ARTIFICIAL NEURAL NETWORKS BASED ON COMMITTEE MACHINE TO PREDICT THE AMOUNT OF SULFUR AND PHOSPHORUS IN THE HOT METAL OF A BLAST FURNACE

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Abstract. Steel is an alloy of iron and carbon containing less than 2% carbon and small amounts of elements such as silicon, manganese, phosphorus, and sulfur, which together do not exceed 1% of the total. Sulfur and phosphorus are undesirable elements in steel because they cause brittleness. The best way to control sulfur and phosphorus content is during the production of cast iron in blast furnace. In the field of simulation and modeling, several models have been proposed for the simulation of blast furnace, which allow progress and detailed information about the fluid flow and mass and heat balances of the blast furnace. However, there are few mathematical models for the prediction of sulfur and phosphorus content. In this context, the main objective of this work was to develop an artificial neural network for predicting the sulfur and phosphorus content in cast iron. A mathematical model was developed based on a committee machine using 8 different artificial neural networks simultaneously. The artificial neural networks with a single hidden layer had neurons varying in 10, 20, 25, 30, 40, 50, 75 and 100 neurons per layer. Pearson's correlation coefficients, RMSE and MAE confirmed that the hidden layer with 25 neurons gave the best results. The conclusion is that high values of mathematical correlation demonstrate the good statistical performance of ANN and show that the mathematical model is an effective predictor of sulfur and phosphorus.

Keywords: artificial neural networks, committee machine, blast furnace, sulfur, phosphorus.

1 Introduction

At the present stage of social development the world is unthinkable without steel. The production of this material is a strong indicator of the level of economic development of a country, as its consumption grows in proportion to the construction of buildings, the manufacture of vehicles, the installation of communications equipment, and the production of household and industrial appliances [5, 19]. These products have already become commonplace in our daily lives, but their production requires techniques that need to be renewed. For this reason, steel companies are investing more and more in research. Steel is an alloy of iron and carbon that contains less than 2% carbon and small amounts of elements such as silicon, manganese, phosphorus and sulfur, which together do not exceed 1% of the total content [3, 15].

Sulfur (S) is usually an undesirable element in steel as it causes brittleness when combined with iron in the form of sulfide. However, when combined with manganese in the form of the respective sulfide, it favors machining. Normally, every effort is made to reduce the sulfur content to the lowest possible level as it can also cause difficulties in welding steel [2, 16]. Phosphorus (P) is considered a harmful element for steels as it greatly reduces their ductility and toughness. Normally, all efforts are made to reduce the content of this element as much as possible. It makes the steel brittle, an effect that increases with increasing carbon content [10]. Coke is the main culprit for the increase in sulfur content in cast iron. This element can also enter the blast furnace via sulfur ores in the form of iron(II)sulfide (FeS), manganese(II)sulfide (MnS), iron(III)sulfide (FeS_2) or sulfates and reaches the gas stream in the form of H_2S or a monoxide compound associated with sulfur [11, 18].

Since the 1980s, the quality of raw materials and fuels used in iron and steel production has steadily deteriorated. This global trend has led to a deterioration in the quality of liquid cast iron in the form of higher impurity levels. At the same time, steel producers are facing an increasing demand for pure steel with low and very low contents, especially of sulfur and phosphorus [4, 8]. In the field of technology and modeling, in order to improve production conditions, in addition to predicting the effects of changes in production parameters, several models have been proposed to simulate blast furnaces, including two- and three-dimensional models that allow progress and detailed information on fluid flow and mass and heat balances within the blast furnace [1, 6, 17].

The modeling of a blast furnace depends on the process-related variables, and one of the main difficulties is to adequately describe the particle-particle and particle-liquid interactions [3, 7].

In the field of simulation of complex processes, the application of solutions based on neural networks has become very popular due to their versatility and the possibility of evolving the answers and making them more reliable, since the neural network receives new data during the training process. The application of neural network technique in steel production is new and there are few works on this topic, mainly for the control of impurities such as sulfur and phosphorus [3, 13, 20].

An artificial neural network (ANN) is a machine that models how the brain performs a specific task. The network is usually simulated through programming and is able to recognize patterns and perform learning processes [3, 14]. In this context, the main objective of this work was to develop an artificial neural network based on a committee machine to find out what is the ideal number of neurons that gives the best results for predicting the sulfur and phosphorus content in cast iron.

