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Discovering key meteorological variables in atmospheric corrosion through an artificial neural network model

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Abstract

This paper presents a deterministic model for the damage function of carbon steel, expressed in μm of corrosion penetration as a function of cumulated values of environmental variables. Instead of the traditional linear model, we designed an Artificial Neural Network (ANN) to fit the data. The ANN numerical model shows good results regarding goodness of fit and residual distributions. It achieves a RMSE value of 0.8 μm and a R^2 of 0.9988 while the classical linear regression model produces 2.6 μm and 0.9805 respectively. Besides, F_{LOF} for the ANN model were next to the critical value.

The improved accuracy provides a chance to identify the most relevant variables of the problem. The procedure was to add/remove one after the other the variables and perform from scratch the corresponding training of the ANN. After some trial and error as well as phenomenological arguments, we were able to show that some popular meteorological variables like mean relative humidity and mean temperature shown no relevance while the results were clearly improved by including the hours with RH < 40%. The results as such might be valid for a limited geographical region, but the procedure is completely general and applicable to other regions.

Keywords: A: Low alloy steel; B: Modeling studies; C: Atmospheric corrosion

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1. Introduction

Uruguay takes part of the collaborative project MICAT [1], operating four atmospheric corrosiveness stations. Standardized metallic samples are exposed in different natural environments, using also standardized procedures and environmental data collection procedures agreed by the MICAT working group. Amongst meteorological ones we include hourly values of relative humidity, temperature, as well as daily precipitation and precipitation run in number of days. Pollution data includes monthly values of sulfur dioxide and chloride deposition rates.

There is a significant research body regarding analytical expressions or models relating penetration and meteorological variables [2–6].

The bibliography shows mainly two alternatives; one models the corrosion rate and the other the corrosion, both as a function of meteorological variables. The second case can be related with the first one through an integral over time. Formally, the first alternative expresses:

$$C = f(X_i(t)) \tag{1}$$

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \frac{\partial f}{\partial X_1}\cdot\frac{\partial X_1}{\partial t} + \frac{\partial f}{\partial X_2}\cdot\frac{\partial X_2}{\partial t} + \frac{\partial f}{\partial X_3}\cdot\frac{\partial X_3}{\partial t} + \cdots \tag{2}$$

If the relation between f and the components of the vector $X(t)$ (pollution and meteorological variables) is linear, the integral of the corrosion rate and therefore C can be modeled with the mean values of the environmental variables in the period of study.

$$\int_0^t \frac{\mathrm{d}C}{\mathrm{d}t}\mathrm{d}t = \int_0^t \left(\frac{\partial f}{\partial X_1}\cdot\frac{\partial X_1}{\partial t} + \frac{\partial f}{\partial X_2}\cdot\frac{\partial X_2}{\partial t} + \frac{\partial f}{\partial X_3}\cdot\frac{\partial X_3}{\partial t} + \cdots\right)\mathrm{d}t = g(X\mathrm{mean})\cdot t \tag{3}$$

If the relation between f and the components of the vector $X(t)$ is not linear, then it will not be mathematically correct to employ the mean values. From a physical point of view the linear relationship hypothesis implies that if the same meteorological and pollution conditions are held constant the corrosion rate reported would be constant, because the mean values will be kept constant. This fact contradicts what is experimentally observed. As the thickness of the film of corrosion products is greater, the corrosion rate diminishes since the reactions do not occur on the naked metal as in the initial phases, but through the defects of a film of corrosion products which is increasingly thicker and compact. So despite its popularity, the linear relationship could not be valid.

In this paper, the function $C = f(X_i(t))$ is modeled assuming that f is not linear and therefore the use of mean values of X is discarded by the arguments exposed before. We will use as a first approximation, more representative of the physical process, accumulated values of the meteorological variables when possible. This is not fully satisfactory however, because it can be argued that the integrated function cannot discriminate if the pollutant was distributed at an uniform rate during the period or if the cumulated value was due to essentially to an episode of high value during a limited time.

It is worthwile noting that in the last decade, Cole et al. [7,8], Graedel [9], Lyon et al. [10], and Cai et al. [11] analysed a different and holistic approach. Graedel and coworkers [12,13], with the Gildes model, performed the first mechanistic study of the atmospheric corrosion of zinc and copper. This model has captured the principal processes involved in the corrosion of these metals under controlled conditions. Cai, using an artificial neural network, presented a phenomenological model of the atmospheric corrosion.

