

## Parametric analysis of carbonation process in reinforced concrete structures through Artificial Neural Networks

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### ABSTRACT

The aim of this paper is parametrically analyze the main factors that influence on the progress of concrete carbonation front. Therefore, a numerical model was developed using Artificial Neural Networks (ANNs), considering the Multi-Layer Perceptron class, designed in a C++ object-oriented program. The software was fed by experimental degradation data available in the current literature. The results obtained in the parametric analysis, besides adding knowledge to the building pathology area, reinforce concepts already known in the literature, demonstrating the efficiency of ANNs in the investigation of concrete carbonation.

**Keywords:** carbonation of concrete; time-to-corrosion initiation; Artificial Neural Network; mathematical modelling.

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## **Análise paramétrica da carbonatação em estruturas de concreto armado via Redes Neurais Artificiais**

### **RESUMO**

O presente trabalho tem como objetivo analisar parametricamente a influência dos principais fatores que afetam o avanço da carbonatação em estruturas de concreto. Para tal, desenvolveu-se um modelo numérico empregando Redes Neurais Artificiais (RNAs) do tipo Multi-Layer Perceptron, sendo concebido em linguagem orientada a objetos C++, o qual foi testado com dados reais de degradação disponíveis na literatura. Os resultados obtidos na análise paramétrica reforçam conceitos já conhecidos na literatura, demonstrando a eficiência de RNAs no estudo da carbonatação do concreto, além de agregar conhecimento à área de patologia das construções.

**Palavras chave:** carbonatação do concreto; tempo de iniciação da corrosão; Redes Neurais Artificiais;

## **Análisis paramétrico de la carbonatación en estructuras de hormigón por Redes Neuronales Artificiales**

### **RESUMEN**

El presente estudio tiene como objetivo analizar paramétricamente los principales factores que influyen en el avance de la carbonatación de las estructuras de hormigón. Por lo tanto, se desarrolló un modelo numérico utilizando Redes Neuronales Artificiales (RNAs o NeuroRed), del tipo Multi-Layer Perceptron, desarrollada en lenguaje orientado a objetos C++, la cual fue probada por datos de degradación reales disponibles en la literatura. Los resultados obtenidos en el análisis paramétrico refuerzan conceptos ya conocidos en la literatura, demostrando la eficiencia de las RNAs en el estudio de la carbonatación del concreto, además aportando conocimientos en el área de patología de las construcciones.

**Palabras clave:** carbonatación del hormigón; tiempo de iniciación de la corrosión; Redes Neuronales Artificiales; modelado matemático.

## **1. INTRODUCTION**

Concrete reinforcement (Rebars) corrosion is the pathology with highest occurrence index in reinforced concrete structures (Taffese et al., 2013; Kari et al., 2014; Possan, Andrade, 2014; Andrade et al., 2017). As an example, this index varies from 14 a 64 % in Brazil, according to the region (Dal Molin, 1988; Andrade, 1992; Aranha 1994).

Carbon dioxide (CO<sub>2</sub>) ingress leads to reduction of calcium hydroxide (Ca(OH)<sub>2</sub>) from the porous concrete matrix and, as a consequence, concrete pH decreases from 13 to approximately 8, letting rebars susceptible to corrosion (Bakker, 1988; Chang et al., 2006). According to Possan et al. (2017), the increasing CO<sub>2</sub> emissions in the atmosphere worldwide with cities development brings several consequences to concrete structures in urban environments. The life cycle of the structures are affected by the elevation of CO<sub>2</sub> emissions in the environment as the rate of carbonation increases, reducing their durability.

There are nowadays several works that explain and model carbonation of concrete. Until mid-1980s, prediction of carbonation depth were obtained by linear and non-linear regressions, based in several factors, such as water/cement ratio, type of binder and exposure conditions (Izumi et

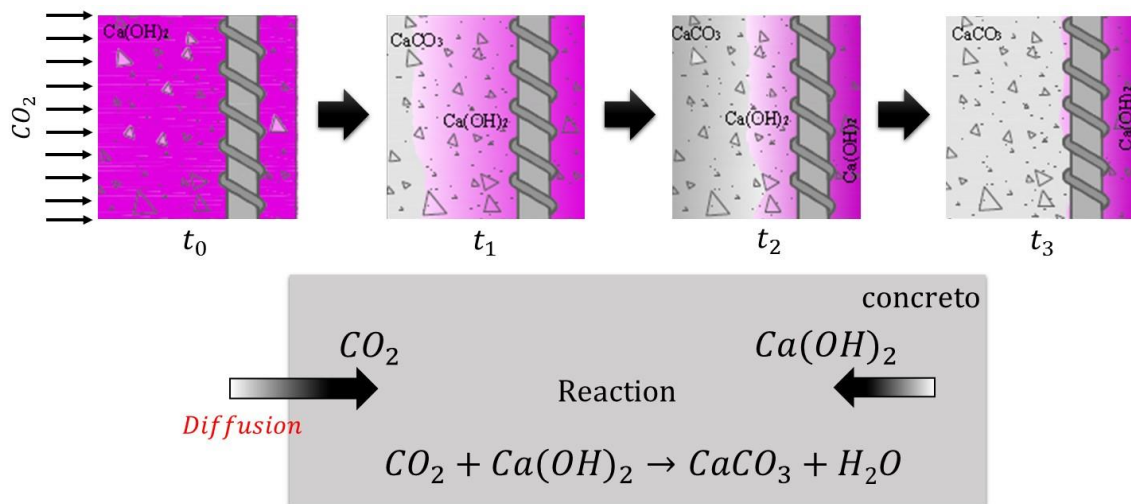
al., 1986; Kobayashi et al., 1990). In the following years, Papadakis et al. (1991), Ishida et al. (2001) e Maekawa et al. (2003) included physico-chemical formulations related to the hydration reaction of the cement paste and the CO<sub>2</sub> dissolution in the concrete porous matrix in their models, which enabled more accuracy in the determination of the carbonation front. However, Possan (2010) point out that these models requires resolution of great complexity equations that govern the diffusion of CO<sub>2</sub> in concrete, and hard to find parameters, such as the diffusion coefficient of carbon dioxide.