2 Experimental

The database for this study comes from a blast furnace of a Brazilian steel company that has an average daily production of 7200 tons. The operating data correspond to 270 registers with 18 input and 2 output variables. During the 1-year period, 270 registers were selected in which the blast furnace did not present major operating variations and was operated with practically the same reactivity value of the coke. Table 1 shows the input variables used in the mathematical modeling.

Table 1. Input variables

Input data	Unit	Mean	Input data	Unit	Mean
Pellet	kg/t	754.1 ± 62.1	Blowing flow	Nm^3/min	6228.2 ± 587.4
Sínter	kg/t	754.1 ± 50.4	Coke ash	%	8.7 ± 0.8
Iron ore	kg/t	37.2 ± 27.1	Coke moisture	%	3.8 ± 0.5
Coke rate	kg/t	300.4 ± 26.1	Nitrogen	Nm^3/t	17.2 ± 11.2
PCI rate	kg/t	198.2 ± 17.4	Oxygen flow	Nm^3/t	14372 ± 415
Fuel rate	kg/t	498.5 ± 21.5	Oxygen enrichment	%	4.2 ± 0.3
Dolomite	kg/t	7.2 ± 4.5	Flame temperature	°C	1205 ± 22
Slag basicity (B2)	%	1.17 ± 0.04	Airspeed tuyère	m/s	222 ± 26
Slag basicity (B4)	%	1.07 ± 0.04	Permeability	-	4.22 ± 0.19

The output variables analyzed in the mathematical model were sulfur and phosphorus. Table 2 shows the descriptive statistics of the output variables. Considering the database related to 270 operating days of the blast furnace, an artificial neural network was modeled based on a committee machine.

Table 2. Output variables

Variable	Minimum	Maximum	Mean
(%S) Sulfur	0.010	0.049	0.020 ± 0.006
(%P) Phosphorus	0.061	0.081	0.070 ± 0.055

The committee method is a field of machine learning that builds a set of classifiers that are more accurate than the best of the one group members. The base classifiers were iteratively trained using the Levenberg-Marquardt algorithm, an optimization method that computes the minimum of a function and converges faster. Simple majority voting is the simplest approach to explain how a committee machine works. Imagine a contest where each judge gives his score, i.e., the final score of the contestant depends on the contest rules. The final score can be the average of the judges' scores or an adjusted average, where the highest and lowest scores are excluded before the final score is calculated. This is the idea of the committee machine where multiple classifiers are combined in a voting strategy. As a final result, the answer that receives the highest number of votes is considered as the committee answer [1, 3, 8].

The number of neurons used in the intermediate layer depends on the complexity of the problem to be modeled, so it is difficult to estimate the number to be considered, which sometimes requires several attempts to obtain the optimal set. Therefore, there is no exact solution for determining the number of neurons in the intermediate layer [3, 8]. In this paper, artificial neural networks with a single hidden layer and a variable number of neurons in the hidden layer (10, 20, 25, 30, 40, 50, 75, and 100 neurons) modeled in MATLAB R2021a are considered. The performance of the committee machine was evaluated using 3 factors: (1) Pearson's mathematical correlation (R); (2) Root Mean Square Error (RMSE); (3) Mean Absolute Error (MAE). In this way, it was possible to assess which layers and which number of neurons gave the best results. In this investigation, the dataset was split into subsets to estimate the model parameters (training, validation and test data). Table 3 illustrates the division of variables for the construction of the mathematical model. Figure 1 illustrates the neural network architecture.