The economical and technological importance of even an empirical model is fairly clear because meteorological and even pollution records are taken routinely, while the direct measurement of corrosion rate of require mid-to-long term experiments. However, identifying the right variables and function has shown to be difficult, because of non-linearity's associated with the physicochemical process responsible for the atmospheric corrosion phenomena, as well as an incomplete understanding of the phenomena itself.

In spite of Graedel, Cai and Cole studies, many of the predictive models used to date are linear regression models that fit the data such that the root mean square error is minimized. Nevertheless, they have been shown to be effective only in limited geographic areas. Such limit might be related with the data or the too simplistic mathematical model. Artificial neural network modeling emerges as a promising tool in corrosion research, because of it potential to model complex non linear processes provided its architecture and parameters are properly set.

This paper describes the modeling of corrosion penetration in terms of standard meteorological variables for low carbon steel alloy. The typical choice by other researchers [2–6] is to use the mean value of the variables instead of the cumulated ones, which is equivalent only for linear models. So we have selected as pertinent meteorological parameters the cumulated time of wetness (in hours), cumulated chloride deposition (in mg Cl/m^2), cumulated sulfate deposition (in mg SO_2/m^2), cumulated hours with relative humidity below 40% (in hours), cumulated precipitation (in mm), as well as mean relative humidity (in %), and mean temperature (in K).

Thus, the problem under investigation is one of nonlinear function estimation. Given a set of n observations at time i of m meteorological variables X_i and the corresponding observed corrosion penetration values f_i, $i = 1,\ldots,n$, we have to find $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{P})$ (boldface denotes a vector) such that the root mean squared error RMSE, defined as

$$\mathrm{RMSE}(\boldsymbol{P}) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(f(\boldsymbol{x}_i,\boldsymbol{P}) - f_i)^2} \tag{4}$$

is minimized with respect to the function parameters $\boldsymbol{P}$.

$\boldsymbol{f}(\boldsymbol{x},\boldsymbol{P})$ is the function providing the corrosion penetration of carbon steel, while $\boldsymbol{x}$ is a vector of cumulated meteorological variables as described before.

2. Materials and methods

Low alloy steel subtracts, with known chemical composition (C 0.05%, Mn 0.37%, S 0.011%, P 0.01%, Cr 0.012%, Ni 0.012%, Cu 0.021%, Ti 0.02%, As 0.01%), prepared according to ISO 8407 Standard [14], were exposed to atmospheric corrosiveness stations, covering very pure rural to industrial-urban polluted atmospheric environments. The experimental design comprised long and short term exposure series. Concerning long-term exposure periods, all the test sites have had the following exposure schedule: 3 series with one-year exposure, and one series with two, three and four years exposure periods, respectively. Concerning short-term, an experiment was designed including five sequences corresponding to: 1, 2, 3, 5 and 7 months of exposure periods for samples located at a continental industrial-urban test site named Site 2. Four samples of each series were exposed in each sequence, three of which were used to evaluate annual corrosion rate.

Table 1
Some climatological parameters for the corrosion test sites

Parameters	Test sites		
	Trinidad	Prado	Melo
t_m[a] (^{o}C)	10.5	10.9	11.1
t_M[b] (^{o}C)	24.3	23.0	23.2
t[c] (°C)	16.9	16.7	17.0
P_m[d] (mm/month)	85.8	81.1	79.3
P_M[e] (mm/month)	121.6	115.3	121.1
R[f] (mm/year)	1201.2	1088.9	1138.1

[a] Mean coldest month temperature.
[b] Mean hottest month temperature.
[c] Mean annual temperature.
[d] Minimum monthly rain.
[e] Maximal monthly rain.
[f] Mean annual rain.

The samples were exposed in each test site, which corresponding major climatological parameters are described in Table 1.

All stations are located in areas classified as Humid Template Without Dry Season, according to Köppen scale.

