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1 Predicting the effect of bed materials in bubbling fluidized bed gasification  
2 using artificial neural networks (ANNs) modeling approach

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10 **Abstract**

11 The effect of different bed materials was included as a new input into an artificial neural network  
12 model to predict the gas composition (CO<sub>2</sub>, CO, CH<sub>4</sub> and H<sub>2</sub>) and gas yield of a biomass  
13 gasification process in a bubbling fluidized bed. Feed and cascade forward back propagation  
14 networks with one and two hidden layers and with Levenberg-Marquardt and Bayesian  
15 Regulation learning algorithms were employed for training of networks. A high number of  
16 network topologies were simulated to determine the best configuration. It was observed that the  
17 developed models are able to predict the CO<sub>2</sub>, CO, CH<sub>4</sub>, H<sub>2</sub> and gas yield with good accuracy  
18 ( $R^2 > 0.94$  and  $MSE < 1.7 \times 10^{-3}$ ). The results obtained indicate that this approach is a powerful  
19 tool to help in the efficient design, operation and control of bubbling fluidized bed gasifiers  
20 working with different operating conditions, including the effect of the bed material.

21 **Keywords:** gasification; bubbling fluidized bed; bed material; artificial neural network

22 **1. Introduction**

23 Biomass gasification is a highly efficient thermochemical conversion process that converts  
24 different biomass feedstocks into a raw gas mainly composed by H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and light

25 hydrocarbons which can be used in further applications such as fuel or for producing chemicals  
26 (Puig-Arnavat et al., 2013). This thermochemical process is a good option to transform different  
27 types of residues into valuable products to produce energy. Thereby, energy is produced in a  
28 renewable way and the problem of residues disposal is reduced. Among the different  
29 techniques used to study this process, modelling is a valuable tool to design and obtain a first  
30 approximation to the expected results, reducing the experimental and human cost. Different  
31 kinds of models, including thermodynamic equilibrium, kinetic rate, computational fluid dynamic  
32 (CFD) and artificial neural network (ANN) have been improved for studying and modelling the  
33 gasification processes (Ahmed et al., 2012; Baruah and Baruah, 2014; Puig-Arnavat et al.,  
34 2010).

35 Equilibrium models are based on the concept of chemical reaction equilibrium based on the  
36 second law of thermodynamics, considering also the transfer phenomena between phases and  
37 the reaction kinetics of the primary reactions (Karmakar and Datta, 2011; Mahishi and  
38 Goswami, 2007). In CFD models, a set of equations for mass, momentum and energy  
39 conservation are solved simultaneously along the gasifier to predict the distribution of different  
40 parameters such as temperature or species concentration (Baruah and Baruah, 2014).

41 The design of new products and processes is a challenge to researchers who face to high cost  
42 and time-consuming experiments to obtain reliable information for different operating conditions.  
43 The advances in soft computing and computer science enhance the interest in the development  
44 of prediction models for time consuming and costly experiments (Ayodele and Cheng, 2015). To  
45 overcome these concerns, artificial intelligence systems such as ANNs are a reliable tool for the  
46 prediction of nonlinear system data due to its accuracy, precision and low cost and time  
47 consuming.

48 ANN analysis is a recent approach for the prediction of the gasification outputs in which a neural  
49 network learns by itself from different sets of experimental data simulating the human brain in  
50 terms of mathematical functions. The theory of the ANN is based in the analogy with the human  
51 brain, which is composed by numerous elements called neurons organized in different layers.  
52 These neurons are interconnected and exchange information between them. When different  
53 stimulus or inputs are received by the neurons, they modify their state and transfer the  
54 information to the next neuron. This way the information travels across the different layers of  
55 neurons until a final response for the initial inputs is obtained. In order to obtain the final  
56 response, the neural network needs to learn and recognize the relationships between inputs  
57 and outputs, in the same way humans do. Thus, an ANN is formed by an input layer, a number  
58 of hidden layers and an output layer, being the number of neurons per layer a parameter that  
59 can be modified. As a modern approach, ANNs are particularly useful to obtain the solution of  
60 an extensive variety of problems in science and engineering, being the prediction performance  
61 and generalization closely related with the training of the network. This tool have an excellent  
62 learning ability and a high capability for recognizing and modeling complex non-linear relations  
63 between the input and the output variables of a process (Mikulandrić et al., 2014). These  
64 characteristics make ANNs very interesting and useful, motivating their use in the modeling of  
65 biomass gasification processes. Therefore, biomass gasification, which is a complex  
66 thermochemical process, can be conveniently simulated using the appropriately designed ANN.

