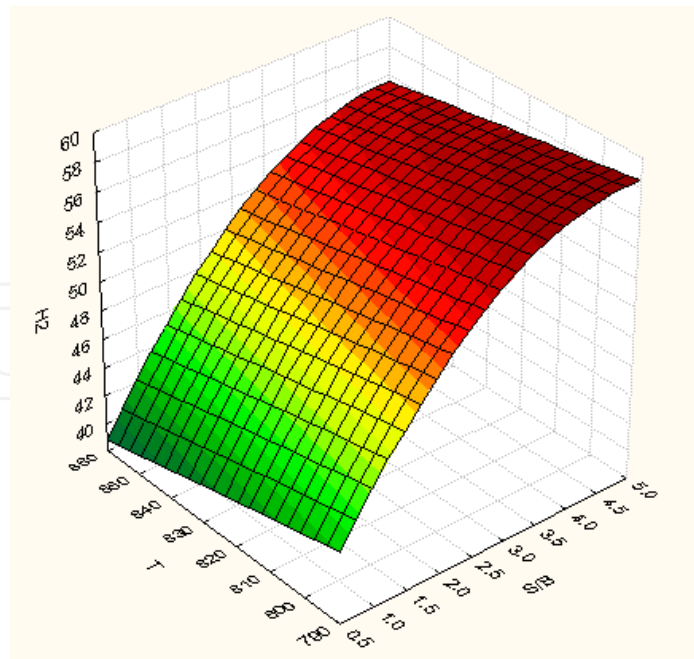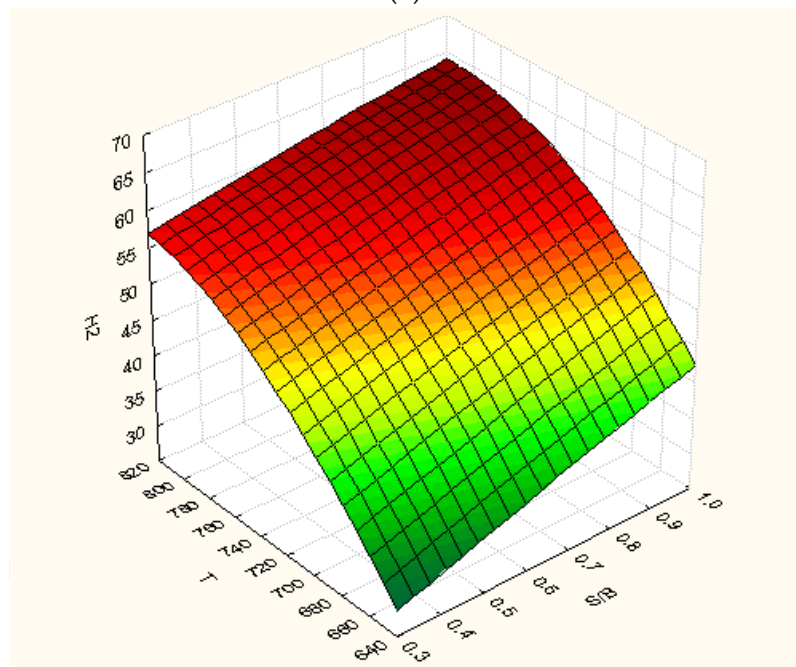

(a)
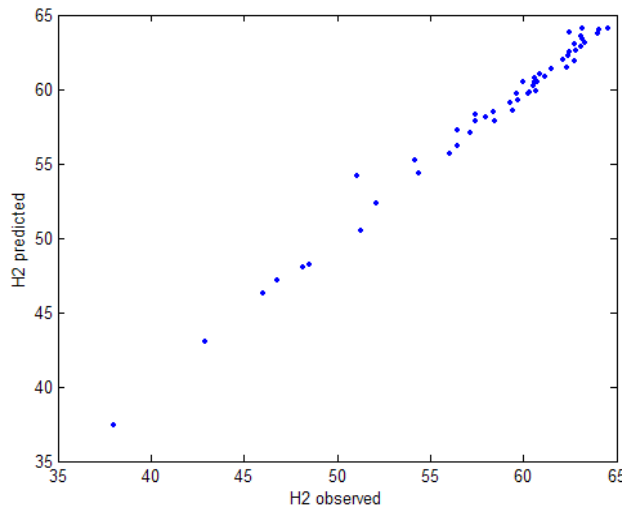
(b)

Figure 8. MLP 7:10:1 for prediction of hydrogen in the produced gas (bubbling gasifier, gasificant agent: steam): (a) illustration; (b) predicted vs. experimental values

	Moisture	Volatiles	C	H	O	S/B	T
Ratio	8.00	4.45	4.85	8.877	8.160	8.27	6.49
Rank	4	7	6	1	3	2	5

Table 4. MLP 7:10:1 for prediction of hydrogen in the produced gas (bubbling gasifier, gasificant agent: steam): sensitivity analysis

(a)

(b)

Figure 9. MLP 7:10:1 for prediction of hydrogen in the produced gas (bubbling gasifier, gasificant agent: steam): response surface for wood (a) and straw (b).

Particle Swarm Optimization (PSO) [36], was applied, in order to find the optimum (maximum yield of H_2 in the produced gas), for a given biomass, considering the whole operating range in the training database. When that approach was applied, as an example, for straw biomass, the PSO algorithm found an optimum for hydrogen production of 81.07 for S/B = 4.7 and T = 700.95 ºC. This result should be analysed very cautiously; the

percentage of hydrogen seems very high – as literature report percentage of 72 % [37] – but it indicates for the operator a region that should be further examined experimentally in order to reach higher percentages of the component of interest in the produced gas. Additional results and details may be found in [35].

5. Conclusions

ANNs are able to capture the latent characteristics present in the experimental data used for training, including nonlinearities [5]. Hence, multilayer perceptron neuron networks were proposed here as an alternative tool for the empirical modeling of biomass gasification. Specifically, ANN models were developed to correlate operating conditions of the gasifier and biomass data with characteristics of the produced gas, using experimental data given in the literature. It was verified that the developed model showed a good performance with a parsimonious number of units, when it was specifically built for a particular gasifier and a particular gasification agent [35]. Very high correlation rates between predictive and observed data were obtained.

The resulting trained ANN model is an algebraic mapping between input-output data, demanding little computational time. That fact makes the use of neural network very attractive in real time control and/or optimization of the process. The preliminary optimization investigation carried out here showed that the ANNs may supply the operator with information of tendencies that should be further experimentally checked in order to reach the target of maximizing the amount of a given component in the produced gas.

Calibration of the ANNs is easily performed, that is, whenever additional data are available, they may be added to the database and the ANN may be retrained, improving its predictive ability.

Presently, works based on hybrid neural-phenomenological [38] are being developed by the group as done before with a biotechnological process [39].

Author details

Maurício Bezerra de Souza Jr., Leonardo Couceiro Nemer and Amaro Gomes Barreto Jr.
Rio de Janeiro Federal University, Chemical Engineering Department, Centro de Tecnologia,
Ilha do Fundão, Rio de Janeiro, Brazil

Cristina Pontes B. Quitete
Petrobras, R&D Center, R&D in Gas, Energy and Sustainable Development,
Av. Horário de Macedo, Cidade Universitária, Rio de Janeiro, Brazil

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