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# Modeling of artificial neural networks for silicon prediction in the cast iron production process

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**ABSTRACT**

The main way to produce cast iron is in the blast furnace. In the production of hot metal, the control of silicon is important. Alumina and silica react chemically with limestone and dolomite to form blast furnace slag. In this work, 12 artificial neural networks (ANNs) were modeled with different numbers of neurons in each hidden layer. The number of neurons varied between 10 and 200 neurons. ANNs were used to predict the silicon content of hot metal produced. The ANN with 30 neurons showed the best performance. In the test phase, the mathematical correlation was 97.5% and the mean square error (MSE) was 0.0006, and in the cross-validation phase, the mathematical correlation was 95.5% while the MSE was 0.00035.



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## 1. INTRODUCTION

Cast iron is the raw material for steel production. The blast furnace is the main way for its production. Originally, blast furnaces produce hot metal, which contains a high percentage of carbon and impurities such as sulfur and silicon. In the production of hot metal, the blast furnace is charged from the top and bottom. In the upper part, the furnace is charged with ores (sinter, pellets, and granulated ore), fluxes (limestone and dolomite), and coke [1]–[3].

In the lower part are the blowing tuyeres, which blow oxygen-enriched hot air into the furnace. It is also possible to blow auxiliary fuels (natural gas and biogas), although pulverized coal is the most commonly used. The hot metal is cast and then sent in torpedo cars to the next stage to be processed into steel. Control of silicon is essential in the production of hot metal, as this impurity is harmful to steels [4]–[6]. During the production process, slag and hot metal are removed from the bottom of the reactor. The cast iron is transported to the torpedo car and sent to the next stage to be converted into steel. The slag is transported to the slag granulators and then sent to the cement industry [7], [8].

The air blown into the tuyeres is preheated in hot stoves to a temperature of 1,075 °C. Before the hot air is blown into the tuyeres, it is enriched with oxygen. Several chemical reactions take place in the furnace to convert the iron ore into hot metal. The hot air reacts chemically with the metallurgical coke to produce carbon monoxide (CO) and carbon dioxide ($CO_2$). This chemical reaction also releases energy to raise the temperature of the blast furnace to 1,650 °C. Alumina and silica react chemically with limestone and dolomite to form blast furnace slag [9]–[11].

The amount of silicon in cast iron depends on the balance between the phases "iron/slag". Currently, several models are proposed to simulate complex processes. The use of neural networks is very popular due to its reliability, as this machine learning technique acquires knowledge to generalize problems [9]–[12]. In this sense, the objective of this work was to create 12 different single-layer neural networks to control the silicon content in cast iron.

## 2. EXPERIMENTAL

### 2.1. Selection of variables

There are many variables that influence the behavior of silicon. Selecting the right samples is neither easy nor trivial. Many variables make the convergence of the model difficult, while few variables impoverish the model. The input variables were classified into 7 groups. Table 1 shows the summary of the classification of the groups of input variables. Table 2 shows the output variables analyzed. The input variable database consists of 81,400 pieces of information from an operating cycle considered normal for the reactor.

Table 1. Variable group division

| Variable group | Number of variables | Number of information |
|---|---|---|
| Hot air blown | 6 | 6,600 |
| Top gas | 7 | 7,700 |
| Temperature | 6 | 6,600 |
| Fuel | 22 | 24,200 |
| Ore | 11 | 12,100 |
| Hot metal | 9 | 9,900 |
| Slag | 13 | 14,300 |
| Total | 74 | 81,400 |

Table 2. Silicon (output)

| Output variable | Number of variables | Number of information |
|---|---|---|
| Silicon | 1 | 1100 |
| Total | 1 | 1100 |

### 2.2. Treatment of outliers

The original database was reduced by about 15%, after processing the resulted in a big data with 1,100 rows and 75 columns. Initially, a big data was selected taking into account the experience of specialists in the steel sector. All reactor maintenance events (10 times) as well as reactor operation change events occurring before and after scheduled maintenance were excluded from this initial big data. Maintenance shutdowns lasted an average of 4 days each.

In general, maintenance events and the 7 days following and preceding these events were excluded from the database. Any operational instability event was also excluded (5 events total). Table 3 shows how many outliers in days were deleted from the big data.

