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An Early Stopping-Based Artificial Neural Network Model for Atmospheric Corrosion Prediction of Carbon Steel

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Abstract: The optimization of network topologies to retain the generalization ability by deciding when to stop overtraining an artificial neural network (ANN) is an existing vital challenge in ANN prediction works. The larger the dataset the ANN is trained with, the better generalization the prediction can give. In this paper, a large dataset of atmospheric corrosion data of carbon steel compiled from several resources is used to train and test a multilayer backpropagation ANN model as well as two conventional corrosion prediction models (linear and Klinesmith models). Unlike previous related works, a grid search-based hyperparameter tuning is performed to develop multiple hyperparameter combinations (network topologies) to train multiple ANNs with mini-batch stochastic gradient descent optimization algorithm to facilitate the training of a large dataset. After that, one selection strategy for the optimal hyperparameter combination is applied by an early stopping method to guarantee the generalization ability of the optimal network model. The correlation coefficients (R) of the ANN model can explain about 80% (more than 75%) of the variance of atmospheric corrosion of carbon steel, and the root mean square errors (RMSE) of three models show that the ANN model gives a better performance than the other two models with acceptable generalization. The influence of input parameters on the output is highlighted by using the fuzzy curve analysis method. The result reveals that TOW, Cl- and SO_2 are the most important atmospheric chemical variables, which have a well-known nonlinear relationship with atmospheric corrosion.

Keywords: Atmospheric corrosion prediction, early stopping, fuzzy curve, grid search, hyperparameter tuning, multilayer neural network.

1 Introduction

The atmospheric degradation of metal materials is essential for the durability of structures and causes high economic costs so that atmospheric corrosion becomes a serious global

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concern. Deterioration of the worldwide infrastructure, mostly made of carbon steel, might cause severe damage and threats to public safety. The World Corrosion Organization (WCO) currently estimates the direct cost of corrosion worldwide at around $2.2 trillion annually. The cost of $660 billion worldwide would be saved by the existing corrosion control technologies [WCO (2020)]. To improve the reliability and endurance of infrastructure and industrial equipment, the prediction of corrosion behavior of material and its lifetime is increasingly urgent.

Existing models with the foundation of power function were lack of the ability to describe the difficulty of atmospheric corrosion kinetics and might not generalize well on new environmental parameters due to minor parameters and simple structure. On the contrary, ANN has been developing as a milestone in machine learning for a decade, replacing traditional models for forecasting tasks and giving satisfactory results by its benefits of generalization, noise tolerance, and fault tolerance. The main benefit of ANN is that it can model problems in which there are no transparent relationships between inputs and outputs, and construct the solutions that cannot be easily formulated within a short time without specifying the form of interactions between variables. Abstracted by ANN's outstanding performance, many researchers applied it to simulate the complicated processes and obtained good results in various materials performance analysis works concerning mechanical property [Forcellese, Gabrielli and Simoncini (2011); Ashtiani and Shahsavari (2016)], metallurgy [Yang, Zhu, Lai et al. (2012)], atmospheric corrosion [Pintos, Queipo, de Rincón et al. (2000); Zhang, Yu, Yang et al. (2011)], civil engineering [Sadowski (2013); Yıldızel and Öztürk (2016)], tribological property [Li, Lv, Si et al. (2017)], thermal property [Zhao and Li (2017)].

As the meteorological variables involved in the atmospheric corrosion process have nonlinear features and timely change, ANN has been paid attention as a solution to predict the atmospheric corrosion. Since the complex interactions between environmental factors bring difficulty for modeling the process of atmospheric corrosion, Lo et al. [Lo, Chiu and Lin (2017)] employed ANN to develop a regional forecasting model to predict atmospheric corrosion rates of copper within general industrial zones and coastal industrial zones in Taiwan. Vera and Ossandón [Vera and Ossandón (2014)] used numerous ANNs to predict the atmospheric corrosion rates of carbon steel, galvanized steel, copper, and aluminum, respectively. Li et al. [Li, Qiu, Xing et al. (2013)] took advantage of ANN to model the atmospheric corrosion behavior of aluminum alloys in 10 typical atmospheric corrosion test sites. Zhang et al. [Zhang, Yu, Yang et al. (2011)] analyzed atmospheric corrosion behavior of bainite steel exposed offshore platforms by applying ANN. Willumeit et al. [Willumeit, Feyerabend and Huber (2013)] demonstrated that ANN was able to function well on predicting corrosion properties of Mg alloys. Turning to carbon steel, Kenny et al. [Kenny, Paredes, de Lacerda et al. (2009)] developed an ANN with linear and sigmoidal functions, aiming to predict low-carbon steel, copper, and aluminum corrosion rates according to meteorological parameters. Pintos et al. [Pintos, Queipo, de Rincón et al. (2000)] proved that an ANN-based methodology was better than a linear regression model and had a good agreement with known or observed data for modeling atmospheric corrosion. Cai et al. [Cai, Cottis and Lyon (1999)] built two different ANNs to model atmospheric corrosion of carbon steel and zinc, respectively. Reddy et al. [Reddy (2014); Jančíková, Zimný and Koštial (2013)]

applied ANN to predict the corrosion loss of structural carbon steel based on the input environmental parameters in the atmospheric environment.

Although ANN performed well in various materials performance predictions, some works [Sun, Qi, Hou et al. (2007); Rajendraboopathy, Sasikumar, Usha et al. (2009)] have reported that to achieve the optimal generalization of the prediction results, the enrichment of adequate training data was a necessity. Unlike other machine learning methods whose optimal performance is limited to a certain extent of a huge dataset, the deep learning nature of ANN takes advantage of the ability to handle data augmentation. The larger the dataset the neural network is trained with, the better generalization the prediction can give.