Table 3. Division of variables

Step	variables
Training	90
Validation	90
Testing	90
TOTAL	**270**

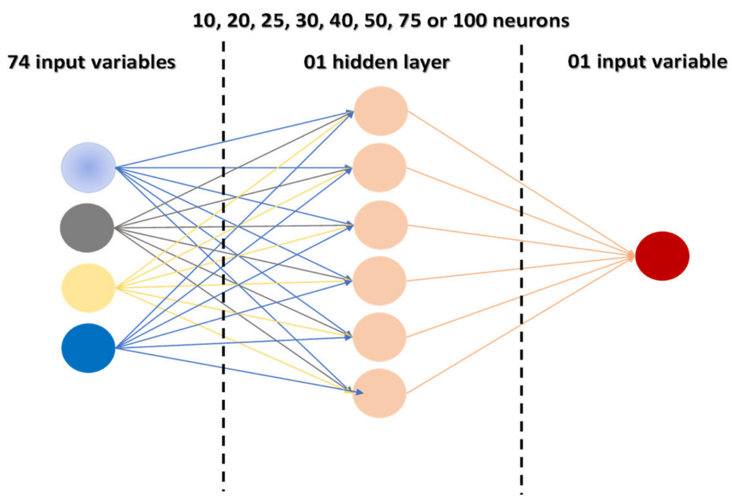

Figure 1. Artificial Neural network architecture

3 Results and discussion

It is not easy to develop a mathematical model to predict the phosphorus and sulfur content of the hot metal. The choice of the best estimation method suggests the use of statistical techniques to evaluate the different methods. The artificial neural network uses three statistical criteria to evaluate the efficiency of the mathematical model: the root mean square error (RMSE), the mean absolute error (MAE) and Pearson's correlation coefficient (R). The RMSE is the root mean square error of the difference between the estimated and measured values, so larger errors are weighted more heavily. Values close to zero indicate better model performance. The RMSE is calculated as shown in Equation (1). MAE calculates the "average absolute error" of the errors between the actual observed values (blast furnace operation) and the predictions (artificial neural network). MAE is calculated as shown in Equation (2). The performance of ANN is also evaluated using Pearson's mathematical correlation coefficient (R). In general, the value (R) aims to evaluate the relationship between two variables based on (n) observations of these variables. It indicates how much the independent variable can be explained by the fixed variable. The correlation coefficient for equations (R) is calculated as indicated in Equation (3).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(C_{neural} - C_{real})^2} \tag{1}$$

$$MAE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}|C_{neural} - C_{real}|} \tag{2}$$

$$R = \sqrt{\left[\sum_{i=1}^{n}(C_{neural} - C_{real})^2\right] \Big/ \left[\sum_{i=1}^{n}(C_{real} - C_{neural})^2\right]} \tag{3}$$

Where (n) represents the number of observations, (C_neural) represents the value calculated by the artificial neural network, and (C_real) represents the value measured during blast furnace operation. Statistical analysis was performed using Minitab statistical software. Figures 2 to 4 illustrate the initial results.