Use of computational tools, such as Artificial Neural Networks (ANNs), is a reliable alternative to overcome hardships imposed by the modeling of carbonation of concrete due to is ability to map and to model complex non-linear problems, without knowing all phenomena involved (Braga et al., 2000, Lu et al., 2009; Kwon et al., 2010; Güneyisi et al., 2014; Taffese et al., 2015; Félix, 2016).

In this study, we analyze several factors on the carbonation phenomenon, such as relative air humidity, CO<sub>2</sub> concentration, concrete composition, cement type, admixtures, exposure conditions to rain, and compressive strength of concrete. A prediction model of the carbonation depth is obtained through Multilayers Perceptron ANN and Backpropagation learning algorithm. Results show the ANN potential to model the depth of carbonation in concrete.

## 2. CARBONATION OF CONCRETE

Carbonation of concrete is a physical-chemical reaction that leads to the reduction of capillary porosity and affects the equilibrium of pore water content. Corrosion of rebar in reinforced concrete is also a consequence (Neville, 1997). According to Vesikari (1988) and Hamada (1969), the depth of carbonation in concrete increases over time (Figure 1), as a function of several intrinsic parameters and the environment.



Label:

■ Non – carbonated zone    ■ Partially carbonated zone    ■ Carbonated zone

Figure 1. Schematic representation of the carbonation of concrete.

Adapted from Possan (2010).

There are several works in which carbonation and its influence factors are described, such as Hamada, 1969; Parrot, 1987; Helene, 1993; Houst et al., 2002; Pauletti et al., 2007; Possan 2010; Talukdar et al., 2012. Pauletti et al. (2007) and Possan (2010) point out that the influence parameters in the carbonation of concrete are related to (i) environmental conditions: temperature, relative air humidity and CO<sub>2</sub> concentration; (ii) concrete: mix design, quality of execution and curing, use of admixtures, and chemical composition of the binder; and (iii) exposure conditions: internal, external environment and rain protection. All these factors must be evaluated both in the study of carbonation phenomenon and in its modeling. In the present work an AAN model is proposed to evaluate the depth of carbonation in concrete considering, as input parameters, relative humidity, CO<sub>2</sub> concentration, concrete compressive strength, cement type, exposure conditions, use and mix design of admixtures, and age of concrete.

### 3. CARBONATION PREDICTION MODEL THROUGH ANN

The proposed methodology is divided in two stages: i) development of a prediction model of depth of carbonation in concrete using ANN; and ii) parametric analysis of the variables employed by the model.

#### 3.1 Model Development

We based our model on the Multilayer Perceptron model trained by Backpropagation Momentum algorithm. The methodology used to obtain the model is presented in flowchart of Figure 2.

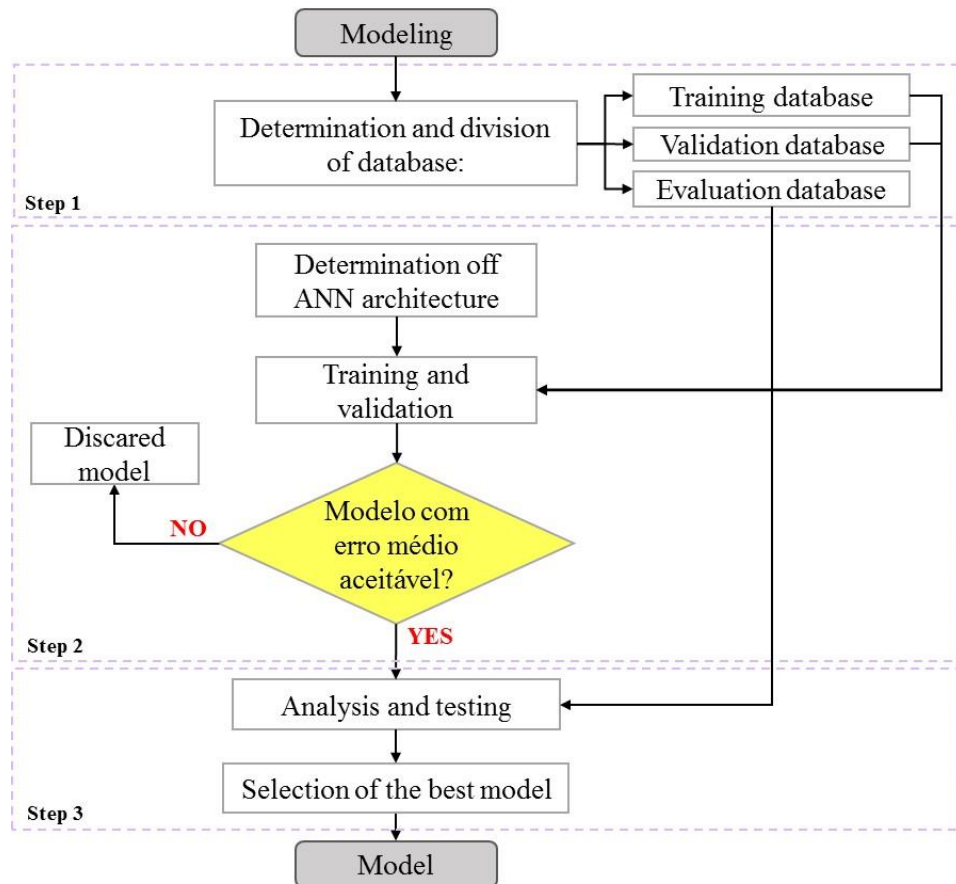


Figure 2. Flowchart of the prediction model of depth of carbonation in concrete

In the first stage, the database is set up to cover all input variables (relative humidity, CO<sub>2</sub> concentration, concrete compressive strength, cement type, exposure conditions, use and mix design of admixtures, and age of concrete). The database is composed by experimental results from Meira et al. (2006) and Vieira et al. (2009), and by Possan (2010) focus group, using respectively 179 and 100 data points. Some input variables were converted to numbers in order to be properly associated to the AAN, such as cement type (CP II-E, CP II-F, CP II-Z, CP III, CP IV and CP V ARI), numbered from 1 to 6. Exposure conditions was also represented by 1.30, 1.00 and 0.65 when exposed to indoor environment, external environment yet protected from rain and unprotected from rain, respectively, as established by Possan (2010). This process defined the model applicability and boundaries for input variables, as presented in Table 1.