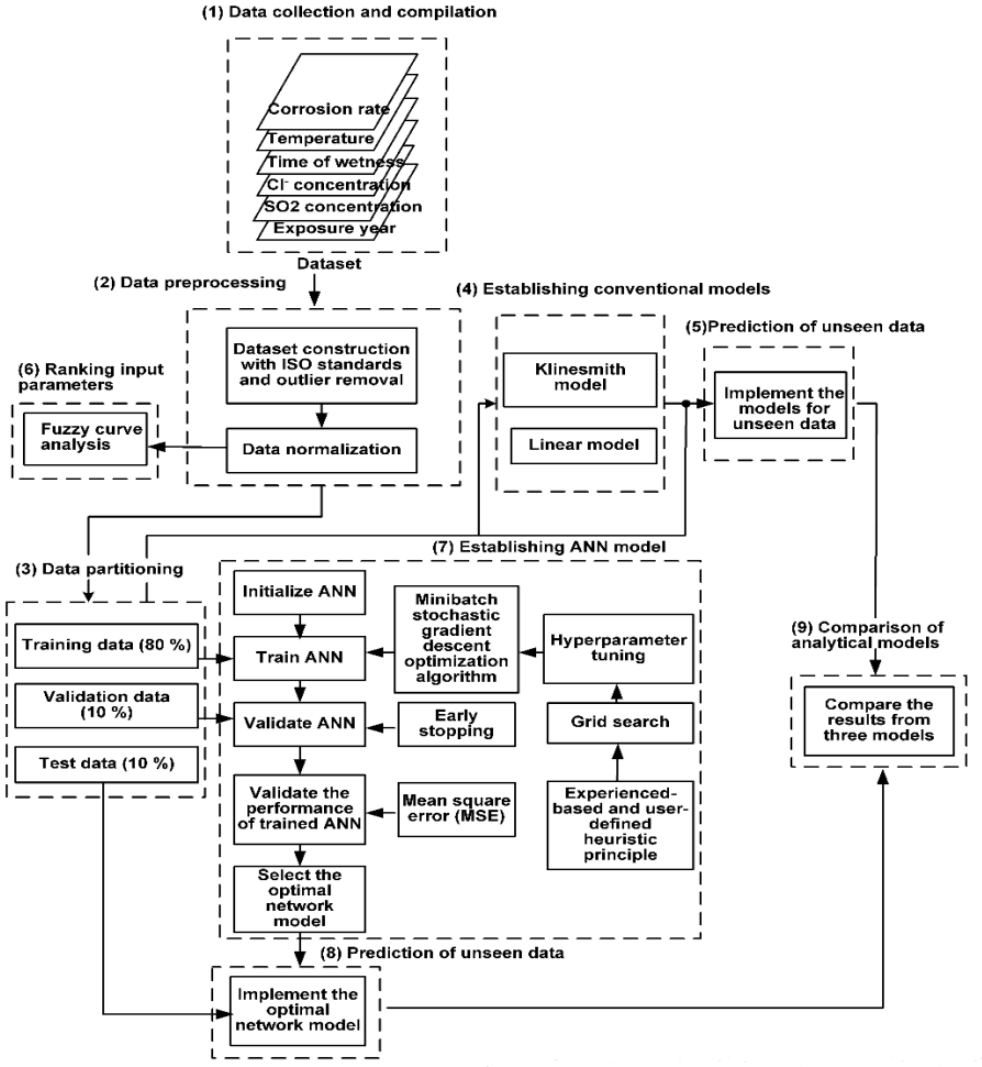

Figure 1: The flowchart showing the overall methodologies of constructing atmospheric corrosion prediction models: conventional models and ANN

Fig. 1 illustrates the overall methodologies used in this work. The procedure of atmospheric corrosion experiments (the long-term exposure tests of carbon steel) is feasible but extremely time-consuming and laborious. The atmospheric corrosion data of carbon steel is collected as much as possible in a limited time so that the related useful information is extracted from published papers to construct a dataset that is big enough for training our neural network model. To retain the generalization ability of ANN instead of memorizing the depth of training history is one of the existing vital challenges for the optimization of network topologies by a stopping criterion. Unlike previous related works adopted Levenberg-Marquardt backpropagation training algorithm, ANN is trained with a deep learning optimization algorithm, mini-batch stochastic gradient descent (SGD) optimization algorithm, which is more appropriate for large scale optimization. Although the dataset is not practically big enough to be expressed as a large scale, mini-batch SGD optimization algorithm is adopted for the intention of establishing a model to deal with future enrichment of dataset. To further reduce the burden of testing, a grid search-based hyperparameter tuning is performed so that different multiple hyperparameter combinations are trained to establish multiple ANN models. A contribution is then made into our work by adopting a stopping criteria-based selection strategy for the optimal hyperparameter combination to guarantee the generalization ability of the optimal ANN model for the estimation of atmospheric corrosion of carbon steel. One simple linear equation and one equation formulated in Klinesmith et al. [Klinesmith, McCuen and Albrecht (2007)] are also evaluated to find out their relevance against the ANN model. The purpose of this paper is to apply ANN to describe the phenomenon of atmospheric corrosion of carbon steel, make a comparison with conventional models and determine the influence of meteorological variables via fuzzy curves.

The rest of the contents are arranged as follows. Section 2 starts with the dataset construction and modeling methodologies for constructing three different models and fuzzy curves are then proposed. Section 3 discusses the analysis of the outcomes of three models by comparing their evaluation metrics and the ranges of fuzzy curves to highlight the impact of each input parameter on the atmospheric corrosion. Section 4 ends with a conclusion and a future research trend.

2. Materials and methods

2.1 Dataset construction

Extracting the relevant data used to train and test the ANN reported here comes from the literature of long-term exposure tests (in published papers, project reports, and researches) of atmospheric corrosion of carbon steel, along with a wide range of climatological variables and pollution parameters. Being collected from nine published works listed in Tab. 1 along with the countries from which the data came, the worldwide atmospheric corrosion data of carbon steel is compiled into a large dataset conformed to corrosivity standardized in (International organization for standardization) ISO 9223, ISO 9224, ISO 9225 and ISO 8044 as much as possible for the construction of prediction model and some outliers are removed.

As seen in the world map of Fig. 2, the atmospheric corrosion data of carbon steel in the colored portions covering 52 countries in 5 continents under various types of climates

(tropical, subtropical, warm, cold, etc.) is accumulated into a big dataset of around one thousand pieces of records used in this work.

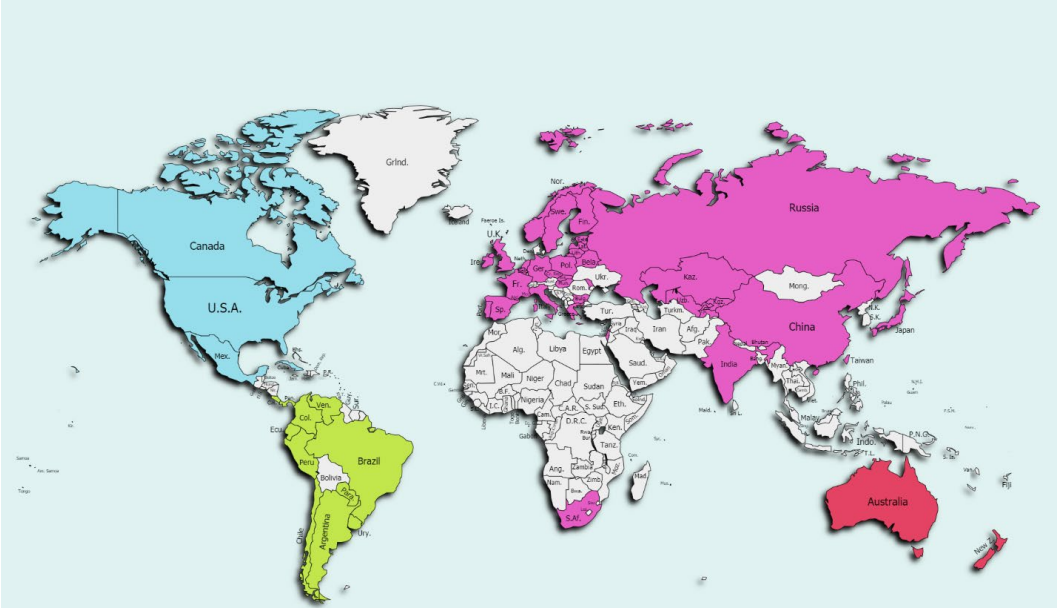

Figure 2: World map covering all countries from which data for this work were collected