2.1. Brief introduction to artificial neural networks

The term "artificial neural network" (ANN) denotes a computational structure intended to model the properties and behavior of the brain structures, particular self-adaptation, learning and parallel processing. It consists of a set of nodes and a set of interconnections between them [15,16]. A node contains a computational element (neuron) which takes inputs through synaptic connections from some other neurons and produces a single output. A typical neuron takes as input the weighted sum of the input links and produces a single output through a given transfer function. The behavior and properties of such a net is dependent of the computational elements, in particular the weights and the transfer function, as well as the net topology. Usually the net topology and the transfer function are specified in advance and are kept fixed, so only the weights of the synaptic connections, and the number of neurons in the hidden layer need to be estimated. The usual procedure is to divide the available dataset in two parts: the *learning* (*or training*) *set* and the *test set.* The former is presented to the ANN, and the Root Mean Squared Errors RMSE ($\boldsymbol{P}$) is minimized by properly choosing of $\boldsymbol{P}$. This process is denoted as *training*. Once $\boldsymbol{P}$ is estimated, an independent verification takes place analyzing the *generalization ability* of the ANN, evaluating the RMSE using now the test set. Usually, this new value is larger than the one obtained for the training set; if it is similar or even smaller, the parameters are accepted and the ANN is ready to be used. Otherwise, some adjustment should be made, and the overall training process is repeated. Notice that the parameters are held constant while evaluating the RMSE with the test set.

The transfer functions can be linear or not. A linear ANN can only map linear functions, severely limiting the usefulness of the model for our purposes. Non linear transfer functions are often used because they allow the network to fit better the training set.

The neurons can be connected in many ways, and thus leading to different architectures. The most popular option is named as Multilayer Perceptron. It is composed of one input layer, where the connection with the input data is performed. Such input is transmitted (lets say, from left to right) to a *hidden layer*. All neurons in the first hidden layer receive a weighted average of all inputs, but there is no connection among them. If available, further hidden layers receive inputs from weighted averages of the outputs of the previous hidden layers. The final layer collects the inputs of the last hidden one, and produced the output of the ANN. In our case, we have just one neuron in the final layer, because we will produce just one function value. Each hidden layer can have any number of neurons, and each neuron can have (in first instance) a different transfer function. The more neurons in the hidden layers, the more sophisticated cases the network is capable of learning.

Each neuron receives as input a weighted average of the outputs of the previous layer; we will denote the weights as w_{ij},. Each synaptic weight w_{ij}, is interpreted as the strength of the connection from the jth unit to the ith unit. It is customary to add a constant bias term in order to improve the training phase. The input to the jth unit can be calculated as

$$\text{NetInput}_j = \mu_j + \sum_i w_{ij} * \text{output}_i \tag{5}$$

where w_{ij} are the synaptic connection weights from neuron j to neuron i, output_i is the output from neuron i, and μ_j is a bias term for neuron j.

The output of each neuron is a simple function of its net input. A number of nonlinear functions have been used by researchers as *transfer* or *activation functions* [15,16].

Cybenko [17] demonstrated that under weak requirements on the transfer function, an ANN with one hidden layer and enough neurons can approximate any continuous function to an arbitrary degree. The synaptic weights in neural networks are conceptually similar to coefficients in regression models. They are adjusted to solve the problem presented to the network.

Learning or training is the term used here to describe the process of finding the most suitable values of these weights. There are many different algorithms for training neural networks. Backpropagation [18] is the most popular one. It modifies the weights by moving in the direction contrary to the RMSE error function gradient. The algorithm is limited by the fact that it is sensitive to the set of initial weights, and it may get trapped in local optima; it requires in addition that the transfer function should be differentiable.

2.1.1. ANN modeling

In order to facilitate the learning process, the input variables were normalized to a zero mean, unitary variance equivalents. We used in the following the same name for the input variable or its normalized version. The output of the ANN needs not to be normalized. In other branches of science, the Π Buckingham Theorem plus the prior knowledge of all significant variables allow a reduction in the number of inputs to the ANN while keeping valid the resulting model. To date it is impossible to take full advantage of this, since the full set of variables that control the corrosion process are not known. Even if they will be identified in the future, we will still need to use the available meteorological data, so the problem analyzed will still be valid.

The data set is rather small, so it has been artificially enlarged. It is well known in the ANN literature that some noise in the input is beneficial in terms of convergence, so the

learning set were duplicated using a random perturbation of at most 5%. After removing the outliers, the final training set was composed of 47 observations, plus 47 more obtained by perturbation. The test set have 18 records.

The number of neurons for the input and output layer are fixed in advance by the number of meteorological variables (five) and the number of variables to be predicted (one). The design of the ANN will be completed once the number of neurons in the hidden layer and the activation function is specified. Usually the activation function has considerable less influence in the final results [17] so the *a*sinh function has been selected for the hidden layer, and the linear one for the output neuron.