Table 1. Database boundaries.

Input Variable	Boundaries / Domain
Cement Type	[CP II-F <sup>1</sup> ; CP II-Z <sup>2</sup> ; CP II-Z <sup>3</sup> ; CP III <sup>4</sup> ; CP IV <sup>5</sup> ; CP V <sup>6</sup> ]
Relative Humidity (%)	[30 - 90]
Exposure conditions	[1.30, 1.00, 0.65]
Content of additions (%)	[0-30]
CO <sub>2</sub> concentration (%)	[0.01-3.0]
Compressive strength (MPa)	[20-90]
Age of concrete (years)	[0-60]

- <sup>1</sup> CP II F: Portland cement composite with filler - NBR 11578. There is no equivalent in ASTM.
- <sup>2</sup> CP II Z: Portland cement composite with Pozzolan - NBR 11578. *Pozzolan-modified Portland* - ASTM C 595.
- <sup>3</sup> CP II E: Portland cement composite with Slag - NBR 11578. *Slag-modified Portland* - ASTM C 595.
- <sup>4</sup> CP III: Portland cement composite with blast furnace - NBR 5735. *Portland blast furnace slag* - ASTM C 595.
- <sup>5</sup> CP IV: *Portland pozzolan cement* - NBR 5736. *Portland pozzolan* - ASTM C 595.
- <sup>6</sup> CP V ARI: Portland cement high initial strength - NBR 5733. *Portland with high early strength* - ASTM C 150.

The boundaries or domain defines limits to use the model, since AAN are unable to extrapolate results, and it is only possible to map and to train an ANN within its domain (Braga et al., 2000). AAN requires splitting the entire database in three smaller databases, one for training, other to validate, and the last to evaluation. Figure 3 shows the amount of data allocated in each database.

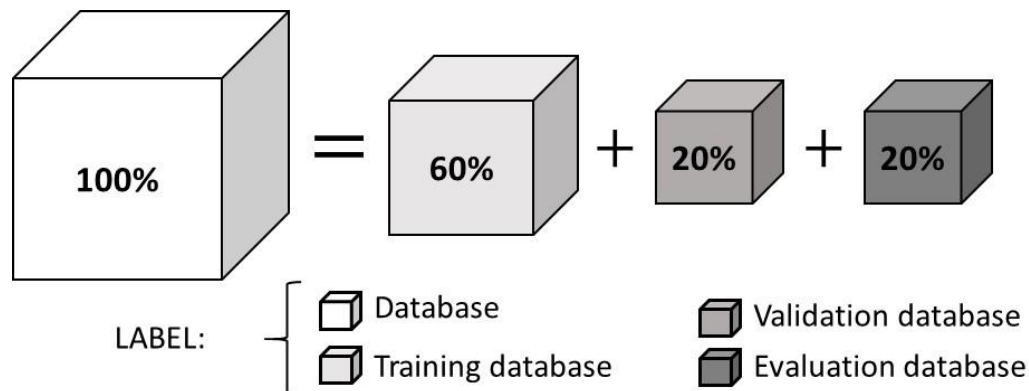


Figure 3. Amount of data allocated in each database.

Each database (training, validation and evaluation) are used in a step of the process of modelling with AAN. The first database is responsible to train the network, through each pair of



input/output. The second database is responsible to validate and to certify the trained network. The third and last database is responsible to test and to check the model capabilities.

AAN trained was then classified by topology, activation function and learning rate of the train algorithm, as described by Félix (2016).

We created 1200 ANN's with different learning rates (0.1, 0.2, 0.3 and 0.4), input entries (4, 5 and 7 perceptron's), number of hidden layers (one or two), and number of perceptron's in the hidden layer (from 0 to 9). With all possible combinations, resulted in 1200 ANN's (4\*3\*10\*10). See figure 4 for details.

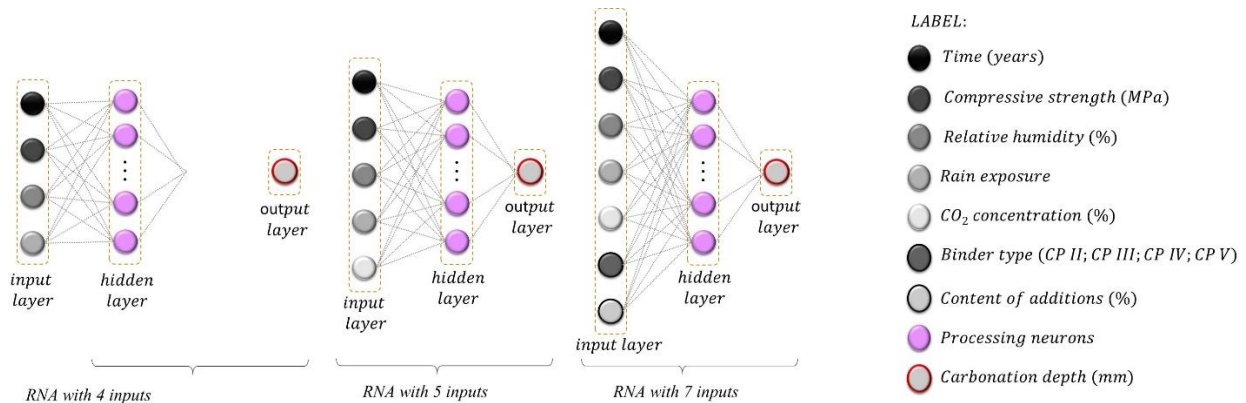


Figure 4. Tested topologies and input entries.