Table 1: Data sources collected for this work

No.	Country	References
1	33 countries	[Cai, Cottis and Lyon (1999)]
2	38 countries (in Europe, America, Asia and Oceania)	[Chico, De la Fuente, Díaz et al. (2017)]
3	14 countries (throughout Iberoamerican)	[Pintos, Queipo, de Rincón et al. (2000)]
4	Colombia	[Castaño, Botero, Restrepo et al. (2010)]
5	Spain (Canary Islands)	[Morales, Martín-Krijer, Díaz et al. (2005)]
6	Argentina, Brazil, Colombia, Ecuador, Spain, Mexico, Peru, Uruguay	[Panchenko and Marshakov (2017)]
7	three Caribbean countries (in Cuba, Mexico and Venezuela)	[Corvo, Haces, Betancourt et al. (1997)]
8	China	[Hou and Liang (1999)]
9	Japan (Tsukuba, Choshi, Miyakojima)	[NIMS (2018)]

Tab. 2 lists the ranges of the corrosion and environmental variables used in this work. Before training, both input and output parameters are normalized between 0 and 1 to avoid the dominance of different dimensions [Zhang, Yu, Yang et al. (2011)]. The meteorological input variables (Temperature and Exposure year) are linearly scaled. The diversity ranges of two input pollution variables (SO_2 concentration and Cl^- concentration) and the output

variable (Corrosion rates) are highly wide so that they are logarithmically scaled to minimize the loss of accuracy. The normalization is done with the following equation.

$$P = \frac{x_i - x_{min}}{x_{max} - x_{min}} \quad (1)$$

where P is the normalized data, x_i is the i[th] input/output parameter, and x_{min} and x_{max} are the minimum and maximum values of i[th] parameter respectively.

The whole dataset (943 data sets in total) is randomly divided into three sets: 754 data sets as the training dataset (80% in total), the other 94 data sets as the validation dataset (10% in total) and the rest 95 data sets as the test dataset (10% in total) under the same sample distribution.

Table 2: The ranges of input and output parameters in the whole big dataset used in this study

Input and Output Parameters	Temperature (T, ^oC)	Time of wetness (TOW)	SO_2 concentration (SO_2, $\mu g/m^3$)	Cl^- concentration (Cl^-, $mg/m^2/day$)	Exposure year (Year, years)	Corrosion rate (μm/year)
Range	-3.1-29.3	0.003-1	0-175	0-260	0.5-12	1.7-1040

2.2 Modeling methodologies

2.2.1 Constructing conventional corrosion models

A simple linear regression model is constructed to predict the atmospheric corrosion of carbon steel as a function of five independent variables: temperature (T), time of wetness (TOW), SO_2 concentration (SO_2), Cl^- concentration (Cl^-) and exposure year (Year). There is nothing special to be set, and all parameters are generated from the least square methods as the following equation.

$$\text{Corrosion rate} = A + B \times T + C \times TOW + D \times SO_2 + E \times Cl^- + F \times \text{Year} \quad (2)$$

where A=0.1691, B=0.0310, C=0.1937, D=0.0656, E=0.1676, and F=0.4484.

The role of environmental parameters has a high impact on long-term atmospheric corrosion. Because existing long-term corrosion prediction models, such as power model [Townsend (2002)], were just mostly time-dependent models and they neglected the influence of environment on atmospheric corrosion process, they could not produce accurate predictions when being used in different conditions or locations. The researchers in Knotkova et al. [Knotkova, Boschek and Kreislova (1995)] established similar corrosion prediction models by considering the impact of one or three environmental variables as predictor variables, but not exposure year that the coefficients of the models might not give enough accuracy to access the influence of other essential predictor variables that were not taken into account in the corrosion process. The authors in Klinesmith et al. [Klinesmith, McCuen and Albrecht (2007)] developed eight reliable prediction models that chewed over the effects of each environment parameter as well as the exposure time in the corrosion process for four materials data from ISO CORRAG, a worldwide collaborative atmospheric exposure program, under a wide range of atmospheric conditions or locations. In this work, the Klinesmith model [Klinesmith, McCuen and Albrecht (2007)] is adopted to access the effects of changes in

environmental conditions in predicting the atmospheric corrosion of carbon steel as a function of environmental parameters and exposed period as well. The Klinesmith model for atmospheric corrosion prediction of carbon steel is established as Eq. (3), where some parts of its parameters (C, E, and G) are obtained from the mean values of the corresponding environmental variables and the rest (B, D, F, H, and J) are acquired by the least square methods.

$$\text{Corrosion rate} = \text{A}\, year^{B}\left(\frac{TOW}{C}\right)^{D}\left(1+\frac{SO_2}{E}\right)^{F}\left(1+\frac{Cl^-}{G}\right)^{H} e^{J(T+T_0)} \quad (3)$$

where A=14.5018, B=0.7528, C=0.4474, D=0.3641, E=22.0902, F=0.4210, G=23.9742, H=0.6684, J=0.0068 and T_0=20 are empirical coefficients.

2.2.2 Constructing artificial neural network model

The role of neural network prediction is increasingly significant in materials science. An artificial neural network is one kind of network model established in a mathematical way that is based on the working principle of biological neurons connected in a biological neural network. The layers of ANN are systematically connected from left to right order, and every layer becomes the input layer for its successive layer. Details of the neural network method itself can be found in Graupe et al. [Graupe (2013); Demuth, Beale, Jess et al. (2014)].