67 The application of ANN in biomass pyrolysis and gasification processes have also been  
68 reported by (Karaci et al., 2016; Souza et al., 2012; Sreejith et al., 2013; Sunphorka et al., 2017;  
69 Xiao et al., 2009). ANN based models were developed for predicting the product yield and gas  
70 composition in an atmospheric steam blow biomass fluidized bed gasifier (Guo et al., 2001). It  
71 was concluded that the feed forward neural network model had better predictive accuracy over  
72 traditional regression models. Chavan et al. used two types of ANN based data-driven models

73 for the prediction of the gas heating value and production in coal gasifiers (Chavan et al., 2012).  
74 Mikulandrić et al. simulated a fixed bed gasifier using an ANN from experimental data, showing  
75 the capability of this tool to predict the results of a gasification process with acceptable accuracy  
76 and speed (Mikulandrić et al., 2014). Puig-Arnavat et al. obtained similar conclusions for the  
77 prediction of the gas composition in circulating and bubbling fluidized beds using ANN (Puig-  
78 Arnavat et al., 2013). Baruah et al. also developed a ANN-based model for the prediction of the  
79 gas composition in a down-draft fixed bed gasifier, using C, H, O, ash and moisture contents for  
80 the biomass and reduction zone temperature as inputs (Baruah et al., 2017). Pandey et al.  
81 predicted the performance of municipal solid waste gasification in terms of lower heating value  
82 of the gas and products, and gas yield (Pandey et al., 2016a). Recently, Shahbaz et al. also  
83 used the ANN approach for the studying the steam gasification of palm oil waste using bottom  
84 ash and CaO, obtaining a good prediction compared to experimental data (Shahbaz et al.,  
85 2019).

86 All the mentioned studies, used similar input data for the models based on the biomass  
87 properties (C, H, O, moisture and ash content) and operating conditions (temperature,  
88 equivalence ratio and steam/biomass ratio). However, a lot of work has been done using  
89 different bed materials in the fluidized bed in order to improve the product gas quality (Arena  
90 and Di Gregorio, 2014; Baratieri et al., 2010; Gómez-Barea et al., 2005). Although ANN based  
91 modeling have been used in biomass gasification, to the authors' knowledge, no study has  
92 focused in the prediction, using ANN and different bed materials, of a bubbling fluidized bed  
93 gasifier. This is parameter has an important influence in the products from the gasifier and is  
94 usually skipped from this type of approaches. Hence, the objective of the present work is to  
95 develop ANN models for the prediction of the producer gas composition and gas yield for  
96 several operating conditions in bubbling fluidized bed gasifiers using different bed materials.  
97 The addition of this new input data to the previous models is studied in order to get a more

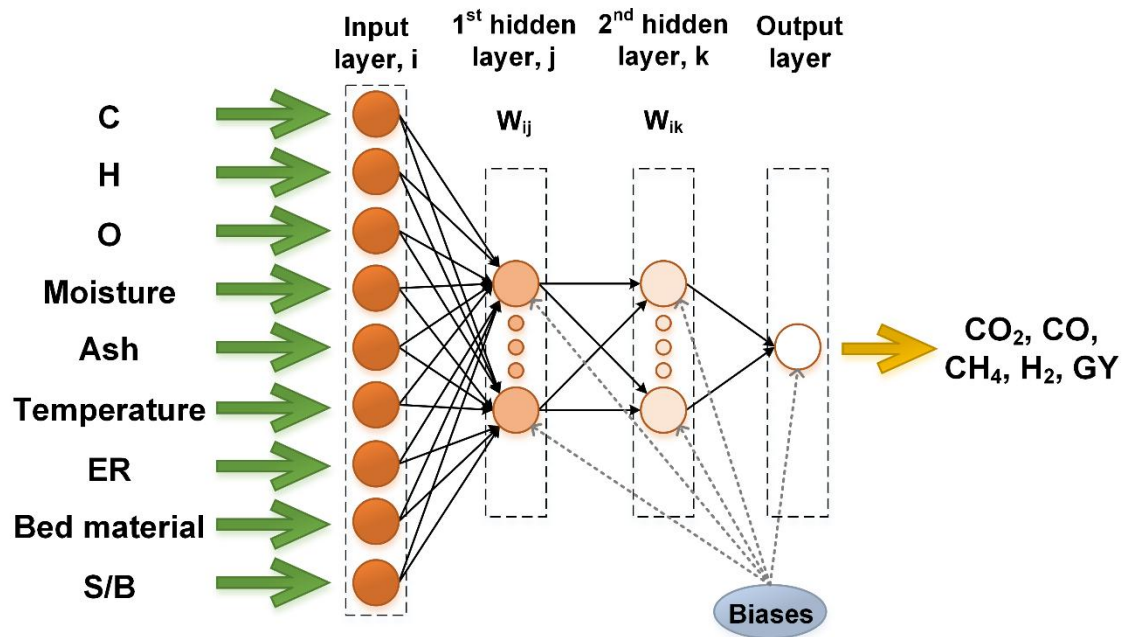
98 complete model for future predictions or, if, on the contrary, it results in a very complicated  
99 model that cannot obtain a relation between the input and output data.