The Matlab Neural Networks Toolbox 2.0, in the context of Matlab 4.2 c. has been used for the whole process.

2.1.2. Linear model

In order to compare the results obtained by the proposed ANN model, a linear model was adjusted with the same input data. The dependent variable results of a lineal combination of the independent variables, plus a constant term. In our case the dependent variable is the penetration in μm, while the independent variables of the model are meteorological and pollution accumulated variables.

The general lineal model can be expressed:

$$Y = \alpha_o + \alpha_1 X_1 + \alpha_2 X_2 + \cdots + \alpha_5 X_5 \tag{6}$$

where variables X_i are again the accumulated meteorological and pollution variables and α_i are the coefficients of the linear model to be calculated.

2.1.3. Validation criteria

There are two fundamental aspects in any experimental problem: the design of experiments and the statistical analysis of the results. In such sense, model validation is a critical phase in this investigation. In this work, we propose to report not only the traditional numbers (Coefficient of correlation R and Root Mean Square Error RMSE) but also reporting the dispersion inherent in the data and the corresponding to the lack of fit of the model. This technique is known as *Test of Lack of Fit* (LOF). We believe that this is a definite advantage over the typical procedures carried out by most of the investigators.

2.1.4. Coefficient of correlation

The coefficient of correlation employed to validate linear models is a technique that provides only an algebraic-analytic evidence upon the kindness of the adjustment of the model but does not report the variation inherent in the data. This dispersion is called "pure error". The coefficient of correlation R is defined as

$$R = \frac{\sum_{i=1}^{n}(x_i - \bar{x}).(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 . \sum_{i=1}^{n}(y_i - \bar{y})^2}} \tag{7}$$

where the x_i are the values of the independent variable, the y_i are the values of the dependent variable and overbars denote the respective average values.

Geometrically this is equal to the cosine of the angle formed by the vectors. If all the points are perfectly aligned these two vectors are collinear and in that case R would be 1 [19]. By continuity of the functions involved, if the points are "almost" aligned the value

of R or in every case that of R^2 (to avoid the problem of sign) will be next to the unit. This ratio does not provide an interval of confidence neither a test of hypothesis that permit to confirm the adjustment or not of a model. This confirmation will be done with the Test of Lack of Fit (whenever there exist replicated values in at least one of the points).

2.1.5. Root mean square error

The RMSE is defined as

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\cdot\sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \widehat{Y^j})^2} \tag{8}$$

where Y_i^j represents the ith value corresponding to the jth point and $\widehat{Y^j}$ is the predicted value for that point. As the criterion of the Coefficient of Correlation, this technique of validation only provides an algebraic-analytic evidence but does not provide an appropriate statistical test. It is interesting to expand the quantity subradical of the RMSE, that we will denoted as SS(RMSE).

For this analysis we will denote as $\overline{Y^j}$ the average of the n_j determinations in the jth point. It results

$$\begin{aligned}
\mathrm{SS(RMSE)} &= \sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \widehat{Y}^j)^2 = \sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \overline{Y}^j + \overline{Y}^j - \widehat{Y}^j)^2 \\
&= \sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \overline{Y}^j)^2 + \sum_{j=1}^{r}\sum_{i=1}^{n_j}(\overline{Y}^j - \widehat{Y}^j)^2 + 2\sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \overline{Y}^j)(\overline{Y}^j - \widehat{Y}^j) \\
&= \mathrm{SS(PE)} + \mathrm{SS(LOF)} + 2\sum_{j=1}^{r}(\overline{Y}^j - \widehat{Y}^j)\left(\sum_{i=1}^{n_j}(Y_i^j - \overline{Y}^j)\right) \\
&= \mathrm{SS(PE)} + \mathrm{SS(LOF)}
\end{aligned} \tag{9}$$

keeping in mind that

$$\sum_{i=1}^{n_j}(Y_i^j - \overline{Y}^j) = \sum_{i=1}^{n_j}(Y_i^j) - n_j\overline{Y}^j = 0 \tag{10}$$

It is concluded that the SS(RMSE) is the sum of squares associated to the pure error SS(PE) and the corresponding to the lack of fit SS(LOF). That is to say that in the RMSE the total error is considered without discriminating the contributions of both sources (pure error and lack of fit). We refer the reader to the specialized literature.