We adopted the root mean square error (RMSE) between depths of carbonation measured and depths of carbonation evaluated by the trained network as convergence criteria, according to Equation (1).

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - x_m)^2} \quad (1)$$

where  $n$  is the number of outputs,  $x_i$  is the value provided by the network for the  $i$ -th output, and  $x_m$  is the average of the values from all outputs.

ANN training is made by the package Project-Yapy (Konzen et al., 2011), provided in C++.

ANN performance was evaluated by the following parameters: correlation coefficient ( $R^2$ ), root mean square error (RMSE), maximum error ( $E_{max}$ , largest error provided), and minimum error ( $E_{min}$ , smallest error provided). These parameters were evaluated both in the training stage and in the validation stage. In the test stage, these parameters were also used to access the performance of the network.

After ordering by their performance, it was possible to select the network that could better represent the carbonation of concrete. Figure 5 shows the selected network, containing three layers of perceptrons. The first layer has seven neurons, responsible for input. The second (or hidden) layer has four neurons, which are responsible to processing information, and the last layer has a single neuron, responsible for output – depth of carbonation in concrete.

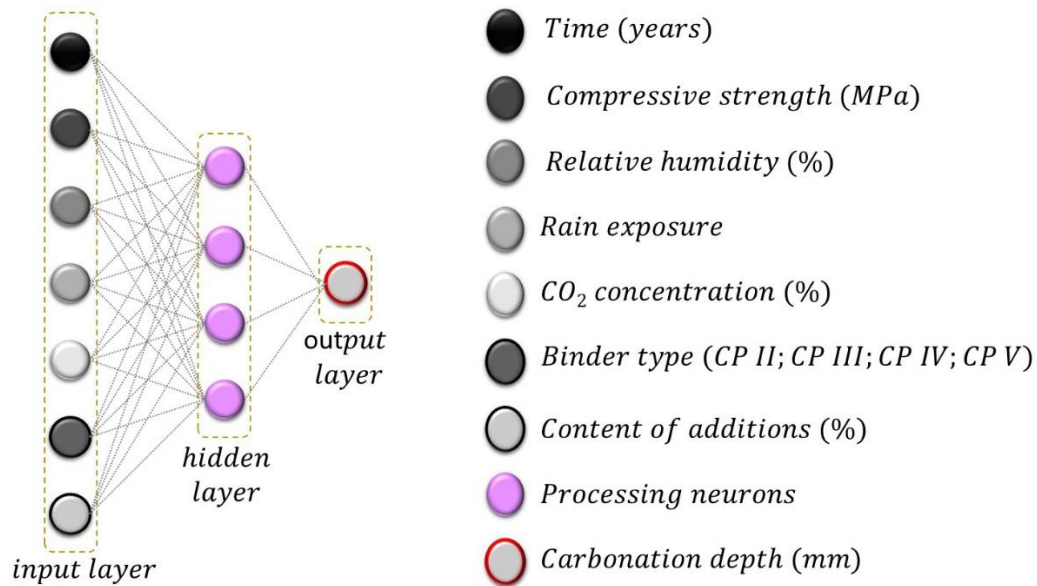


Figure 5. Chosen topologies and input entries.

Correlation charts between the carbonation depths modeled by the program (modeled depth) and the natural carbonation depths (observed depth, provided by Possan (2010)) are shown in Figures 6(a) and 6(b).

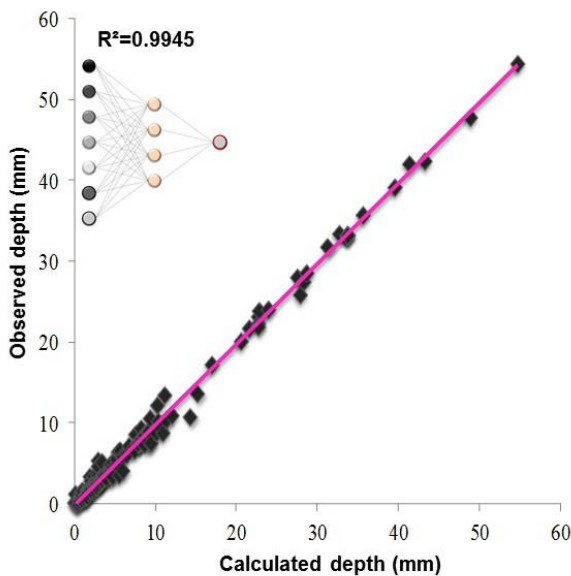


Figure 6(a). Training correlation.

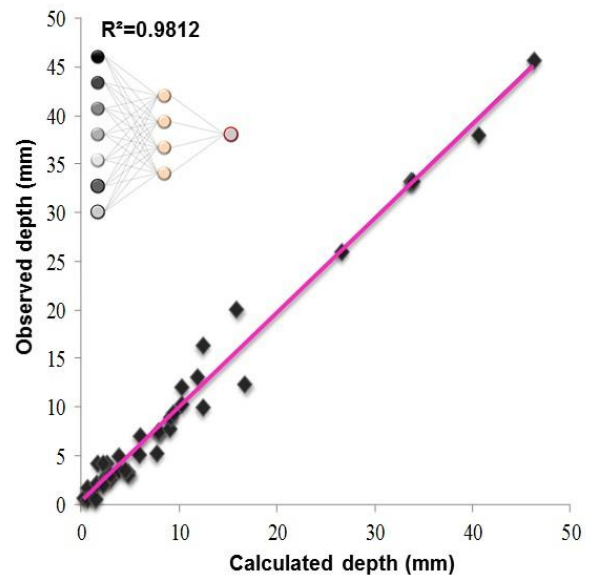


Figure 6(b). Validation correlation.