## 100 **2. Material and methods**

### 101 **2.1. Artificial neural network (ANN) design**

102 In this study, the Neural Network Toolbox from MATLAB software R2018b was used to design  
103 and train the ANN, validating the obtained results. Figure 1 shows the topology of developed  
104 neural network with the input and output variables. Nine input parameters were selected for this  
105 work: carbon (C), hydrogen (H), oxygen (O), moisture (MC) and ash (Ash) contents for the  
106 biomass, equivalence ratio (ER), reaction temperature (T), steam/biomass mass ratio (S/B), and  
107 bed material. The first eight inputs are the usually employed in this type of studies as the give  
108 important information about the type of biomass and the most important operating conditions.  
109 The ninth input variable is added in this work as it also has an important relation with the final  
110 composition of the product gas and it is usually avoided in gasification ANN models. This  
111 variable has been accounted as a discrete variable ranging from 1 to 4, corresponding each  
112 value to one different bed material. This way, the network can be able to distinguish between  
113 bed materials. In the case of the outputs, five variables have been considered separately (i.e.:  
114 one ANN per output): H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and gas yield (GY). The experimental data needed for  
115 the ANN have been collected from previous biomass gasification experiments of the authors  
116 (Serrano et al., 2017, 2016) and completed with more experimental data collected from  
117 literature, using all of them a fluidized bed gasifier (Arena et al., 2010; Arena and Di Gregorio,  
118 2014; Baratieri et al., 2010; Campoy Naranjo, 2009; Christodoulou et al., 2014; De Andrés et al.,  
119 2011a, 2011b; Gómez-Barea et al., 2005; Huynh and Kong, 2013; Kaewluan and  
120 Pipatmanomai, 2011b, 2011a; Lahijani and Zainal, 2011; Lan et al., 2019; Loha et al., 2013; Lv  
121 et al., 2004; Mansaray et al., 1999; Miccio et al., 2009; Narváez et al., 1996; Pandey et al.,

122 2016b; Roche et al., 2014). Table 1 shows the boundaries and levels for the nine inputs and five  
 123 outputs used in this study. The range of this variables in addition to the type of gasifier (fluidized  
 124 bed) and gasifying agent (air), defines the range of validity of the present model.



125  
 126 Figure 1. Proposed ANN architecture to predict the five main producer gas components in a  
 127 bubbling fluidized bed gasifier.

128 A multi-layer feed forward and a cascade forward neural network based on back propagation  
 129 (BP) learning rule with different numbers of hidden layers (one and two) were simulated using  
 130 the experimental data to obtain the best prediction for the outputs during bubbling fluidized bed  
 131 gasification with different bed materials. Optimal number of hidden neurons in each hidden layer  
 132 has been determined for one and two hidden layers under 9–x–1 and 9–x–y–1 architectures,  
 133 respectively, where x and y represents the number of neurons in the first and second hidden  
 134 layer, respectively.

135 Table 1. Characteristics of input and output variables in the ANN based model.

Input variables	Range	Output variables	Range
C [%wt db]	27.30-85.17	GY [Nm <sup>3</sup> /kg daf]	0.23-6.26
H [%wt db]	1.61-14.04	CH <sub>4</sub> [%vol N <sub>2</sub> free]	2.31-28.97
O [%wt db]	0-59.42	CO <sub>2</sub> [%vol N <sub>2</sub> free]	2.27-58.06
Moisture [%wt ar]	0.20-27	H <sub>2</sub> [%vol dry]	2.60-56.88
Ash [%wt db]	0.33-44	CO [%vol N <sub>2</sub> free]	6.80-47.29
ER [-]	0.15-0.49		
T [°C]	650-1050		
Bed material	1-4		
S/B [-]	0-4.04		

136 For bed material: 1: Silica sand; 2: Ofite; 3: Olivine; 4: Alumina  
137 db, dry basis; ar, as received

138 During the BP training, the weights and biases of the different neurons are updated iteratively in  
139 order to reproduce the expected results. This algorithm uses the supervised training procedure  
140 where the network weights and biases are initialized randomly at the beginning of the training  
141 phase. The process for the error minimization is obtained using a gradient descent rule by  
142 changing the weights via an activation function for improving the performance of the network.  
143 The network minimizes the error by adjusting weights and biases until the minimum error is  
144 obtained.

145 The input data is repeatedly presented to the ANN and the error is computed for each repetition  
146 by comparing the output of the neural network with the desired output. Cascade forward back  
147 propagation (CFBP) operation by the use of the BP algorithm for weights updating is similar to  
148 the feed forward back propagation (FFBP) network, although the major characteristic of the  
149 network configuration is that each layer of neurons is connected to all neurons of previous  
150 layers. Levenberg-Marquardt (LM) training algorithm was applied to update the network weights.  
151 The selection of the number of hidden layers and the number of neurons in each layer is a very  
152 crucial part in the development of neural network as it improves the capacity and ability of  
153 network.