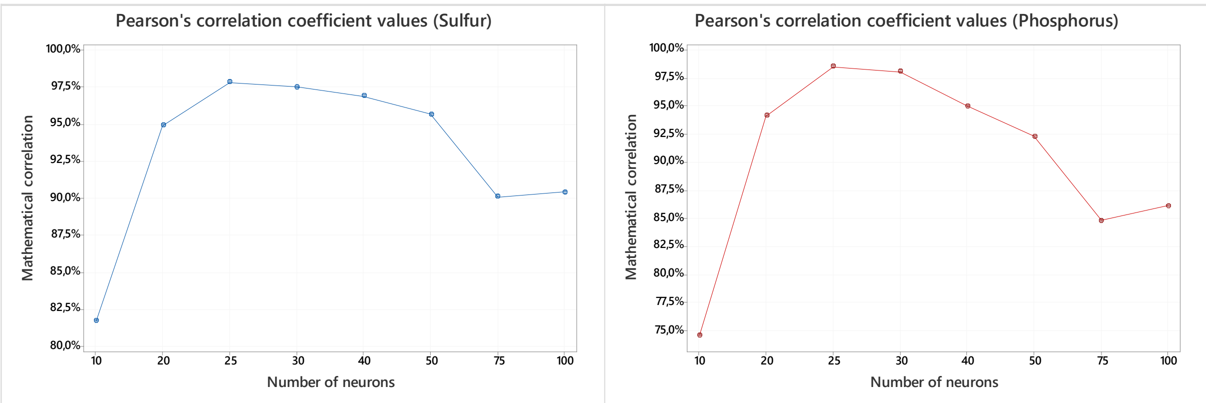

Figure 2. Correlation coefficients

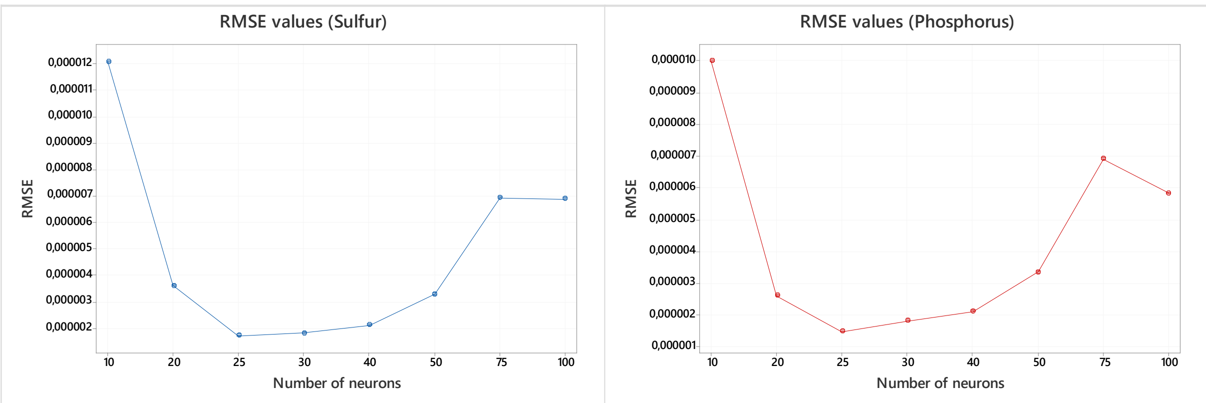

Figure 3. RMSE values

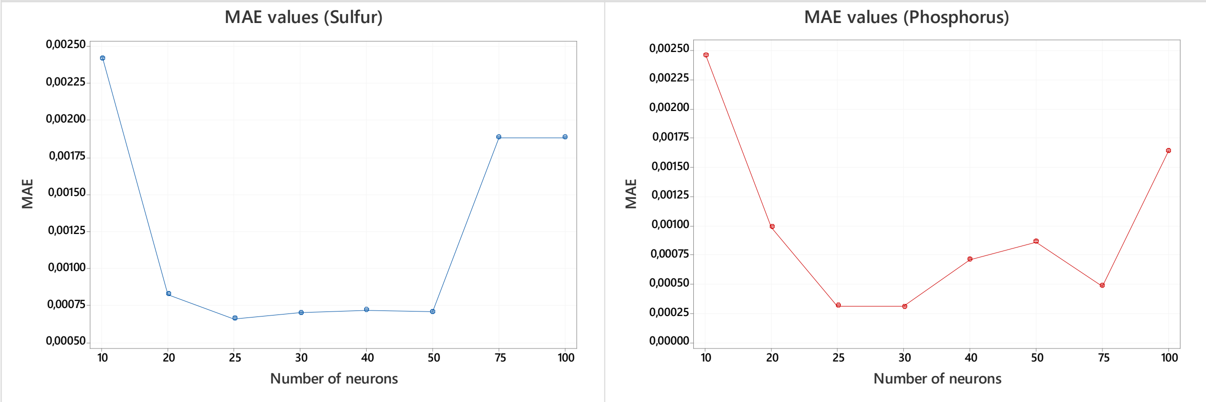

Figure 4. MAE values

It is generally accepted in the literature that in most cases the use of a single hidden layer is sufficient, since this structure is able to approximate any nonlinear equation (such as quadratic equations or exponentials) [3, 8].

Two hidden layers are already able to represent any relationship between the data, even those that cannot be represented by equations [3, 8]. More than two hidden layers are only needed for even more complex problems such as time series and computer vision, where there is a relationship between the dimensions that contain the data (time in the first case and geometric shapes in the second).

According to the literature, the number of neurons in the hidden layer must be determined empirically, and there are no explicit rules for an ideal calculation [3, 8]. Scientist Jeff Heaton [8], the author of the book "Introduction to Neural Networks for Java", proposes four initial approaches to determine the optimal number of neurons, which were used in this research. Based on these four estimates, the number of hidden layers was determined. In this work, 18 input variables and 2 output variables were used following the approach of Jeff Heaton [8], it is concluded that: **(1)** The number of neurons in the hidden layer should be fixed between the size of the input layer and that of the output layer. **(2)** The number of neurons in the hidden layer must be at least 2/3 of the size of the input layer plus the size of the output layer. **(3)** The number of hidden neurons must be less than twice the size of the input layer. **(4)** The number of hidden neurons must be at least twice the size of the input layer.

The proposal to develop a neural network based on a committee machine has shown excellent results. From the analysis of Figures 2 to 4, the best results were obtained with 25 and 30 neurons in each hidden layer. The neural network with 25 neurons in the hidden layer showed about 5% better result than the ANN with 30 neurons.