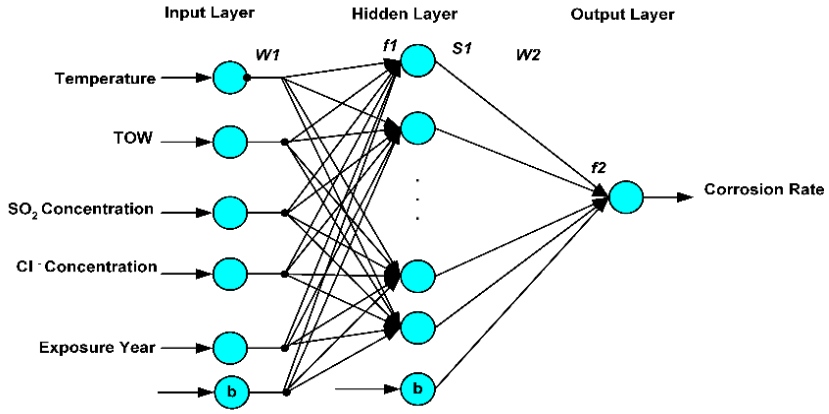

Figure 3: The architecture of ANN for predicting the atmospheric corrosion rate of carbon steel

ANN can be tolerant of any faults and noises in data. It can deal well with the nonlinear relationship between variables in function approximation problems, such as prediction of atmospheric corrosion of materials which has a complex interaction between input variables and meteorological variables [Cai, Cottis and Lyon (1999); Jančíková, Zimný and Koštial (2013)]. To compare with the results of two corrosion prediction models above, the neural network model established in this work is the multilayer backpropagation neural network (ANN). ANN is a neural network composed of at least three or more layers: one input layer, at least one or more hidden layers and one output layer. As illustrated in Fig. 3, ANN starts from the input layer, the input parameters

consecutively go through the hidden layers and output layer and are continuously transformed by activation functions contained in the neurons of each layer during the propagation process, which is known as feedforward propagation. The learning algorithm used for training ANN is a mini-batch SGD optimization algorithm. The generalization ability of ANN can be improved by the use of mini-batch sizes because it uses fewer samples to estimate the actual gradient so that the computational efficiency is improved [Zhang, Lipton, Li et al. (2020)].

Three-layer ANN is constructed to predict the atmospheric corrosion rate and establish the relationship between five input meteorological parameters (T, TOW, SO_2 Concentration, Cl^- Concentration, Year) and one output parameter (Corrosion rate) of carbon steel. Tab. 3 lists the network features applied in ANN. After multiplying the corresponding weights (W) and then pulsing with the bias (b) in Eq. (4), the weighted input values generated from the previous layer are brought into logistic sigmoid function expressed in Eq. (5) to produce the activation of the neuron in a hidden layer.

Table 3: Network parameters adopted in the ANN model

Network Parameters	Value
Number of layers	3
Initial weights and biases	Randomly between 0 and 1
Number of neurons in the input layer	5
Number of neurons in the output layer	1
Learning algorithm	Mini-batch stochastic gradient descent
Activation function	Logistic sigmoid
Method for avoiding over-training	Early stopping criteria

$$z = WX + b = \sum_{i=1}^{m} x_i w_{ni} + b_n \tag{4}$$

$$f(z) = \frac{1}{1+e^{-z}} \tag{5}$$

where X represents all of the input variables in ANN, W is the weight value of the input variable X, z is the weighted sum of input variables, b is the bias value, n is the number of neurons, m is the number of input, and f(z) is the logistic sigmoid activation function of the node. Weights and biases contained in neural networks are adjusted continuously by backpropagation during the training process. The error of each neuron between predicted and actual values is obtained from forwarding propagation, and the predicted target is minimized from the chain rule. The output layer receives the calculation results from the hidden layer and generates the output. The mathematical model of the result of the output layer in ANN can be expressed as follow:

$$Y = f2(W2 \times [f1([W1 \times X] + b) + b) = f2\ (W2\ \times S1 + b) \tag{6}$$

where X and Y represent the input and output values, b is the bias value, $W1$ and $W2$ denote the corresponding weight values between the input and hidden layers, and between the hidden and output layers, respectively. The functions $f1$ and $f2$ are the

logistic sigmoid functions applied to generate the output from the weighted data in the nodes of each layer.

There are several rules of thumb for defining the number of hidden nodes in the hidden layer. Since it is difficult to pre-define the number of hidden neurons in the hidden layer and there is no unique formula to define it [Cao, Zhu, Zhang et al. (2010)], the trial-and-error approach is implemented in this work. To restrain the scale of possible network topologies and the number of combinations between each hyperparameter (number of hidden neurons, the size of mini-batches and the value of learning rate), one experienced-based and user-defined heuristic thought is adopted that the total number of parameters (the number of weights, the number of biases, the number of input parameter N_{input} and the number of output parameter N_{output}) contained in the neural network should be less than or equal to the number of the training datasets, implying $7N_{hidden}+N_{input}+N_{output}+1\leq 754$ and then $N_{hidden}\leq 107$ where N_{hidden} is the hyperparameter indicating the number of hidden neurons in the hidden layer, $N_{input}=5$ and $N_{output}=1$.

Based on the stated heuristic thought, all hyperparameters (learning rates, mini-batch sizes, and the number of hidden neurons) of ANN are tuned with a particular step size by grid search strategy described in Tab. 4. Since grid search iterates over all possible combinations of hyperparameter values, mini-batch SGD optimization algorithm is used for training multiple ANN models with multiple network topologies by each hyperparameter pair (number of hidden neurons, learning rate, and mini-batch size), giving a total of 770 (10 different numbers of hidden neuron×11 mini-batch sizes×7 learning rates=770) different hyperparameter combinations to construct the optimal neural network model with better generalization and establish the relationship between inputs and output.

Table 4: Defining all possible hyperparameters by grid search

Hyperparameters for ANN	Number of neurons in the hidden layer	Mini-batch size	Learning rate
Grid search	From 10 to 107, step size 11 (10, 21, 32, 42, 53, 64, 74, 85, 96, 107)	From 1 to 754, step size 75 (1, 75, 150, 226, 301, 377, 452, 527, 603, 678, 754)	From 10^{-5} to 10, step factor 10 (0.00001, 0.0001, 0.001, 0.01, 0.1, 1, 10)

The optimum number of hidden neurons does not yield overfitting problems that are caused by using the excessive number of hidden neurons and will degrade the performance of the neural network by slowing down the convergence rate or overestimating the complexity of the problem [Xu, Zhu, Xiao et al. (2014)]. It is vital to know how the ANN model can generalize well to unseen data outside the training data. Mean square error (MSE) is used as the loss function for evaluating the performance of the ANN model. MSE can be calculated as the following equation.

$$\mathrm{MSE}=\frac{1}{N}\sum_{k=1}^{N}(y_k-\hat{y}_k)^2 \tag{7}$$

where y_k and $\hat{y}_k$ are the k[th] values of real (actual) and predicted rates of atmospheric corrosion, respectively, and N represents the number of data records.