154 An optimum neural network architecture is proposed by varying the number of hidden layers  
155 (from 1 to 2), transfer functions and number of neurons in each hidden layer (up to 30 neurons).  
156 This selection is made considering previous works using ANNs (Pandey et al., 2016a; Puig-  
157 Arnavat et al., 2013). Different transfer functions including linear (purelin), hyperbolic tangent  
158 sigmoid (tansig) and logarithmic sigmoid (logsig) transfer functions, given in the following  
159 equations, have been utilized to reach the optimum network structure (Chayjan et al. 2014):

$$160 \quad Y = A \quad \text{(purelin)} \quad (1)$$

$$161 \quad Y = \frac{2}{(1+e^{-2A})} - 1 \quad \text{(tansig)} \quad (2)$$

$$162 \quad Y = \frac{1}{1+e^{-A}} \quad \text{(logsig)} \quad (3)$$

163 where  $A_j$  is computed as follows:

$$164 \quad A = \sum_{i=1}^m W_i X_i + b \quad (4)$$

165 and where  $X_i$  is the input value for the  $i^{\text{th}}$  input neuron,  $W_i$  is the weight between the  $i^{\text{th}}$  input and  
166 the hidden layer,  $b$  is the bias for the corresponding neuron of the layer, and  $m$  is the number of  
167 input neurons. The number of transfer functions for each ANN depends on the number of  
168 hidden and output layers. Each hidden layer needs its transfer function and the same for the  
169 output layer.

170 In order to check the robustness, validation and prediction ability of the models, 203 data  
171 patterns obtained from different experimental conditions of experiments were randomly selected  
172 in 162 for training (80 %) and 41 for validation (20 %). These percentages are in agreement with  
173 the ones used by (Shahbaz et al., 2019). Additionally, another 10 new data patterns were used  
174 for testing (Table 3). This classification was maintained for all configurations, being the same  
175 training, validation and test data patterns in all networks. The details of ANN model parameters

176 are presented in Table 2. Combining these parameters (network type, number of hidden layers,  
 177 number of neurons and number of transfer functions), a total of 49140 ANN configurations were  
 178 simulated for each output variable. The selected data for testing was presented to the trained  
 179 and validated networks in order to compare the prediction performance over the same data  
 180 sets.

181 Table 2. Details of the ANN models

No	Particulars	Specifications
1	Network type	Feed Forward Backpropagation (FFBP) Cascade Forward Backpropagation (CFBP)
2	Training function or Training algorithm	Levenberg-Marquardt (LM) backpropagation (TRAINLM)
3	Adaption learning function	Gradient Descent with Momentum Weight and Bias (LEARNGDM)
4	Performance function	Mean Square Error (MSE)
5	Transfer functions	Hyperbolic Tangent Sigmoid (TANSIG) Logarithmic sigmoid (LOGSIG) Linear (PURELIN)
6	Data division	Random (Dividerand)
7	Number of input layer unit	9
8	Number of output layer unit	1
9	Number of hidden layers	1 and 2
10	Number of neurons in the hidden layer	From 1 to 30
11	Number of epoch (Learning cycle)	2000 iterations

182

183 **2.2. Data normalization and error evaluation**

184 As a first step in ANN modelling to predict the outputs, all datasets (input and output) should be  
 185 normalized as it increases the ability of model and the performance of the network for  
 186 diagnosing relation among inputs and outputs, guaranteeing the convergence and the stability  
 187 of the process (Hasanipanah et al. 2015). Data normalization has been carried out using the  
 188 following equation

$$189 \quad Z_{norm} = \frac{Z_r - Z_{min}}{Z_{max} - Z_{min}} \quad (5)$$

190 where  $Z_r$  and  $Z_{norm}$ , represent the measured and normalized values, respectively,  $Z_{min}$ ,  $Z_{max}$  are  
 191 the minimum and maximum values of the measured parameters, respectively.

192 The mean square error (MSE) and the coefficient of determination ( $R^2$ ) have been used to  
 193 compare the performance of the different ANN models. These parameters have been  
 194 calculated by using the following equations for the experimental and ANN predictions so the  
 195 best network performance is statistically obtained by the MSE and the  $R^2$  (Chayjan et al.2014;  
 196 Golpour et al. 2015):

$$197 \quad \underline{MSE = \frac{1}{n} \sum_{k=1}^n (S_k - T_k)^2} \quad (6)$$

$$198 \quad \underline{R^2 = 1 - \frac{\sum_{k=1}^n (S_k - T_k)^2}{\sum_{k=1}^n \left( S_k - \frac{\sum_{k=1}^n S_k}{n} \right)^2}} \quad (7)$$

199 where  $S_k$  is the network output for  $k^{\text{th}}$  dataset,  $T_k$  is the target output for  $k^{\text{th}}$  dataset and  $n$  is the  
 200 number of datasets. A low value for MSE indicates a small error between the targets and the  
 201 outputs, and values of  $R^2$  close to 1 indicates how well the model reproduces the desired  
 202 outputs.