2.1.6. Test of Lack of Fit

If the Linear General Model is considered with the usual hypothesis that the errors ε_i are normally distributed and besides are available repetitions or replicas for some of the points, then is possible to apply the LOF test. Intuitively this test compares the self dispersion of the data (which explains why it is necessary the repetition) against the dispersion of the mean data with regard to the predicted values. Formally the former is determined with the Pure Error Mean Square ($\mathrm{CM_{PE}}$), while the latter is calculated with the Lack of Fit Mean Square ($\mathrm{CM_{LOF}}$). The quotient of these two mean squares provides a statistical value, F_{LOF} that is compared against a critical value that is obtained from the F-Table of Fisher [20,21].

This statistical technique employs all the individual experimental values instead of mean values The test requires the existence of replicas in at least one of the points in order to estimate the pure error (PE) or dispersion inherent to the experimental data. This pure error is compared with the Lack of Fit Error corresponding to the model.

To assure the applicability of the test is necessary to work with true replicas and to verify other hypothesis associated to residuals, like independence and identical distribution. This distribution should be normal of zero mean and homogeneous variances.

Another consequence is that if mean values were employed in modeling, it will not be possible to estimate the pure error. Beyond this technical difficulty, there is a conceptual fact and is that we are not able to say that a model fits or not without comparing its eventual lack of fit against the own errors of the method. If the pure error was very large, practically any model would fit independently of the value of the coefficient of correlation.

Specifically in the LOF Test are presented two possible hypothesis (H_0 and H_1)

H_0: the linear model in the parameters is adjusted to the data
H_1: not H_0

As mentioned previously, this Test allows to discriminate if a linear model is applicable or not but in turn requires that replicas were available. In other words, for the same value of X there should be several measured values of Y, being

$$\boldsymbol{Y}_i^j = \boldsymbol{g}(\boldsymbol{X}_i) + \varepsilon_i^j, \quad \text{with } \varepsilon_i^j \; iid \sim N(0,\sigma^2),\ 1 \leqslant i \leqslant n_j,\ 1 \leqslant j \leqslant r,\ y\ \exists j/n_j > 1.$$

If a linear model is assumed, $Y = A\alpha + \varepsilon$, then:

$$\mathrm{SS(E)} = \|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|^2, \quad \text{where } \widehat{\boldsymbol{Y}} = \boldsymbol{A}\hat{\alpha} \tag{11}$$

$$\mathrm{SS(PE)} = \sum_{j=1}^{r}\sum_{i=1}^{n_j}(Y_i^j - \overline{Y^j})^2 \tag{12}$$

where $\overline{Y^j} = \frac{1}{n_j}\sum_{i=1}^{n_j} Y_i^j$ and $\mathrm{SS(LOF)} = \mathrm{SS(E)} - \mathrm{SS(PE)}$.

The critical region is defined as

$$W = \left\{ \frac{\mathrm{SS(LOF)}/(r-k-1)}{\mathrm{SS(PE)}/(n-r)} \geqslant F_{1-\alpha}(r-k-1, n-r) \right\} \tag{13}$$

$$W = \left\{ \frac{\mathrm{CM(LOF)}}{\mathrm{CM(PE)}} \geqslant F_{1-\alpha}(r-k-1, n-r) \right\} \tag{14}$$

with $\boldsymbol{n} = \sum_{j=1}^{r}\boldsymbol{n}_j$ and $k+1$ number of parameters in the linear model $(\alpha_0, \alpha_1, \ldots, \alpha_k)$.

2.1.7. Residual analysis

When validating the models, the analysis of the residual distributions turns out to be fundamental. In effect, practically all the tests and statistical methods assume that the residuals should be independent and identically distributed, with Normal distribution, of zero mean and homogeneous variance. These residuals are defined as the difference between observed values and predicted ones.

2.1.8. Normal distribution

Keeping in mind that kinetics studies were carried out employing three replicas for each experimental series, it would not have sense to carry out a verification of normality because of the lack of a sufficient number of data. Instead of this, the normality of the

residuals of all experimental series were analyzed altogether. The tests of normality employed were: Test of Kolmogorov, Test of Lillieforfs, and Test of Shapiro Wilk. [22–26]. Corresponding results were presented in Figs. 2 and 3 in terms of *p*-values.