Table 3. Operacional outlier

| Operacional outlier | Number of events | Number of days |
|---|---|---|
| Blowing air | 05 | 15 |
| Permeability | 02 | 10 |
| Operational maintenance | 10 | 30 |
| Weeks before/after maintenance | 20 | 140 |
| Total | 37 | 195 |

The second technique for identifying outliers is based on the statistical principle of exploratory data analysis. In (1) and (3) identify moderate outliers, while (2) and (4) identify severe outliers. Where 1st quartile ($Q_1$); 3rd quartile ($Q_3$); and interquartile range (IQR) [12]. All points outside the range (-3σ and +3σ) were excluded. Table 4 shows how the database was treated.

$$Lower\ inner\ fence = Q_1 - 1.5 \times (IQR) \tag{1}$$

$$Lower\ outer\ fence = Q_1 - 3 \times (IQR) \tag{2}$$

$$Lower\ inner\ fence = Q_3 - 1.5 \times (IQR) \tag{3}$$

$$Lower\ outer\ fence = Q_3 - 3 \times (IQR) \tag{4}$$

Table 4. Database outlier removal

| | Number of days | Eliminated | Sustained |
|---|---|---|---|
| Raw big data | 1309 | * | * |
| Operational date | * | -196 | * |
| Moderate variables | * | * | 24 |
| Severe variables | * | -9 | * |
| Final database | 1100 (1309-202) | 205 | 24 |

### 2.3. Database standardization

The big data in this work contains several data of different magnitudes (pig iron temperature and chemical composition) that should not be used to model artificial neural networks (ANNs) without proper treatment, since samples with large magnitudes affect the processing of ANN and the incorrect storage of synaptic weights. In this context, it was necessary to standardize the big data considering the interval [0, 1] as shown in (5):

$$Z = \frac{x-\mu}{\sigma} \tag{5}$$

where (Z) is the standardized variable, ($x$) is the variable to be standardized, ($\mu$) is the mean, ($\sigma$) the standard deviation [12].

### 2.4. Splitting database variables

In this paper the big data (database) was segmented into 4 parts. The segmentation of the database, according to Table 5, is important so that during the modeling there are no overfitting or underfitting. Using this technique, after the ANN has converged with the information from the training dataset, it is re-trained with the validation dataset to confirm that the neural network has recognized patterns and is able to generalize the knowledge [12].

If the error converges after the validation step, it can be assumed that the trained network can be used as a process model. The test data set is used for the model test. At this stage, the neural network does not know the variables of this database and there are no new corrections to the synaptic weights. After testing, it is possible to check the final result with an additional database to cross-validate the results obtained after the training, validation and testing steps [12]–[14].

Table 5. Database split

| Step | Variables |
|---|---|
| Training | 700 |
| Validation | 150 |
| Test | 150 |
| Cross-validation | 100 |
| Total | 1,100 |

### 2.5. Network architecture

The ANN is a computational model that mimics the human brain, as it recognizes patterns and acquires knowledge. The ANN has interconnected neurons that compute the input and output values simulating the behavior of a biological neuron. The algorithm for training was the Levenberg-Marquardt (LM) that is used to minimize functions and allows fast convergence. The performance of the ANN is evaluated by the mean square error (MSE) and [15]–[19].

According to the literature [3]–[5], [16]–[22], modeling single layer ANNs is sufficient to generalize solutions and approximate results for any nonlinear equation. However, ANN with 2 layers consumes more memory and computation time but manages to classify and represent every pattern in the sample set. More than two layers are needed only for even more complex problems, such as time series. The ANN in this paper has 74 input variables and 1 output variable.

According to the literature, there are no rules or an ideal mathematical calculation to determine the number of neurons in a layer of a neural network [3], [5], [9], [14]. This paper evaluated 12 different single-layer neural networks using the Levenberg-Marquardt training algorithm. ANNs consist of an input, an output, and a hidden layer according to Figure 1 which illustrates the architecture of a typical ANN.