203 Table 3. Test data.

Test ID	C [%wt db]	H [%wt db]	O [%wt db]	Moisture [%wt]	Ash [%wt db]	ER [-]	T [°C]	Bed material	S/B
1	50.54	7.08	41.11	8.00	0.55	0.22	800	sand	2.70
2	49.00	6.10	44.40	7.00	0.40	0.25	750	alumina	0
3	50.00	6.20	36.30	7.60	6.30	0.31	820	ofite	0
4	49.30	5.90	44.37	8.40	0.33	0.17	780	olivine	0.65
5	32.31	5.37	14.38	8.70	41.70	0.30	800	sand	1
6	27.30	4.80	18.9	7.00	44.00	0.40	850	sand	0
7	85.17	13.83	0.00	0.20	1.00	0.31	825	olivine	0
8	37.60	5.42	33.20	9.08	23.40	0.35	670	alumina	0
9	49.47	5.79	41.94	6.28	0.71	0.23	752	ofite	0.18
10	42.68	3.30	31.72	9.95	21.68	0.35	850	sand	0.8

204

205 In addition, the mean average percentage error (MAPE) was also calculated to measure the  
206 performance of the models with the test data. This value accounts for the absolute value of the  
207 average magnitude of errors in predicting each variable (Sreejith et al., 2013). This parameter,  
208 being a percentual value, is simpler to quantify and understand the error produced by the model  
209 for new data as it gives information how far the predictions are from the target values. This way,  
210 the accuracy of the prediction of new data can be better addressed.

211  $MAPE = \frac{1}{n} \sum_{i=1}^n \frac{|y_i - \hat{y}_i|}{y_i}$  (8)

### 212 3. Results and discussion

#### 213 3.1. ANN using silica sand as bed material

214 Before analyzing the results of the different ANN using different bed materials, only datasets  
215 with silica sand as bed material (135 datasets) were used to obtain the best ANN configuration  
216 for each output. As in this case the bed material is the same for all experimental datasets, the  
217 number of inputs is reduced, having the ANN topology 8 inputs for both one and two hidden  
218 layers (8-x-1 and 8-x-y-1). Table 4 shows the results of this analysis for the different  
219 configurations in each ANN developed. The results have been selected to show the best  
220 topology and threshold functions for FFCP and CFBP, respectively. As it can be observed,  
221 configurations with one hidden layer, either FFBP or CFBP, always produced worst results than  
222 configuration with two hidden layers for all the outputs.

223 In the case of CO<sub>2</sub>, the best result was obtained with a FFBP network with two hidden layers (21  
224 and 4 neurons, respectively) and tansig-tansig-logsig as transfer functions (for the two hidden  
225 layers and the output layer). This structure generated a MSE and R<sup>2</sup> of 1.26·10<sup>-3</sup> and 0.9737,  
226 respectively. A FFBP network with two hidden layers (24 and 7 neurons, respectively) and  
227 tansig-tansig-logsig as transfer functions was the best configuration for CO prediction. The  
228 performance outputs for this architecture resulted in a MSE = 1.13·10<sup>-3</sup> and a R<sup>2</sup> = 0.9713. The  
229 most promising results for CH<sub>4</sub> prediction were obtained with a FFBP network with two hidden  
230 layers (3 and 22 neurons, respectively) and tansig-logsig-purelin as threshold functions. This  
231 composition produced a MSE = 7.50·10<sup>-4</sup> and a R<sup>2</sup> = 0.9553. In the case of H<sub>2</sub>, a FFBP network  
232 with two hidden layers (23 and 19 neurons, respectively) was the best topology. The logsig  
233 transfer function was the same for all layers (hidden and output), with a MSE and R<sup>2</sup> values  
234 equal to 3.19·10<sup>-3</sup> and 0.8979, respectively. The gasification performance is measured in terms  
235 of the GY. A FFBP network with two hidden layers (19 in both first and second hidden layers)  
236 and purelin-logsig-purelin as threshold functions performed the best. In this structure, the MSE  
237 and R<sup>2</sup> values were 4.44·10<sup>-4</sup> and 0.9762, respectively.

238 Table 4. Best-selected topologies including different layers and neurons for FFBP and CFBP  
 239 configurations using silica sand as bed material.