Considering that the neural network with 25 neurons gave the best results, it can be mentioned that sulfur had a Pearson correlation coefficient of 97.8%, while the root mean square error (RMSE) was 1.7129 $x10^{-6}$ and the mean absolute error (MAE) was 0.7 $x10^{-3}$, i.e. these results were the best compared to other artificial neural networks. It can also be mentioned that phosphorus had a Pearson correlation coefficient of 96.6%, while the root mean square error (RMSE) was 1.489 $x10^{-6}$ and the mean absolute error was 1.1 $x10^{-3}$ (MAE). These results were the best compared to other artificial neural networks. Figure 5 illustrates the scatter plot of the output variables.

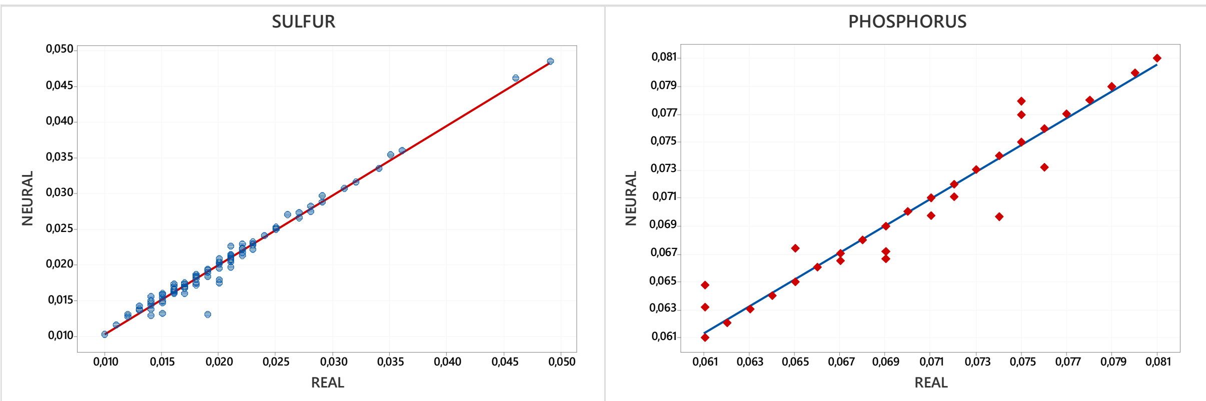

Figure 5. Scatter plot of output variables considering 25 neurons in the hidden layer

In the analysis of Figure 5, the x-axis shows the real variables, i.e. the variables measured during the blast furnace operation, while the y-axis shows the neural variables, i.e. the values calculated by the artificial neural network. Figure 5 shows the results of the initial modeling (training, validation and testing) with a database of 270 operating days and 25 neurons in the hidden layer. The artificial neural network (ANN) was able to predict the results even if the blast furnace had small operational changes.

4 Conclusions

The artificial neural network model developed in this paper to predict the sulfur and phosphorus content in cast iron is based on a committee machine. It is concluded that:

- The neural model is a useful tool to support the operation of a blast furnace;
- It is concluded that high values of mathematical correlation prove the good statistical performance of ANN and show that the mathematical model is an effective predictor of sulfur and phosphorus;
- Pearson, RMSE and MAE correlation coefficient values confirmed that the hidden layer with 25 neurons gave the best results;
- The obtained results demonstrate the ability of ANN, to generalize the acquired knowledge;
- Artificial neural networks with more than 40 neurons fit the dataset very well but proved ineffective in predicting new results, indicating that the statistical model was overfitted.
- To circumvent the problem of overfitting, it is proposed to insert a regularization function that leads to the elimination of unimportant numerical parameters and thus to a more convex model that should better represent reality.
- For future work, it is proposed to test the neural network with additional values by performing a cross-validation where the model is tested with a reserved part of the dataset that has not been used for training and validating the model in question. In this way, it can be accurately determined whether or not the model suffers from overfitting.
- It is clear that this research does not intend to exhaust the study on the importance of controlling the phosphorus and sulfur content during the production of cast iron, however, it is widely known that the discussion of this argument, deleterious impurities, is a relevant factor influencing the productivity, quality, gas flow through the load, melt bed calculation, operational stability and thermal losses.

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Declaration of competing interest
The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authorship contribution statement
Wandercleiton S. Cardoso: methodology, writing - original draft, data interpretation, results, interpretation, recommendations, writing manuscript draft, investigation, results interpretation, reading manuscript and revision.
Raphael C. Baptista: formal analysis, data curation, laboratory operations, laboratory physico-chemical analysis, analysis and data interpretation, reading manuscript, and revision.
Renzo di Felice: reading manuscript, critical review of the article for intellectual content, methodology, and revision.

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