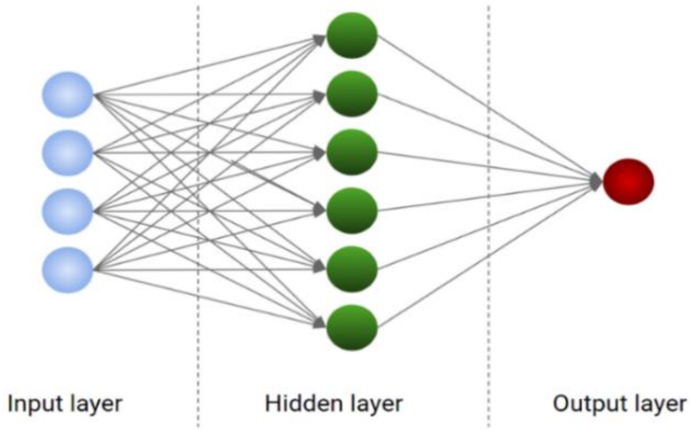


Figure 1. Simplified illustration of an ANN

### 2.6. Statistical analysis

Descriptive statistics apply techniques to describe and summarize a database. Some measures used to summarize a database are mean, median, standard deviation, maximum, minimum, skewness and kurtosis. Table 6 presents the descriptive statistics of silicon.

Table 6. Descriptive statistics of silicon

| Variable | Unit | Mean | Standard deviation | Minimum | Median | Maximum | Skewness | Kurtosis |
|---|---|---|---|---|---|---|---|---|
| Silicon (%) | % | 0.336 | 0.101 | 0.106 | 0.314 | 0.728 | 0.94 | 0.82 |

## 3. RESULT AND DISCUSSION

### 3.1. Model variables

In selecting input variables, it was decided to select the most important variables that affect the working of the reactor. The variables were selected considering seven groups of Table 1. Flow measurements are important for process control of the blast furnace and provide information on operating deviations. Operational control of top gas is important information for the application of thermochemical models and the frequency of its analysis is important to determine specific carbon rate and specific air flow. Thermal control is important to ensure the performance of the blast furnace and the quality of the final product.

Silicon is a variable that depends on the operating temperature and the quality of the raw material used in the reactor. Control of blast furnace fuels, metallurgical coke, and pulverized coal is the most important group of variables. The blast furnace understudy operated with seven types of coal with different grain sizes and chemical compositions.

Metallurgical coal and coke play an important role in production, as they allow high temperatures (about 1,550 ºC) to be reached. They are responsible for melting the iron ore, as they act as a reducing agent that reacts chemically with oxygen and converts the ore into pig iron at high temperatures [22]–[24]. Regarding the reduction of the level of unwanted impurities, it is important to control the quality of the raw material. During the production process it is important to control the composition of pig iron to reduce the costs of the operational process. The production of pig iron with a high amount of dissolved silicon makes secondary refining unprofitable [25].

Slag is obtained by melting and separating the gangue from the raw materials and fluxes. It consists mainly of thermodynamically stable oxides ($MgO$, $CaO$, $Al_2O_3$ and $SiO_2$) which constitute up to 96 wt% in the slag. The hot metal/slag control is important because the silicon must preferentially migrate to slag [26].

### 3.2. Descriptive statistics

Analyzing the descriptive statistics, it is conclude that the database has little noise, a low standard deviation, asymmetry, and a kurtosis close to zero. The ANN showed excellent results for all neurons. The hypothesis test proved that all sample groups calculated by the ANN are equal in the database considering 99% confidence interval using Welch method. Table 7 illustrates the number of neurons in each hidden layer and a hypothesis test was performed, which proves the assertiveness of the modeling.

Table 7. Silicon variables (%)

| | Mean | Standard deviation | Minimum | Median | Maximum | Skewness | Kurtosis |
|---|---|---|---|---|---|---|---|
| Database | 0.336 | 0.101 | 0.101 | 0.314 | 0.728 | 0.94 | 0.82 |
| 10 neurons | 0.338 | 0.096 | 0.121 | 0.316 | 0.718 | 0.96 | 0.83 |
| 20 neurons | 0.337 | 0.097 | 0.135 | 0.315 | 0.706 | 0.91 | 0.68 |
| 25 neurons | 0.338 | 0.098 | 0.106 | 0.318 | 0.730 | 0.92 | 0.75 |
| 30 neurons | 0.334 | 0.098 | 0.115 | 0.313 | 0.701 | 0.91 | 0.73 |
| 40 neurons | 0.336 | 0.100 | 0.062 | 0.317 | 0.771 | 0.87 | 0.91 |
| 50 neurons | 0.335 | 0.098 | 0.124 | 0.315 | 0.707 | 0.81 | 0.57 |
| 75 neurons | 0.337 | 0.098 | 0.114 | 0.317 | 0.724 | 0.91 | 0.82 |
| 100 neurons | 0.339 | 0.100 | 0.101 | 0.315 | 0.723 | 0.85 | 0.73 |
| 125 neurons | 0.335 | 0.101 | 0.092 | 0.311 | 0.691 | 0.85 | 0.58 |
| 150 neurons | 0.327 | 0.095 | 0.141 | 0.312 | 0.691 | 0.91 | 0.82 |
| 175 neurons | 0.337 | 0.096 | 0.106 | 0.316 | 0.765 | 1.02 | 1.12 |
| 200 neurons | 0.338 | 0.105 | 0.122 | 0.319 | 0.712 | 0.93 | 0.91 |