Element	Network	Threshold function	Topology	R <sup>2</sup>	MSE
CO <sub>2</sub>	FFBP	logsig-tansig	8-8-1	0.9052	4.55·10 <sup>-3</sup>
	<b>FFBP</b>	<b>tansig-tansig-logsig</b>	<b>8-21-4-1</b>	<b>0.9737</b>	<b>1.26·10<sup>-3</sup></b>
	CFBP	logsig-tansig	8-5-1	0.7554	1.17·10 <sup>-2</sup>
	CFBP	logsig-logsig-logsig	8-3-11-1	0.9627	1.79·10 <sup>-3</sup>
CO	FFBP	logsig-purelin	8-23-1	0.8348	6.51·10 <sup>-3</sup>
	<b>FFBP</b>	<b>tansig-tansig-logsig</b>	<b>8-24-7-1</b>	<b>0.9713</b>	<b>1.13·10<sup>-3</sup></b>
	CFBP	logsig-logsig	8-5-1	0.8847	4.54·10 <sup>-3</sup>
	CFBP	purelin-tansig-purelin	8-18-27-1	0.9698	1.19·10 <sup>-3</sup>
CH <sub>4</sub>	FFBP	logsig-purelin	8-28-1	0.7586	4.05·10 <sup>-3</sup>
	<b>FFBP</b>	<b>tansig-logsig-purelin</b>	<b>8-3-22-1</b>	<b>0.9553</b>	<b>7.50·10<sup>-4</sup></b>
	CFBP	logsig-logsig	8-16-1	0.7871	3.57·10 <sup>-3</sup>
	CFBP	tansig-tansig-purelin	8-28-13-1	0.8264	2.91·10 <sup>-3</sup>
H <sub>2</sub>	FFBP	logsig-logsig	8-5-1	0.7576	7.58·10 <sup>-2</sup>
	<b>FFBP</b>	<b>logsig-logsig-logsig</b>	<b>8-23-19-1</b>	<b>0.8979</b>	<b>3.19·10<sup>-3</sup></b>
	CFBP	logsig-tansig	8-11-1	0.6419	1.12·10 <sup>-2</sup>
	CFBP	tansig-logsig-logsig	8-14-8-1	0.8869	3.54·10 <sup>-3</sup>
GY	FFBP	logsig-purelin	8-26-1	0.6469	6.59·10 <sup>-3</sup>
	<b>FFBP</b>	<b>purelin-logsig-purelin</b>	<b>8-19-19-1</b>	<b>0.9762</b>	<b>4.44·10<sup>-4</sup></b>
	CFBP	logsig-logsig	8-2-1	0.8983	1.90·10 <sup>-3</sup>
	CFBP	logsig-tansig-purelin	8-3-15-1	0.9716	5.30·10 <sup>-4</sup>

240

241 Once the best ANN topology for each element has been selected, the test data (Table 3) were  
 242 introduced in the network to assess the accuracy of the ANN estimations. In this case, only 4  
 243 test data were used, the ones using silica sand as bed material. Figure 2a-e shows the

244 experimental versus the predicted values, using the different ANN selected for each output.  
 245 These figures also include the regression coefficient for the linear fitting. In general, all the ANN  
 246 models reproduced rather good results for the testing points. In the case of H<sub>2</sub>, the model did  
 247 not estimate the testing point 6 with a good accuracy, obtaining a relative error of 90% with  
 248 respect to the experimental value. This leads to a very poor regression coefficient for this element.  
 249 However, the rest of the points, including this one for CO<sub>2</sub>, CO, CH<sub>4</sub> and GY, were near enough  
 250 to the experimental ones. The MAPE for the test data is shown in Table 6, with values around  
 251 10% for CO<sub>2</sub>, CO and CH<sub>4</sub>, around 25% for H<sub>2</sub> and 2% for GY. These results can be acceptable  
 252 for ANN prediction models, as also obtained in previous works (Pandey et al., 2016a; Sreejith et  
 253 al., 2013).

### 254 3.2. ANN using silica sand, ofite, olivine and alumina as bed material

255 In this section, the effect of the bed material in the fluidized bed reactor was introduced in the  
 256 model, using all datasets obtained from the literature (see supplementary information).  
 257 According to the information in Table 2, 49140 ANNs have been simulated for each output  
 258 variable. Table 5 shows the results in terms of MSE and R<sup>2</sup> for the different configurations in  
 259 each ANN developed. In this case, configurations with one hidden layer, either FFBP or CFBP,  
 260 also produced worst results as in the ANN using only sand as bed material.

261 Table 5. Best-selected topologies including different layers and neurons for FFBP and CFBP  
 262 configurations using different bed materials.

Element	Network	Threshold function	Topology	R <sup>2</sup>	MSE
CO <sub>2</sub>	FFBP	logsig-logsig	9-2-1	0.6092	1.31·10 <sup>-2</sup>
	<b>FFBP</b>	<b>tansig-tansig-logsig</b>	<b>9-16-15-1</b>	<b>0.9734</b>	<b>8.91·10<sup>-4</sup></b>
	CFBP	logsig-tansig	9-17-1	0.6745	1.09·10 <sup>-2</sup>