A complete description of the training process of the networks and the parameters used in the modeling can be found in Felix (2016).

### 3.2 Parametric analysis of carbonation

We decided to perform a parametric analysis of the influence of the input variables on the evaluation of the carbonation depth in concrete. The analysis was divided into four, evaluating the influence of a single or two input variables, as shown in Figure 7.

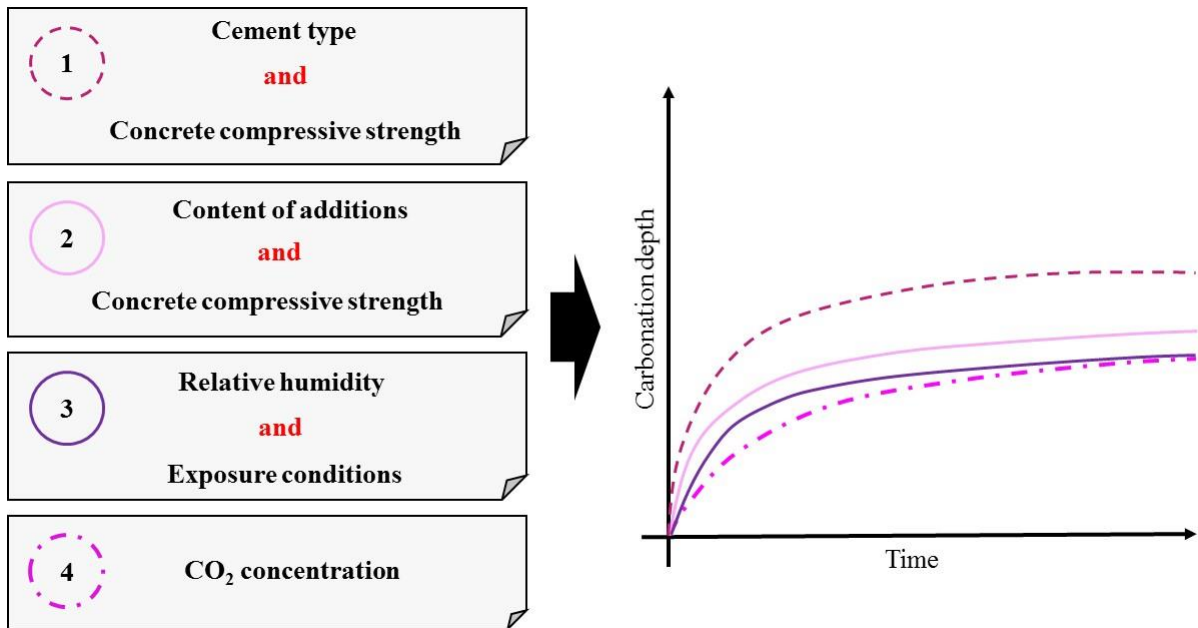


Figure 7. Input parameters evaluated in each parametric analysis.

## 4. RESULTS

### 4.1 Validation with reference

Initially, in order to certify the performance of the developed model, we compared our results with others proposed models and degradation values provided by Possan (2010). Equation (2)-(6) introduces carbonation models provided by Smolczyk (1976), Vesikari (1988), Bob & Afana (1993), EHE (2008) and Possan (2010), respectively.

$$y = a \cdot \left( \frac{1}{\sqrt{10f_c}} - \frac{1}{\sqrt{10f_{clim}}} \right) \cdot \sqrt{52 \cdot t} \quad (2)$$

$$y = [26 \cdot (ac - 0.3)^2 + 1,6] \quad (3)$$

$$y = 150 \cdot \left( \frac{c \cdot k \cdot d}{f_c} \right) \cdot \sqrt{t} \quad (4)$$

$$y = C_{amb} \cdot C_{ar} \cdot a \cdot f_{cm}^b \cdot \sqrt{t} \quad (5)$$

$$y = k_c \cdot \left( \frac{20}{f_c} \right)^{k_{fc}} \cdot \left( \frac{t}{20} \right)^{\frac{1}{2}} \cdot \exp \left[ \left( \frac{k_{ad} \cdot ad^3}{40 + f_c} \right) + \left( \frac{k_{CO_2} \cdot CO_2^{\frac{1}{2}}}{60 + f_c} \right) - \left( \frac{k_{RU} \cdot (UR - 0.58)^2}{100 + f_c} \right) \right] \cdot k_{ce} \quad (6)$$

where  $y$  is the carbonated depth (mm),  $a$  is the rate of carbonation,  $f_c$  is the concrete compressive strength (Mpa),  $f_{clim}$  is a limiting value for the carbonated concrete compressive strength (MPa),  $t$  is the age of concrete (years) and  $ac$  is water/cement ratio. The input parameters that are function of the type of binder and exposure conditions are defined using tables provided by each author in their work. More details can be found in Félix (2016).



Some scenarios are provided in Table 2 and compared in Figure 8(a)-(d), showing the depth of carbonation vs time.

Table 2. Test Stage – Trail Scenarios.

Scenario	CO <sub>2</sub> (%)	Relative humidity (%)	Exposure conditions	Binder type	Compressive Strength (MPa)
I	0.01	70.00	Protected	CP II – F	30.00
II	0.01	70.00	Protected	CP III	40.00
III	0.01	65.00	Unprotected	CP IV	40.00
IV	0.01	65.00	Unprotected	CP V	40.00

OBS.: Time of analysis: 60 years; No chemical addition is considered.