### 3.3. Model evaluation

The ANN architecture was trained with 700 datasets. The training validation was performed with 150 datasets. The testing step was performed with 150 datasets. After generating the source code of the ANN, cross validation was performed with 100 datasets to evaluate the performance of the source code.

The training, validation and testing phase was performed with up to 1,000 iterations and automatically interrupted when it converged to the smallest error. The model was validated using Pearson's correlation coefficient and MSE. Five correlation coefficients were calculated: training; validation; test; cross-validation; and general correlation. The general correlation was calculated using the training, validation, and test variables.

Training an ANN is a type of optimization problem where one wants to minimize the error of a function. In this case, the function is the MSE of the output layer of the ANN. Five MSE were calculated: training; validation; testing; cross-validation; and general correlation. The MSE was calculated with the training, validation, and testing variables. Figures 2 and 3 shows the results of model validation.

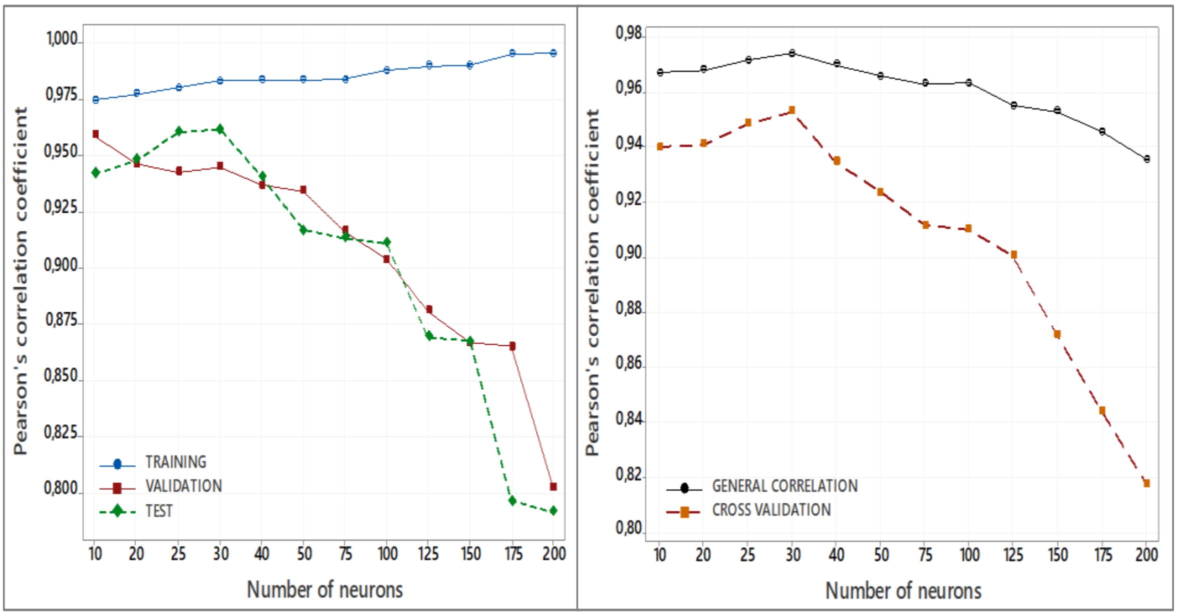


Figure 2. Model validation (Pearson)

Analyzing Figures 2 and 3, one can see that the best results were obtained with 25 and 30 neurons. The neural network with 30 neurons showed about 1% better result than the ANN with 25 neurons. Considering that the best results were those of the neural network with 30 neurons, it can be mentioned that silicon had a Pearson correlation coefficient of 97.5%, while the MSE was 0.0006.