	CFBP	tansig-tansig-logsig	9-15-24-1	0.9659	$1.14 \cdot 10^{-3}$
CO	FFBP	logsig-logsig	9-21-1	0.9544	$1.67 \cdot 10^{-3}$
	<b>FFBP</b>	<b>tansig-tansig-purelin</b>	<b>9-21-19-1</b>	<b>0.9712</b>	<b><math>1.05 \cdot 10^{-3}</math></b>
	CFBP	logsig-logsig	9-9-1	0.8340	$6.07 \cdot 10^{-3}$
	CFBP	tansig-logsig-logsig	9-2-17-1	0.9694	$1.12 \cdot 10^{-3}$
CH <sub>4</sub>	FFBP	logsig-tansig	9-12-1	0.7353	$6.16 \cdot 10^{-3}$
	FFBP	tansig-tansig-logsig	9-26-15-1	0.9328	$1.56 \cdot 10^{-3}$
	CFBP	logsig-logsig	9-16-1	0.9068	$2.17 \cdot 10^{-3}$
	<b>CFBP</b>	<b>tansig-tansig-logsig</b>	<b>9-7-27-1</b>	<b>0.9462</b>	<b><math>1.25 \cdot 10^{-3}</math></b>
H <sub>2</sub>	FFBP	logsig-logsig	9-22-1	0.4856	$1.43 \cdot 10^{-2}$
	<b>FFBP</b>	<b>tansig-tansig-logsig</b>	<b>9-5-30-1</b>	<b>0.9394</b>	<b><math>1.69 \cdot 10^{-3}</math></b>
	CFBP	logsig-purelin	9-30-1	0.4810	$1.44 \cdot 10^{-2}$
	CFBP	purelin-logsig-logsig	9-24-21-1	0.9231	$2.14 \cdot 10^{-3}$
GY	FFBP	logsig-purelin	9-3-1	0.7676	$5.28 \cdot 10^{-3}$
	<b>FFBP</b>	<b>tansig-tansig-logsig</b>	<b>9-18-19-1</b>	<b>0.9872</b>	<b><math>2.90 \cdot 10^{-4}</math></b>
	CFBP	tansig-purelin	9-2-1	0.7699	$5.23 \cdot 10^{-3}$
	CFBP	logsig-logsig-logsig	9-8-10-1	0.9843	$5.56 \cdot 10^{-4}$

263

264 The best result for CO<sub>2</sub> was obtained with a FFBP network with two hidden layers with 16 and  
265 15 neurons, respectively. The threshold function for this network was tansig-tansig-logsig. This  
266 structure generated a MSE =  $8.91 \cdot 10^{-4}$  and  $R^2 = 0.9734$ . According to the results (not presented  
267 here), another FF network configuration produced rather similar results with a  $R^2$  higher than  
268 0.97, with different transfer functions and neurons configuration. In the case of CO, a FFBP  
269 network with two hidden layers (21 and 19 neurons) and tansig-tansig-purelin as threshold  
270 functions was the best configuration. The performance outputs for this architecture resulted in a  
271 MSE =  $1.05 \cdot 10^{-3}$  and  $R^2 = 0.9712$ . In this case, the FFBP configuration with one hidden layer  
272 also produced rather good results ( $R^2$  higher than 0.95). The most promising results for CH<sub>4</sub>  
273 were obtained with a CFBP network, two hidden layers with 7 and 27 neurons, respectively, and



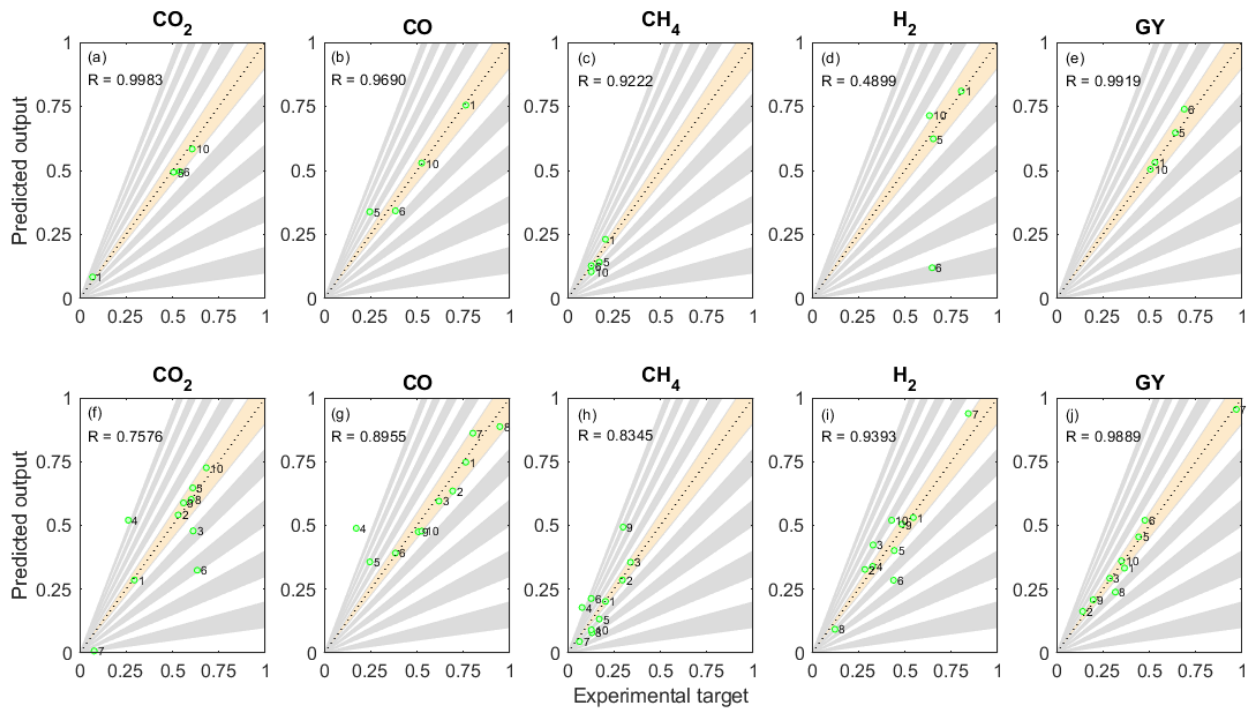
274 tansig-tansig-logsig threshold functions. This composition produced a MSE =  $1.25 \cdot 10^{-3}$  and  $R^2 =$   
 275 0.9462. The best configuration for H<sub>2</sub> was a FFBP network with two hidden layers (5 and 30  
 276 neurons, respectively) and tansig-tansig-logsig threshold functions, with a MSE and  $R^2$  values  
 277 equal to  $1.69 \cdot 10^{-3}$  and 0.9394, respectively. Up to 12 network FF topologies also resulted in  $R^2$   
 278 values higher than 0.93. In the case of GY, the best configuration was a FFBP network with two  
 279 hidden layers (18 and 19 neurons, respectively) and tansig-tansig-logsig as threshold functions.  
 280 In this structure, the MSE and  $R^2$  values were  $2.90 \cdot 10^{-4}$  and 0.9872, respectively.