The optimization of the network topologies, such as stopping criteria that decides when to stop training a neural network with the lowest generalization error estimated by validation set error, is one of the existing vital challenges to retain the generalization ability of the network instead of memorizing the depth of training history. Different stopping criteria were proposed in Shao et al. [Shao, Taff and Walsh (2011); Prechelt (2012)]. Chaushev et al. [Chaushev, Raynard, Goad et al. (2019); Liu and Ciucci (2020)] adopted early stopping strategy inspired by Prechelt [Prechelt (2012)]. In this work, to improve the generalization of ANN and avoid overtraining, the early stopping strategy [Prechelt (2012)] is implemented as a stopping criterion in which the validation dataset and validation MSE are used to minimize the size of the dimension of each parameter and maximize the probability of finding a good solution to evaluate the performance of hyperparameters whether they are fine-tuned and as a selection strategy for the optimal hyperparameter combination to construct the optimal neural network model with better generalization. The generalization loss over the validation data set during training is calculated by the following equations.

$$\mathrm{GL(t)} = 100 \times \left(\frac{E_{va}(t)}{E_{opt}(t)} - 1\right) > \alpha \tag{8}$$

$$E_{opt}(t) = min\, E_{va}(t')(t' \leq t) \tag{9}$$

where GL(t) is the generalization loss at epoch t (in percent), $E_{va}(t)$ is the mean square error on the validation set measured after epoch t, $E_{opt}(t)$ is the lowest validation set error obtained in epochs up to t and α is the threshold value.

ANN stops training after the first epoch as soon as GL exceeds 20% and one complementary rule for early stopping criteria to guarantee the termination is applied that the training stops after a maximum of 100000 epochs. The final weights and biases after training are used as the analytical tools for the prediction of unseen data.

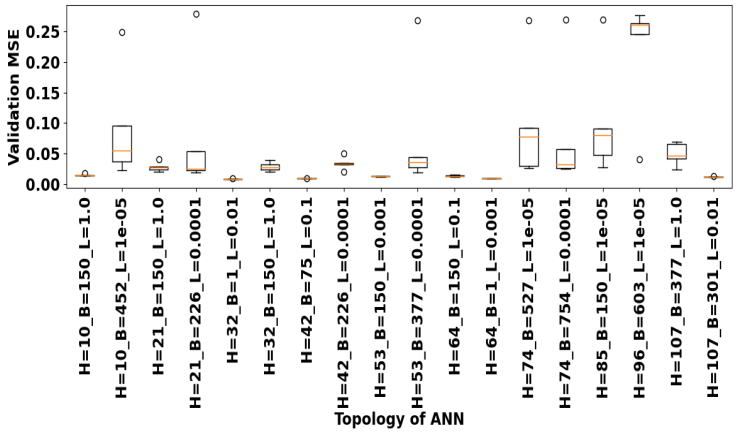

Figure 4: Box plot for the performance of different topologies in the five training runs

The analytical performance of the neural network is repeated for five training runs to remove the uncertainty from the randomly generated weights and biases, giving 3850 topology performance records for the 770 hyperparameter combinations. Fig. 4 represents the performance of some different topologies in five training runs. The results for each hyperparameter combination averaged over all five runs are graphed as a parallel coordinate plot in Fig. 5 which depicts the relationship between the hyperparameters (number of hidden neurons, mini-batch size, and learning rate) and the mean square error values on the validation set. It can be seen that the minimum validation MSE (0.008472) occurs at the point representing the hyperparameter combination of 32-hidden neurons,1-mini-batch size, and 0.01-learning rate along the blue colored line. Thus, the optimal topology of the ANN to predict the atmospheric corrosion of carbon steel can be defined as Tab. 5.

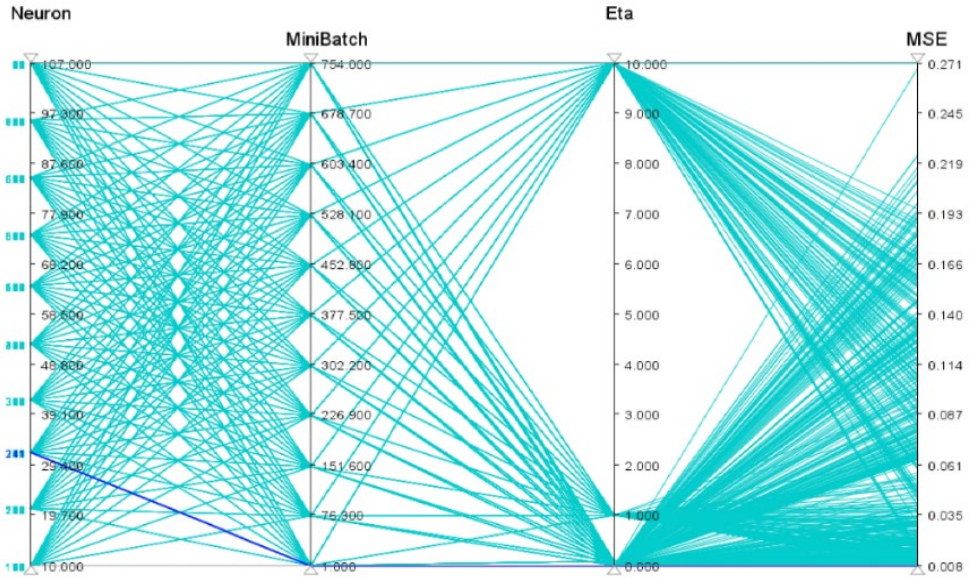

Figure 5: Parallel coordinate plots showing the relationship between hyperparameter combinations (number of hidden neurons (Neuron), mini-batch size (MiniBatch), and learning rate (Eta)) and their corresponding MSE values on validation data

Table 5: The optimized hyperparameters of the optimal ANN model

Hyperparameter	Value
Number of hidden neurons (Hidden Neurons)	32
Mini-batch size (Mini-batch)	1
Learning rate (Eta)	0.01
Epoch (Epoch)	83000

2.2.3 Fuzzy curve analysis

Ranking the importance of meteorological factors on the corrosion rate of metal, specifically carbon steel in this work, provides valuable guidance for the adoption of appropriate procedures to protect the construction made of metal. Sensitivity analysis, change of MSE (mean square error), and fuzzy curves are commonly used to obtain the order of importance of input parameters of ANNs.

The employments of sensitivity analysis and change of MSE (COM) require previous training of ANN. However, the usage of fuzzy curves proposed by Lin and Cunningham [Lin and Cunningham (1994)] is computationally simple, has linear time complexity concerning to the number of input parameters, and needs only the input and output parameters. In this work, fuzzy curves are constructed with data normalized in Section 2.1 to rank the influence of each input on the output.