2.1.9. Outlier detection

It is well known that the mean and standard deviation are badly affected if there are outliers in the dataset. A number of procedures have been devised in the statistics literature to identify unlikely events and thus producing more reliable estimates of the expected value and variance. In this paper, we have used the Minimum Covariance Determinant (MCD) [27,28] as a criteria. It considers all possible subsets of h points out of N, computes its covariance and determinant, and records its minimum value. The procedure as described is impractical for large N, but some well thought algorithms (FASTMCD) circumvent such problem. The scalar value h is selected in advance if one knows how many outliers are likely to exist in the set. The safest value is $N/2$ (rounded upwards) which assumes that nearly half of the data is an outlier.

Once identified the "optimum" subset of h elements, its statistics (mean and standard deviation) are calculated and assumed to be representative of the whole population. For all points the Mahalanobis distance is calculated, defined for the ith point as

$$d_i = (\mathbf{x}_i - \bar{\mathbf{x}})^{\mathrm{T}} \mathbf{C}^{-1} (\mathbf{x}_i - \bar{\mathbf{x}}) \tag{15}$$

being $\mathbf{C}$ the sample covariance matrix, and the overbar the mean value. In the case of univariate data, $\mathbf{C}$ is equivalent to variance. The distribution of d_i is assumed to be known, and thus critical values exist to discriminate between likely ith points and unlikely ones. In the case of dimension 1, the critical value is commonly taken as 3.0, leaving inside 99.865% of the events.

If the dataset does not have any outliers and the underlying population is multivariate normal, the estimates of the mean and variance are equal to the traditional ones.

3. Results and discussion

This section presents an artificial neural network model for the estimation of a damage function for low carbon steel substrates as a function of some input variables. Later we will discuss the performance of the model in terms of goodness of fit and the residual distributions for training and testing data sets.

The inputs variables considered are: X_1 time of wetness (in hours), X_2 sulfate deposition (in mg SO_2/m^2), X_3 precipitation (in mm), X_4 hours with relative humidity below 40% (in hours), X_5 chloride deposition (in mg Cl/m^2), all of them cumulated over the considered period. The target value (y_2) is the penetration (in μm). We recall that during training, we normalized the input variables to zero mean, unit variance.

The approximation commonly used to estimate the time of wetness, X_1, included in ISO 9225, cannot be directly derived from an understanding of surface wetting process, as it was stated by Cole and coworkers [29]. Salts and thus surfaces they were on, may wet over a range of RH, depending the deliquescent RH of the salt. The input variable denoted as X_4 (hours with relative humidity below 40%) is proposed in order to refine the time of wetness concept so as derive in better statistical fit with the available corrosion data. The surface wetting in relation to hygroscopy salts with low deliquescent RH (below 40%) is represented in this input variable.

The full ANN model's output can be expressed as follows

$$y_2 = b_2 + \boldsymbol{w}_1 * a\sinh(\boldsymbol{W}_1 \cdot \boldsymbol{x}^T + \boldsymbol{b}_1) \tag{16}$$

where $\boldsymbol{x}$ is the vector of input variables normalized to a zero mean, unitary variance. The scalar output y_2 should fit the measured penetration (without normalization).

After trial and error, we found that the model with two neurons in the hidden layer shown the best fitting capabilities, exhibiting the smallest RMSE both for learning and testing data sets. It will be presented below. The final weights for the ANN with two neurons in the hidden layer are:

$$\boldsymbol{W}_1 = \begin{pmatrix} -0.2564 & -2.8854 & -0.0718 & 0.0292 & 0.6335 \\ -2.3593 & 3.6564 & -1.0513 & 1.6426 & -2.7169 \end{pmatrix}; \quad b_1 = \begin{pmatrix} -0.1673 \\ 0.0914 \end{pmatrix}$$

$$\boldsymbol{W}_2 = (-14.5092 \quad -5.1597); \quad b_2 = 28.4583 \; [\boldsymbol{W}_2] = [b_2] = \mu\text{m}$$