Em todos os cenários o teor de adição (no concreto) é zero e o tempo de análise é de 60 anos.

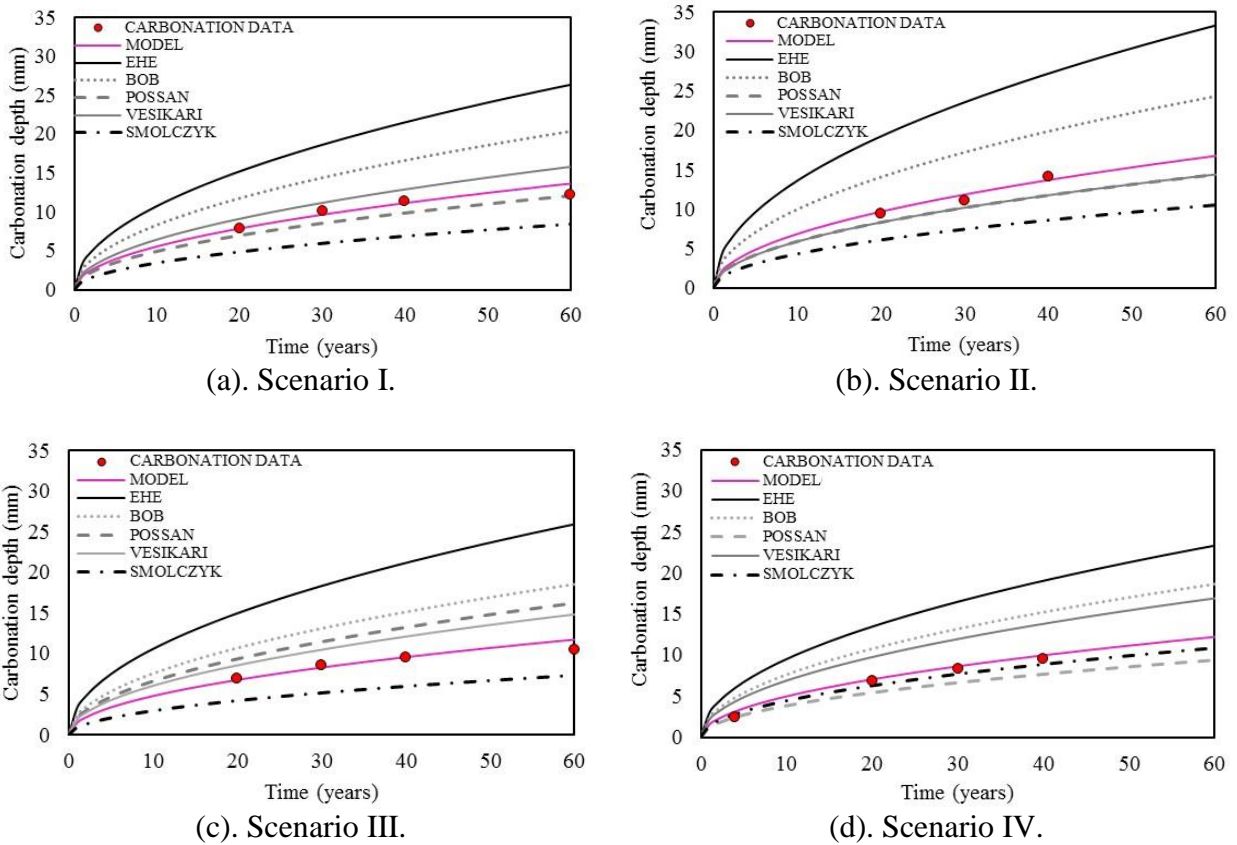


Figure 8. Test Stage – Trail Scenarios.

The results show the applicability of the model and that the proposed model is an efficient tool for estimating the depth of carbonation in concrete.

#### 4.2 Parametric Analysis

Figure 9 shows depth of carbonation in concrete after 50 years obtained in the proposed model varying only the type of binder and the compressive strength. In this simulation, we considered an environment protected from rain, with 65% of relative humidity, 0.04% CO<sub>2</sub>, and no additions in the concrete production.

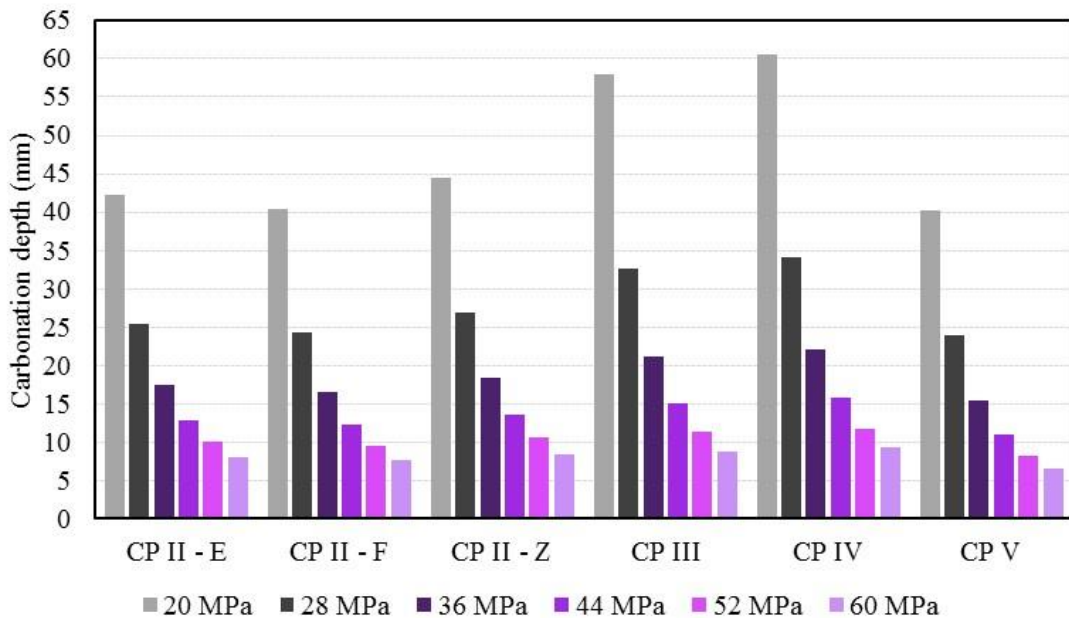


Figure 9. Depth of carbonation as a function of type of binder and compressive strength.