Assuming a neural network with multiple inputs $\boldsymbol{x_i}$ ($i = 1,2,3,\ldots,n,\ i < n$) and single output y, and taking x_{ik} and y_k as the input and output variables in the k^{th} sample of m training sample set (k=1,2,…,m, k<m) respectively, the fuzzy curves are constructed by a fuzzy membership function u_{ik} in Eq. (10) and the centroid defuzzification function c_i in Eq. (11), respectively, as follows.

$$u_{ik}(x_i) = e^{-\left(\frac{x_{ik}-x_i}{b}\right)^2} \tag{10}$$

$$c_i(x_i) = \frac{\sum_k^m u_{ik}(x_i)\cdot y_k}{\sum_k^m u_{ik}(x_i)} \tag{11}$$

where ($k = 1,2,\ldots,m,\ k < m$), (i=1, 2, 3, …, n, i< n) and b is taken around 10% of the length of the input interval of x_i.

The fuzzy curves plotted in the $x_i - c_i(x_i)$ space can demonstrate whether an individual input has a significant influence on the output or not. The importance of the inputs can be sorted explicitly by the ranges that they cover on fuzzy curves. The input variable that has the most significant impact on the output is obtained with the largest value c_i.

3 Results and discussion

3.1 Conventional models and ANN

The following two evaluation metrics (correlation coefficient (R) and root mean square error (RMSE)) are resorted to measuring the predictivity and the accuracy of the trained ANN model and the conventional models on novel unseen datasets.

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^N (E_i - P_i)^2}{N}} \tag{12}$$

$$\mathrm{R} = \frac{\sum_{i=1}^N (E_i - \overline{E})(P_i - \overline{P})}{\left[\sum_{i=1}^N (E_i - \overline{E})^2 \sum_{i=1}^N (P_i - \overline{P})^2\right]^{1/2}} \tag{13}$$

where E and P are the actual and predicted values of atmospheric corrosion respectively, N is the number of data records used in the models, $\overline{E}$ and $\overline{P}$ are the average values of E and P respectively.

There is a linear relevance, which can determine the reliability of the model, between the actual and predicted atmospheric corrosion rates of carbon steel on the test dataset for three individual models, as illustrated in Fig. 6. Deliberating to the prediction of unseen data, according to Ratner [Ratner (2009)], both of the correlation coefficient R=0.5656 for linear model and the correlation coefficient R=0.68596 (that is higher than the linear model) for Klinesmith models indicate moderate positive linear relationships between predicted and actual atmospheric corrosion rates while our early stopping criteria-based ANN model gives a strong positive linear relationship and a better agreement between them with R=0.78877. Alternatively, the ANN model can explain about 80% (more than 75%) of the variance of the actual value in the forecasting of atmospheric corrosion of carbon steel.

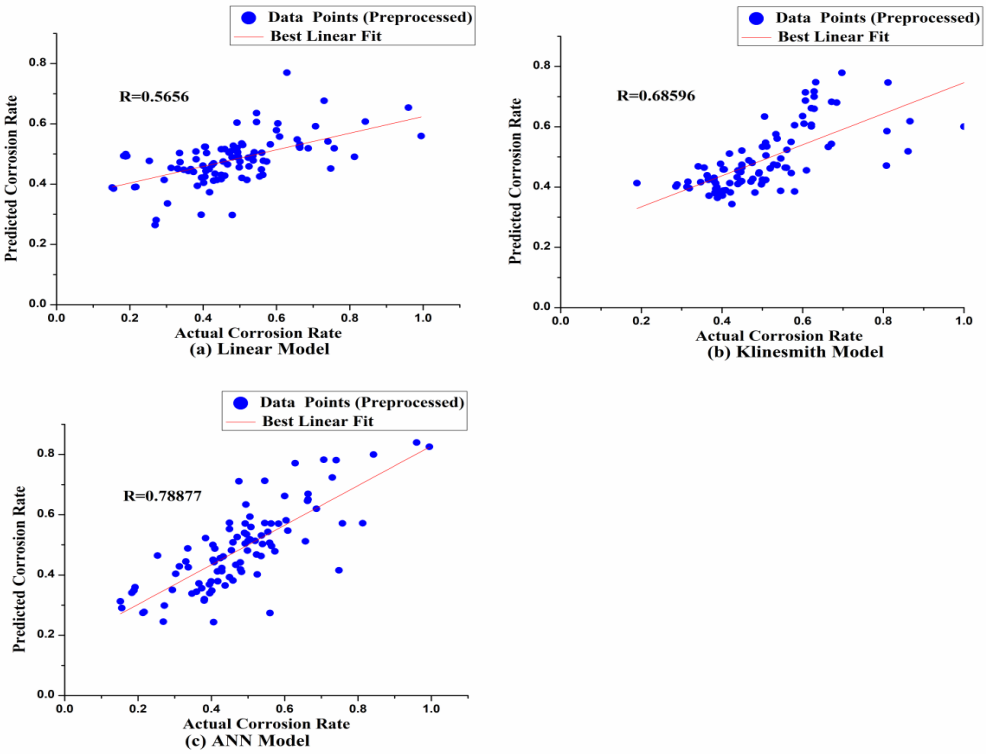

Figure 6: Relevance between the actual and predicted atmospheric corrosion rates of three analytical models on the test dataset

Tab. 6 lists the comparison of evaluation metrics of three models. It can be seen that the RMSE of the linear model (RMSE=0.1356) is the highest value and ANN has a slightly lower RMSE value (RMSE=0.1011) than the Klinesmith model. According to the comparison results of the evaluation metrics for three models for new data, it can be

concluded that the ANN model gives a better performance than conventional models for predicting atmospheric corrosion of carbon steel and the Klinesmith model provides better prediction results than the linear model. Thus, the integration of early stopping method with ANN makes a significant contribution to ANN performance with acceptable generalization.

Table 6: Performance evaluation metrics of three models for test data

Model	RMSE	Correlation Coefficient (R)
Linear Model	0.1356	0.5656
Klinesmith Model	0.1027	0.68596
ANN	0.1011	0.78877

Despite using a large dataset in this work, those data were measured from different sources by different methods so that corrosion data might have inherently scattered. Although this work does not consider other possibly more critical parameters on atmospheric corrosion (such as the effect of microclimate) for the prediction model, it can be seen that ANN can still give more satisfactory results by its fault-tolerance ability than the conventional analytical models.