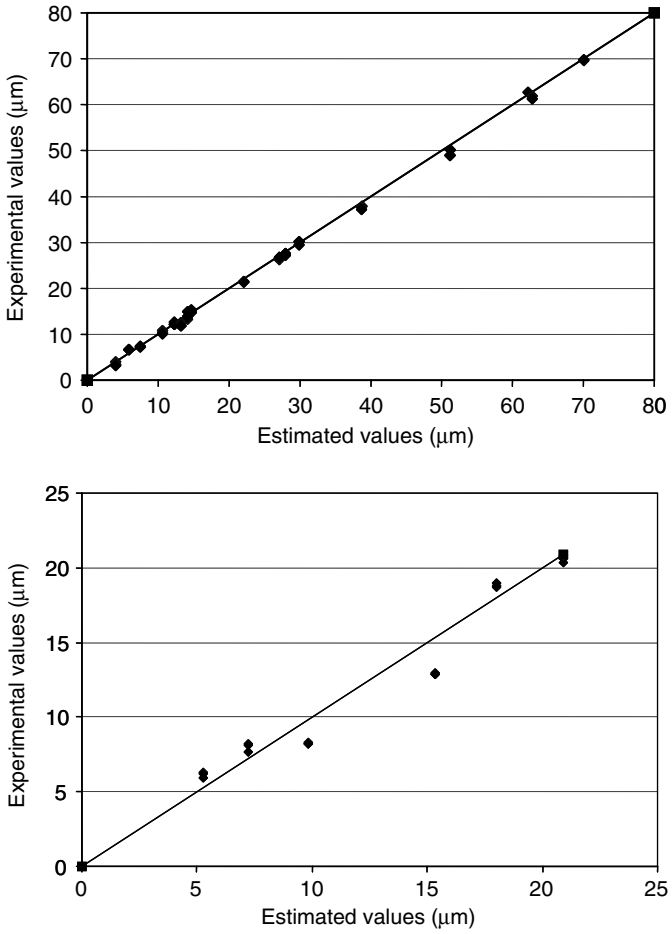

Fig. 1. Above, comparison of measured vs. calculated penetration values (in μm) for the training set. Below, the same for the testing set.

The mean and standard deviation are required for the normalization

$$\text{Mean} = (\,7341.3 \quad 3113.1 \quad 1905.3 \quad 218.2 \quad 2802.1\,)$$

$$\text{Standard deviation} = (\,6529.5 \quad 4820.6 \quad 1665.6 \quad 227.8 \quad 4523.3\,)$$

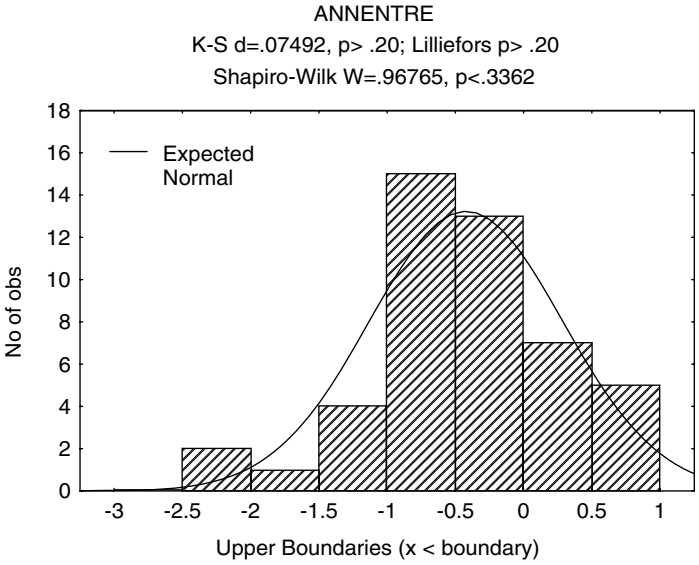

Fig. 2. Distribution of the discrepancies between the ANN output and the measurements for the training set.