One may notice in Figure 9 that concretes produced with CP III and CP IV present greater depth of carbonation, notably with low compressive strength concretes. Jiang et al. (2000) and Possan (2010) noticed a negative influence of additions on the depth of carbonation, due to the reduction of the alkali reserve when the concrete is produced with CP III and CP IV, which have high levels of slag (from 35 to 70%) and pozzolan (from 15 to 50%) in their compositions, respectively. CP II-E and CP II-Z are also composed cements (with slag and pozzolan, respectively), however with lower levels of admixtures. That would explain the lower depth of carbonation in concrete produced with CP II-E and CP II-Z than CP III and CP IV.

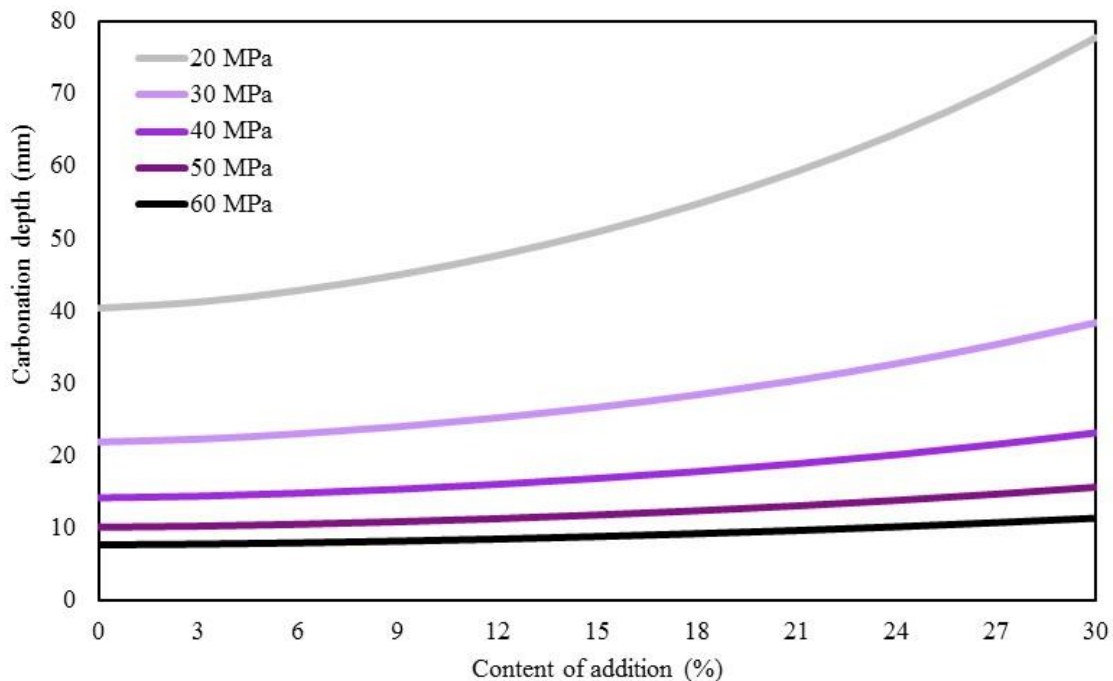


Figure 10. Depth of carbonation as a function of levels of additions and compressive strength.

One may notice in Figure 10 the influence of additions content (silica fume) on the depth of carbonation. It is observed that the depth of carbonation is barely affected by the addition in concretes with higher compressive strength (40, 50 and 60 MPa). It is also noted that the higher the addition content, greater is the depth of carbonation for concretes with lower compressive strength than 40 MPa. Kulakowski et al. (2009) report that, in concrete with higher compressive strengths (greater than 30 MPa), the CO<sub>2</sub> intake is smaller due to porosity, even for concretes with low alkaline reserves. The authors point out that, for concrete with compressive strength greater than 40 MPa, the depth of carbonation is independent of additions and type of cement. In the case of lower compressive strength, the presence of additions increases the depth of carbonation, and the alkali reserve effect predominates (Kulakowski et al., 2009).