3.2 Fuzzy curve analysis

The fuzzy curve is used as an input ranking method to evaluate the influence of each climatological variable and each pollution parameter on the atmospheric corrosion of carbon steel. The fuzzy curve is derived from fuzzy theory, which is still be applied successfully in many areas [Wang, Wang, Zheng et al. (2018)]. A plot of the fuzzy curves constructed for atmospheric corrosion is presented in Fig. 7 and each input variable is expressed with the corresponding range of c_i in the legend. The significance of the input variable is ranked by the range of c_i such that the input variable with a broader range has a higher impact on the atmospheric corrosion. Fig. 8 shows the different ranges of all fuzzy curves for each input parameter. In this work, the ranking of the influence of input variables on the atmospheric corrosion can be defined as TOW>Cl^->SO_2>T>Year which is conformed to the fact that TOW, Cl^- and SO_2 are the most significant meteorochemical variables with a well-known nonlinear relationship in atmospheric corrosion of carbon steel [Pintos, Queipo, de Rincón et al. (2000)].

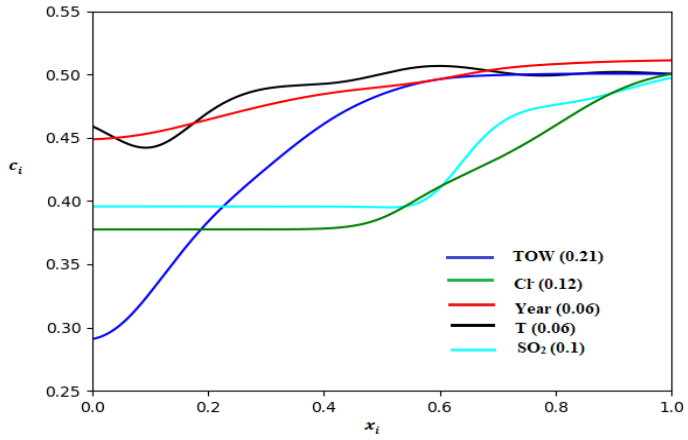

Figure 7: Fuzzy curves determining the influence of each input parameter on atmospheric corrosion rate

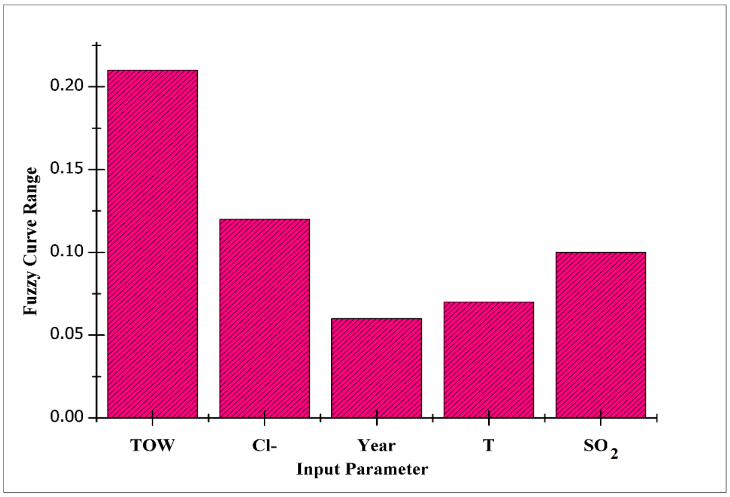

Figure 8: Plot showing the ranges of all fuzzy curves for all input parameters

4 Conclusions

In this work, the result of the linear model exploits its weaknesses of being still not perfect, limited to capture non-linearities of data, and its poor ability to handle a large amount of data. The Klinesmith model predicts acceptable results by considering the impact of possible environmental variables. Thanks to the abilities of noise-tolerance and fault-tolerance, our stopping criteria-based ANN model yields the most satisfactory result among three models so that ANN can deal well with real-world data that are somewhat noisy, uncertain, complex and incomplete, and is an appropriate solution to complicated problems to give the satisfactory result.

It is expected that ANN can also be used as an analytical model for high-throughput experiment data that are quite different from traditional data. The nature of non-linearity, complexity, data similarity and data accumulation of high-throughput data can decrease the performance of existing analytical models. Some new methods may be applied to our prediction model to get the robust result [Yu, Liu, Xiao et al. (2019)]. To highlight the significance of ANN, it is a typical state-of-the-art application to solve the prediction problems in materials science by considering more affecting parameters and more accurate data.

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References

Ashtiani, H. R. R.; Shahsavari, P. (2016): A comparative study on the phenomenological and artificial neural network models to predict hot deformation behavior of AlCuMgPb alloy. *Journal of Alloys and Compounds*, vol. 687, pp. 263-273.

Cai, J.; Cottis, R. A.; Lyon, S. B. (1999): Phenomenological modelling of atmospheric corrosion using an artificial neural network. *Corrosion Science*, vol. 41, no. 10, pp. 2001-2030.

Cao, A.; Zhu, Q.; Zhang, S.; Hou, B. (2010): BP neural network predictive model for stray current density of a buried metallic pipeline. *Anti-Corrosion Methods and Materials*, vol. 57, no. 5, pp. 234-237.

Castaño, J. G.; Botero, C. A.; Restrepo, A. H.; Agudelo, E. A.; Correa, E. et al. (2010): Atmospheric corrosion of carbon steel in Colombia. *Corrosion Science*, vol. 52, no. 1, pp. 216-223.

Chaushev, A.; Raynard, L.; Goad, M. R.; Eigmüller, P.; Armstrong, D. J. et al. (2019): Classifying exoplanet candidates with convolutional neural networks: application to the next generation transit survey. *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 4, pp. 5232-5250.

Chico, B.; De la Fuente, D.; Díaz, I.; Simancas, J.; Morcillo, M. (2017): Annual atmospheric corrosion of carbon steel worldwide. An integration of ISOCORRAG, ICP/UNECE and MICAT databases. *Materials*, vol. 10, no. 6, pp. 601.

Corvo, F.; Haces, C.; Betancourt, N.; Maldonado, L.; Véleva, L. et al. (1997): Atmospheric corrosivity in the Caribbean area. *Corrosion Science*, vol. 39, no. 5, pp. 823-833.

Demuth, H. B.; Beale, M. H.; Jess, O. D.; Hagan, M. T. (2014): Neural network design. Martin Hagan.

Forcellese, A.; Gabrielli, F.; Simoncini, M. (2011): Prediction of flow curves and forming limit curves of Mg alloy thin sheets using ANN-based models. *Computational Materials Science*, vol. 50, no. 11, pp. 3184-3197.

Graupe, D. (2013): *Principles of Artificial Neural Networks*. World Scientific Pub. Co. Inc.

Hou, W.; Liang, C. (1999): Eight-year atmospheric corrosion exposure of steels in China. *Corrosion*, vol. 55, no. 1, pp. 65-73.

Jančíková, Z.; Zimný, O.; Koštial, P. (2013): Prediction of metal corrosion by neural networks. *Metalurgija*, vol. 52, no. 3, pp. 379-381.

Kenny, E. D.; Paredes, R. S. C.; de Lacerda, L. A.; Sica, Y. C.; de Souza, G. P. et al. (2009): Artificial neural network corrosion modeling for metals in an equatorial climate. *Corrosion Science*, vol. 51, no. 10, pp. 2266-2278.