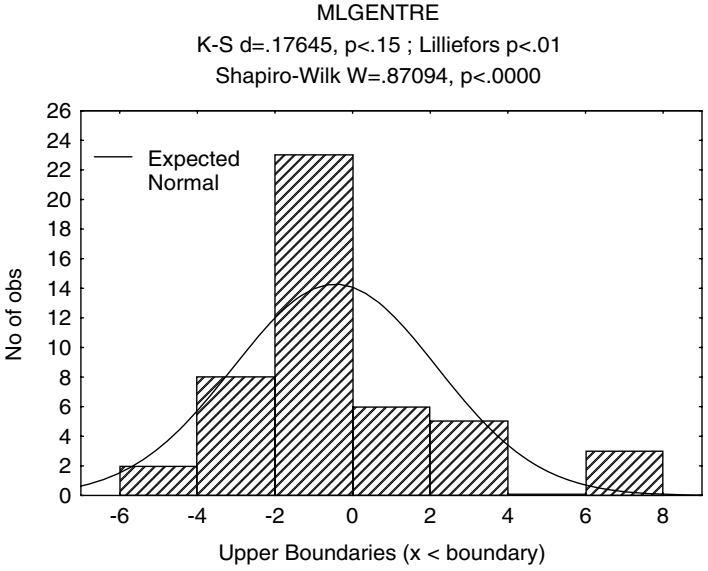

Fig. 3. Distribution of the discrepancies between the classical linear regression model output and the measurements for the training set.

Table 2
R^2, RMSE and F_{LOF} ($\alpha = 0.05$, $\alpha = 0.01$) for training data set

	Model	
	ANN	Linear
F_{LOF}	4.86	112.80
$F_{(0.95\ 16,\ 34)} = 1.95$	No fit	No fit
$F_{(0.99\ 16,\ 34)} = 2.60$	No fit	No fit
RMSE	0.8 μm	2.6 μm
R^2	0.9988	0.9805

Table 3
R^2, RMSE and F_{LOF} ($\alpha = 0.05$, $\alpha = 0.01$) for validation data set

	Model	
	ANN	Linear
F_{LOF}	170.78	993.21
$F_{(0.95\ 5,\ 12)} = 3.11$	No fit	No fit
$F_{(0.99\ 5,\ 12)} = 5.06$	No fit	No fit
RMSE	1.3 μm	3.1 μm
R^2	0.9468	0.6942

With such parameters and after removing the outliers, the RMSE for the training set was 0.8 μm and the regression coefficient R^2 was 0.9988, while for the test set it was 1.3 μm and 0.9468 respectively. These results have been considered acceptable and are graphically represented in Fig. 1. The distribution of the discrepancies between the ANN output and the measurements, as well as the residual distribution corresponding to the classical linear regression model are respectively represented in Figs. 2 and 3.

To make a comparison, we also used a classical linear regression model with the same normalized inputs. The weights were $\mathbf{W} = (30.8375\ 15.5205\ -16.7111\ -7.1684\ 03490)$ and the constant term was 24.8248 μm. In this case, the training set were fitted with an RMSE of 2.6 μm, and the same figure for the test data set was 3.1 μm. This shows that the generalization capabilities of the linear model were good. However, the comparison with other values in the literature should be made with caution, because the researchers usually made the fit with all the available data, and reports the RMSE with such set; in that case, the ANN produces 0.96 μm while the linear model 3.6 μm.

Results are presented in Tables 2 and 3 for training and validation data sets respectively.

4. Conclusions

This paper presents an ANN-based methodology for the modeling of atmospheric corrosion functions, and the full model obtained with data from Uruguay.

It showed excellent results regarding goodness of fit and residual distributions on learning and testing data sets. It achieves a RMSE value of 0.8 μm and a R^2 of 0.9988 while the classical linear regression model produces 2.6 μm and 0.9805 respectively. Its validity to other environments is yet to be ascertained.

It is believed that a properly adjusted ANN model can be useful in the prediction of corrosion damage under different climatological and pollution conditions, while linear models cannot.

The ANN concept is expected to be an effective and efficient tool for the construction of models associated with atmospheric corrosion processes for other metals, and in general, in the modeling of corrosion processes from experimental data.

This investigation has been able to confirm the relevance on the corrosion values of meteorological and pollution variables such as the time of wetness, precipitation and sulphate and chloride, and the negligible effect of considering others. Such conclusion arises after adjusting an artificial neural network with different sets of input variables, and analyzing the differences in terms of goodness of fit.

In particular, the average relative humidity (in %), and average temperature (in K) shown no relevance in modeling both training and testing data sets. Taking into account these meteorological variables the RMSE for the training set is 0.8 μm while for the test set is 3.02 μm.

Theoretical arguments and experimental evidences have been given to prefer the accumulated variables to the mean values, as well as to incorporate a representative variable of the dry periods. Results were clearly improved by including the total number of hours with RH $< 40\%$. If this variable is not included the results are a RMSE of 0.8 μm for the training set, and 9.96 μm for the test set.

Neither the traditional linear nor the ANN model achieved the standard level of confidence of the 95% and 99%.

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