In terms of cross-validation, it can be noted that the best results were also obtained with 25 and 30 neurons. The cross-validation of the neural network with 30 neurons in the hidden layer showed a Pearson correlation coefficient of 95.5%, while the MSE was 0.00035. The ANN was able to predict the results even if the blast furnace had small operation changes. When looking at the MSE values between training and testing as shown in Figure 3, no overfitting was observed. This is the case when the neural network response during the test has a very large error compared to the response in the training phase. Also, no underfitting was found, i.e., when the modeling cannot find an answer to the problem or when the model does not converge during the training phase.

From the technical point of view, we can mention that the silicon content in pig iron is an important quality parameter to be monitored, as it acts as an indicator of the thermal condition and its decrease indicates the cooling of the blast furnace, which requires countermeasures to avoid serious problems in operation [27]. Since the silicon in the process comes from the raw materials, especially from the coke ash and gangue of the metallic charge, the use of raw materials with small variations in composition is one of the ways to control the content obtained in production and keep it as constant as possible with respect to its optimum level, which is intended to minimize the cost of secondary refining in the converters of steel mills [28]. It is also worth noting that the excess of silicon in pig iron requires a larger amount of calcium oxide (CaO) in the steel mill to perform refining, resulting in a larger slag volume and higher cost. Therefore, silicon content prediction models are useful tools to operate with lower safety margins to optimize fuel consumption and improve the efficiency of the steelmaking process [29], [30].

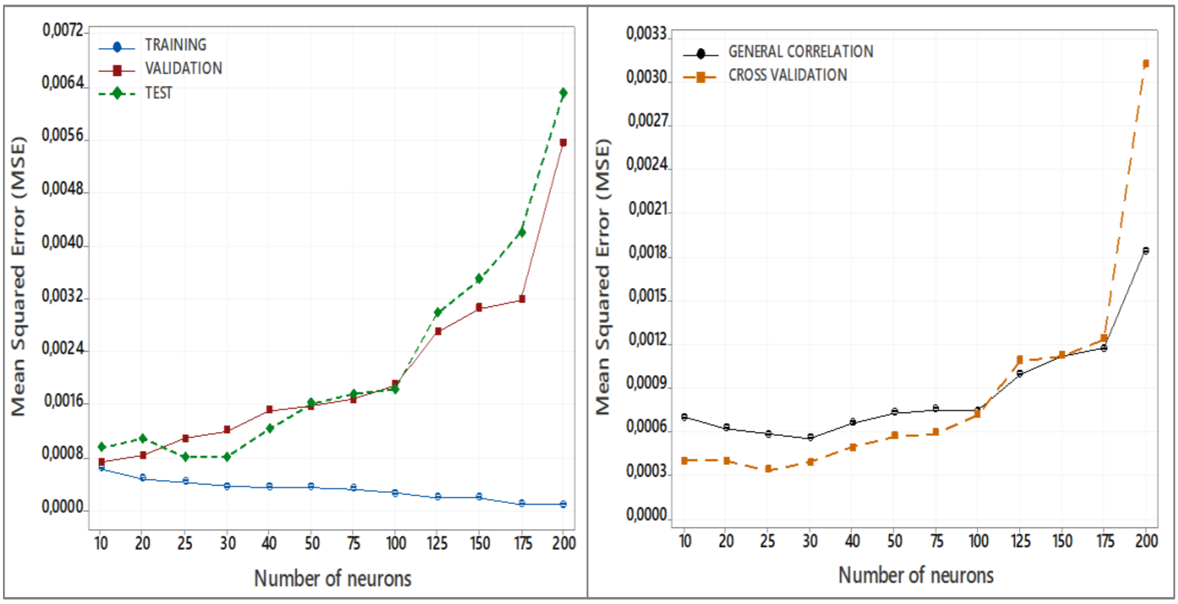


Figure 3. Mean squared error

## 4. CONCLUSIONS

The ANN developed in this work to predict the silicon content in cast iron concluded that the increasing development of computing capacity, leading to cheaper devices with higher capacity, drives the development of more complex algorithms with better results, as in the case of neural networks. Dealing with databases is an important part of the model development process. This process is lengthy, as information must be evaluated and outliers identified to finally obtain the data set that will be standardized for model development. The neural model is a useful tool to support the operation of a blast furnace for iron. High values of mathematical correlation show the good statistical performance of ANN and prove that the mathematical model is an effective predictor for silicon. Pearson and MSE correlation coefficient values confirmed that the hidden layer with 30 neurons gave the best results. The obtained results show the ability of ANN, to generalize the acquired knowledge.

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