Klinesmith, D. E.; McCuen, R. H.; Albrecht, P. (2007): Effect of environmental conditions on corrosion rates. *Journal of Materials in Civil Engineering*, vol. 19, no. 2, pp. 121-129.

Knotkova, D.; Boschek, P.; Kreislova, K. (1995). Results of ISO CORRAG program: processing of one-year data in respect to corrosivity classification. Atmospheric corrosion. *Symposia Papers & STPs. ASTM International*.

Li, D.; Lv, R.; Si, G.; You, Y. (2017): Hybrid neural network-based prediction model for tribological properties of polyamide6-based friction materials. *Polymer Composites*, vol. 38, no. 8, pp. 1705-1711.

Li, L.; Qiu, P.; Xing, S. B.; Su, X. (2013): Research on corrosion rate prediction of aluminum alloys in typical domestic areas based on BP artificial neural network. *Advanced Materials Research*, vol. 652, pp. 1088-1091.

Lin, Y.; Cunningham, G. A. (1994). A fuzzy approach to input variable identification. *Proceedings of IEEE 3rd International Fuzzy Systems Conference*.

Liu, J.; Ciucci, F. (2020): The deep-prior distribution of relaxation times. *Journal of The Electrochemical Society*, vol. 167, no. 2, 026506.

Lo, C. M.; Chiu, Y. P.; Lin, M. D. (2017). Predicting atmospheric corrosion rates of copper in Taiwan industrial zones using artificial neural network. *IEEE International Conference on Industrial Engineering and Engineering Management*.

Morales, J.; Martín-Krijer, S.; Díaz, F.; Hernández-Borges, J.; González, S. (2005): Atmospheric corrosion in subtropical areas: influences of time of wetness and deficiency of the ISO 9223 norm. *Corrosion Science*, vol. 47, no. 8, pp. 2005-2019.

NIMS (2018): *Corrosion Data Sheet (CoDS)*. National Institute for Materials Science. https://smds.nims.go.jp/.

Panchenko, Y. M.; Marshakov, A. I. (2017): Prediction of first-year corrosion losses of carbon steel and zinc in continental regions. *Materials*, vol. 10, no. 4, pp. 422.

Pintos, S.; Queipo, N. V.; de Rincón, O. T.; Rincón, A.; Morcillo, M. (2000): Artificial neural network modeling of atmospheric corrosion in the MICAT project. *Corrosion Science*, vol. 42, no. 1, pp. 35-52.

Prechelt, L. (2012): *Early Stopping-But When*? Springer Berlin Heidelberg.

Rajendraboopathy, S.; Sasikumar, T.; Usha, K.; Vasudev, E. (2009): Artificial neural network a tool for predicting failure strength of composite tensile coupons using acoustic emission technique. *The International Journal of Advanced Manufacturing Technology*, vol. 44, no. 3-4, pp. 399-404.

Ratner, B. (2009): The correlation coefficient: Its values range between+1/−1, or do they? *Journal of Targeting, Measurement and Analysis for Marketing*, vol. 17, no. 2, pp. 139-142.

Reddy, N. (2014): Neural networks model for predicting corrosion depth in steels. *Indian Journal of Advances in Chemical Science*, vol. 2, no. 3, pp. 204-207.

Sadowski, L. (2013): Non-destructive investigation of corrosion current density in steel reinforced concrete by artificial neural networks. *Archives of Civil and Mechanical Engineering*, vol. 13, no. 1, pp. 104-111.

Shao, Y.; Taff, G. N.; Walsh, S. J. (2011): Comparison of early stopping criteria for neural-network-based subpixel classification. *IEEE Geoscience and Remote Sensing Letters*, vol. 8, no. 1, pp. 113-117.

Sun, L.; Qi, F.; Hou, Z.; Xiao, Y. (2007). The prediction of Sn-Ag solder properties based on BP algorithm of artificial neutral network. *8th International Conference on Electronic Packaging Technology*.

Townsend, H. E. (2002): Estimating the atmospheric corrosion resistance of weathering steels. *ASTM Special Technical Publication*, vol. 1421, pp. 292-300.

Vera, R.; Ossandón, S. (2014): On the prediction of atmospheric corrosion of metals and alloys in Chile using artificial neural networks. *International Journal of Electrochemical Science*, vol. 9, no. 12, pp. 7131-7151.

Wang, X. F.; Wang, L.; Zheng, Y. H.; Wang, J. (2018): An event-driven plan recognition algorithm based on intuitionistic fuzzy theory. *Journal of Supercomputing*, vol. 74, no. 12, pp. 6923-6938.

WCO (2020): *Bringing Corrosion Awareness to the Public*. World Corrosion Organization. http://corrosion.org/Corrosion+Resources/Videos.html.

Willumeit, R.; Feyerabend, F.; Huber, N. (2013): Magnesium degradation as determined by artificial neural networks. *Acta Biomaterialia*, vol. 9, no. 10, pp. 8722-8729.

Xu, Y.; Zhu, Y.; Xiao, G.; Ma, C. (2014): Application of artificial neural networks to predict corrosion behavior of Ni-SiC composite coatings deposited by ultrasonic electrodeposition. *Ceramics International*, vol. 40, no. 4, pp. 5425-5430.

Yang, X. W.; Zhu, J. C.; Lai, Z. H.; Kong, Y. R.; Zhao, R. D. et al. (2012): Application of artificial neural network to predict flow stress of as quenched A357 alloy. *Materials Science and Technology*, vol. 28, no. 2, pp. 151-155.

Yıldızel, S.; Öztürk, A. (2016): A study on the estimation of prefabricated glass fiber reinforced concrete panel strength values with an artificial neural network model. *Computers, Materials & Continua*, vol. 52, no. 1, pp. 42-51.

Yu, F.; Liu, L.; Xiao, L.; Li, K.; Cai, S. (2019): A robust and fixed-time zeroing neural dynamics for computing time-variant nonlinear equation using a novel nonlinear activation function. *Neurocomputing*, vol. 350, pp. 108-116.

Zhang, A.; Lipton, Z. C.; Li, M.; Smola, A. J. (2020): Dive into deep learning. http://www.d2l.ai.

Zhang, M.; Yu, J. F.; Yang, S. W.; He, X. L. (2011): Analysis in atmospheric corrosion behavior of bainite steel exposed in offshore platform based on the artificial neural network. *Advanced Materials Research*, vol. 291-294, pp. 1212-1216.

Zhao, N.; Li, Z. (2017): Experiment and artificial neural network prediction of thermal conductivity and viscosity for alumina-water nanofluids. *Materials*, vol. 10, no. 5, pp. 552.