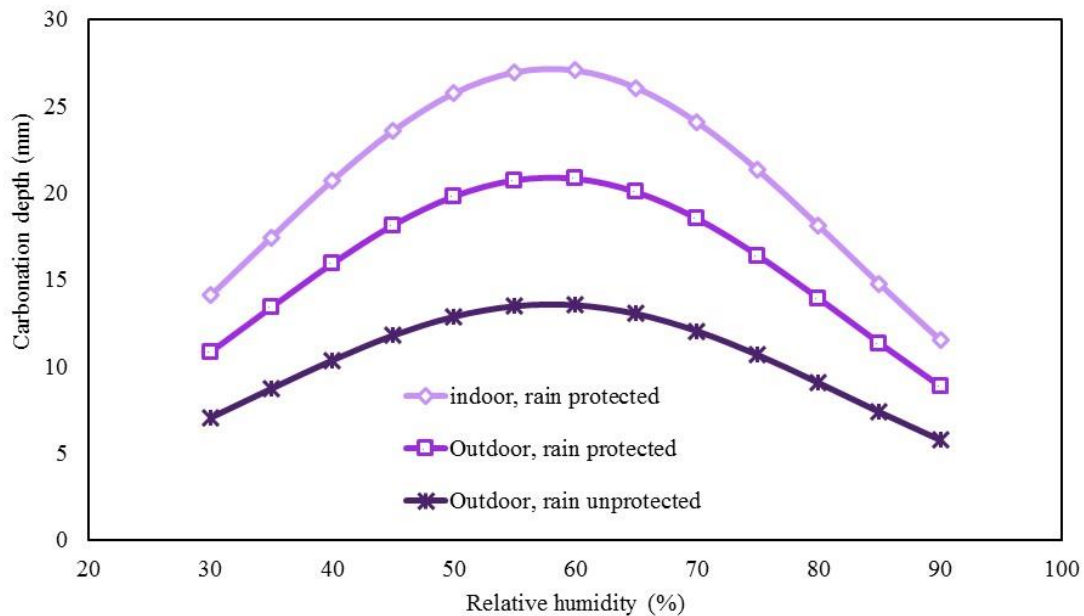


Figure 11. Depth of carbonation as a function of relative humidity and exposure conditions.

Figure 11 shows the depth of carbonation in a 50 years old concrete obtained in the proposed model when relative humidity and the environment exposure conditions are modified. In this simulation, we considered a concrete structure with compressive strength of 30 MPa, CP III, 0.04 % CO<sub>2</sub>, and no additions in the concrete production.

One may notice in Figure 11 that the depth of carbonation reach maximum when relative humidity is close to 60%. Parrot (1987), Neville (1997) and Possan (2010) point out that depth of carbonation reaches its maximum value when the relative humidity is between 50 and 80%. They also mention that the relative humidity can be considered as the environmental factor with the greatest influence on carbonation. Possan et al. (2017) observed in a 35 years old concrete dam that the larger the internal humidity, the lower the depth of carbonation depth. The authors also notice that no carbonation was observed when moisture was about 100%.

Figure 12 shows the depth of carbonation as a function of the exposure conditions to different CO<sub>2</sub> concentrations. In this simulation, we considered a concrete structure with compressive strength of 30 MPa, CP III, relative humidity of 65%, no additions in the concrete production, and in an unprotected outdoor environment.

One may notice that higher degree of exposure to CO<sub>2</sub>, greater the depth of carbonation in concrete over time. An increase of 0.1% of CO<sub>2</sub> concentrations leads to an increase of carbonated depth in 2.15%.

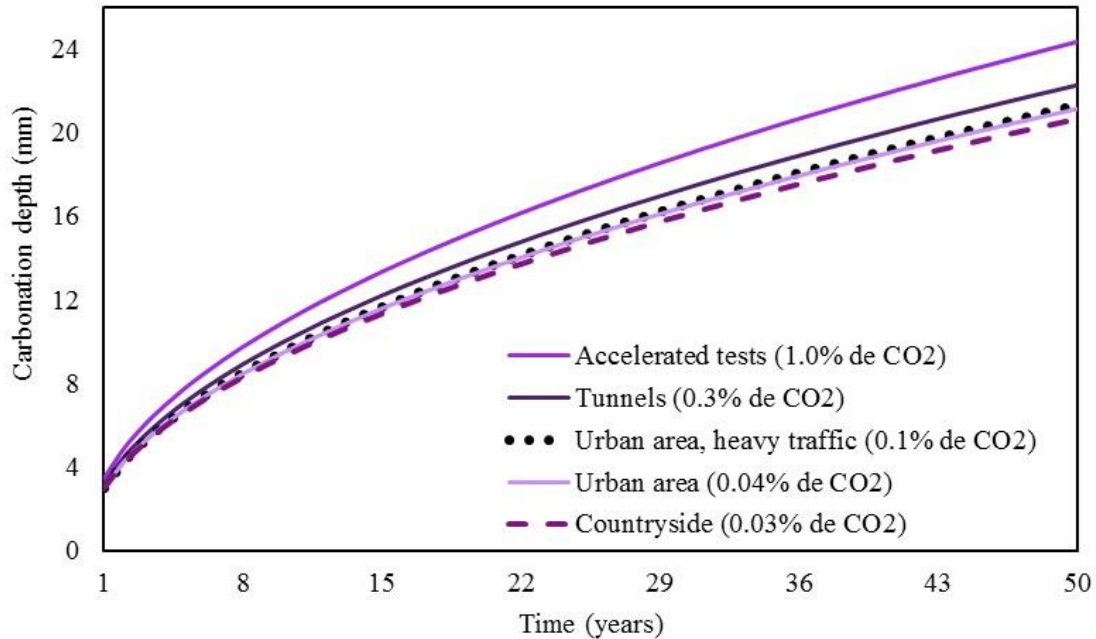


Figure 12. Depth of carbonation as a function of CO<sub>2</sub> concentrations.

## 5. CONCLUSIONS

In this work, we present an Artificial Neural Network for the prediction of the depth of carbonation in concrete structures. Results show the great potential of ANN to model the carbonation phenomenon, considering the several types of cements commercialized in Brazil.

The multilayer perceptron network developed in this work is capable to provide the depth of carbonation as function of relative air humidity, CO<sub>2</sub> concentration, concrete composition, cement type, admixtures, exposure conditions to rain, and compressive strength of concrete.

The parametric study carried out on the developed model confirmed results described by others, such as:

1. The carbonation decreases as the compressive strength of the concrete is increased;
2. The type of cement has a secondary influence on the carbonation phenomenon, since the carbonation is modified by the content of admixtures present in the cement;
3. Additions only has influence on depth of carbonation on concretes with low compressive strength (up to 60% carbonate depth), which is reduced or even eliminated in concretes with high resistance.
4. Exposure to environments with high CO<sub>2</sub> concentrations, such as tunnels, parking lots, urban environment with heavy vehicle traffic, increases carbonation rate.

The results obtained in the parametric analysis demonstrate the efficiency of ANNs in the study of the carbonation rate in concrete, improving the study of constructions pathology.

## 6. ACKNOWLEDGMENTS

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