281 Figure 2f-j shows the results when the test data (Table 3) was introduced in the different  
 282 models. In this case, the regression coefficients were a bit worse than in the previous case  
 283 using silica sand as bed material, influenced by the higher number of test data and the higher  
 284 complexity of the ANNs as they have to differentiate between different bed materials. Then, the  
 285 test data produced rather good correlation between experimental and predicted data, been most  
 286 of the test points below a relative error of 10%. It can be observed that for each output the test  
 287 data points with higher error are not always the same. Although test number 4 (olivine as bed  
 288 material) is always quite far from the experimental target. Attending to the MAPE, this parameter  
 289 resulted in higher values than in the previous scenario with silica sand as bed material. Due to  
 290 the higher complexity of the models and the heterogeneity of the data, these results could be  
 291 satisfactory.

292 Table 6. MAPE for the test data in the different ANN models.

	CO <sub>2</sub>	CO	CH <sub>4</sub>	H <sub>2</sub>	GY
<i>Silica sand as bed material</i>					
	8.78	12.54	12.21	24.89	2.25
<i>Silica sand, ofite, olivine and alumina as bed materials</i>					
	28.21	27.30	38.91	15.64	8.18

293



294

295 Figure 2. Testing results for the selected ANNs: (a)-(e) using silica sand as bed material; (f)-(j)  
 296 using all bed materials. Each shadowed region corresponds with a relative error of 10%.

297 The R values shows a good fitting during training and validation, while for testing process that  
 298 indicator is a bit worse due to the big error introduced with test data set 4. It is clearly apparent  
 299 that the accuracy of the network during the training process is better than testing or validation.  
 300 During the training process, the network modifies the values of its input and output weights to  
 301 get the best fitness whereas in the testing or validation process the output shows the actual  
 302 predictive performance of the trained model on new data without adjusting the weights.  
 303 Therefore, the observed  $R^2$  and MSE values show a good indication of well-trained ANN model.  
 304 The performance of the model is an indication of the appropriate selection of the input variables.  
 305 The obtained networks are highly accurate and consume a short time to obtain the results.  
 306 These findings are in agreement with the reported results in the literature (Souza et al., 2012). It  
 307 can be stated that ANN are powerful tools for gasification modeling in different conditions.

#### 308 **4. Conclusions**

309 The FFBP models with two hidden layers show an improved performance over the CFBP  
310 models and those with only one hidden layer to predict product gas composition in terms of  
311 CO<sub>2</sub>, CO, CH<sub>4</sub>, H<sub>2</sub> and GY, producing a higher coefficient of determination (R<sup>2</sup>). The results  
312 show that the degree of agreement between experimental and predicted values justifies the  
313 accuracy of the proposed ANN models. Therefore, for a given bubbling fluidized bed gasifier,  
314 the developed models are capable of simulate the producer gas composition for selected  
315 biomasses at specified operating conditions, including the effect of the bed material in the  
316 reactor.

#### 317 **Supplementary information**

318 E-supplementary data associated with this work can be found in online version of the paper.

#### 319 **Abbreviations**

320	ANN	artificial neural network
321	BP	back propagation
322	CFBP	cascade forward back propagation
323	CFD	computational fluid dynamics
324	ER	equivalence ratio
325	FFBP	feed forward back propagation
326	GY	gas yield
327	LM	Levenberg-Marquardt

328 MAPE mean average percentage error

329 MC moisture content

330 MSE mean square error

331  $R^2$  determination coefficient

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