ISSN 2070-2051, Protection of Metals and Physical Chemistry of Surfaces, 2009, Vol. 45, No. 5, pp. 610–615. © Pleiades Publishing, Ltd., 2009.

INVESTIGATION METHODS FOR PHYSICOCHEMICAL SYSTEMS

Prediction of Time to Failure in Stress Corrosion Cracking of 304 Stainless Steel in Aqueous Chloride Solution by Artificial Neural Network[1]

S. A. Lajevardi[a], T. Shahrabi[a], V. Baigi[a], and A. Shafiei M[b]

[a] *Department of Materials Engineering, Tarbiat Modares University, Tehran, Iran*

[b] *Department of Materials Science and Engineering, Sharif University of Technology, Tehran, Iran*

e-mail: tshahrabi34@modares.ac.ir

Received June 09, 2008

Abstract—Despite the numerous researches in Stress Corrosion Cracking (SCC) risk of austenitic stainless steels in aqueous chloride solution, no formulation or reliable method for prediction of time to failure as a result of SCC has yet been defined. In this paper, the capability of artificial neural network for estimation of the time to failure for SCC of 304 stainless steel in aqueous chloride solution together with sensitivity analysis has been expressed. The output results showed that artificial neural network can predict the time to failure for about 74% of the variance of SCC experimental data. Furthermore, the sensitivity analysis also demonstrated the effects of input parameters (Temperature, Applied stress and Cr concentration) on SCC of 304 stainless steel in aqueous chloride solutions.

PACS numbers: 84.35.+i, 61.20.Mk

DOI: 10.1134/S2070205109050207

INTRODUCTION

Although austenitic stainless steels have an excellent general corrosion resistance in water, but they are susceptible to chloride stress corrosion cracking (C1–SCC) under specific stress and environmental conditions and limits their usability in some elevated temperatures and/or oxygenated environments at certain chloride levels [1]. Until now, most of the parameters which are effective to cause SCC on stainless steels have been identified but a specific formula is not found to estimate the time to failure. Therefore, a researcher should test a specimen in an aqueous solution to find its SCC resistance in the given environment but if a parameter changes shortly then taking decision about the risk of SCC would be very difficult. In spite of the numerous studies about SCC on austenitic stainless steels, the lack of an effective tool to predict the time to failure as a result of SCC has still been felt.

Artificial Neural Networks (ANNs) are computational systems that correlate a pattern between groups of input observations (real data) and a group of output observations (results). This technique could be useful aids for making corrosion predictions from laboratory data. More recently, artificial neural systems have aroused interest and many examples have been reported in the field of corrosion.

One of the first attempts to implement a Neural Network (NN) for solving a corrosion problem was that of Smets and Bogaerts [1], which employed the features of the NN to predict the risk of stress corrosion cracking for AISI 304 stainless steel. They developed a neural network to evaluate the SCC risk by temperature, chloride concentration and oxygen content and the effect of their combinations by probability of 20%, 50%, and 80%. The aim of this study was to predict the influence of all three factors on SCC risk at the same time by means of an umbrellalike network. The network was composed of two and three input neurons, two output neurons, and two hidden layers. At the input layer, temperature (20–370°C) and chloride content (0.02–10 000 ppm) for the first network and oxygen (0.01–1200 ppm) and chloride content (0.1–1000 ppm) for the second network and combined parameters for third network have been used respectively. The authors showed the feasibility of this approach to predict the susceptibility of AISI 304 to SCC. They defined SCC and NO SCC regions as well as delimit regions where the risk of the onset of SCC increases.

Lu and Urquidi-Macdonald [2] designed a NN for describing the intergranular stress corrosion cracking of AISI 304 sensitized stainless steel at high temperature in aqueous solutions. The network predicted the growth rate of the crack as a function of oxygen concentration, flow rate, stress intensity, hydrogen concentration and corrosion potential (E_{corr}). These NN predictions were compared with real experimental data, derived from the coupled environment fracture deter-

[1] The article is published in the original.

ministic model showing reasonably good agreement between the two approaches.

Silverman and Rosen [3] developed a NN, supported by an expert system to predict corrosion from polarization diagrams. The objective was to predict the type of corrosion from the shape of the polarization curve, since polarization curves are commonly used to characterize the corrosion behavior of an alloy in a given environment. The authors employed the characterizing parameters derived from the polarization curves as the input to the first network. At the output, the network predicted the occurrence of crevice corrosion, pitting or uniform attack.

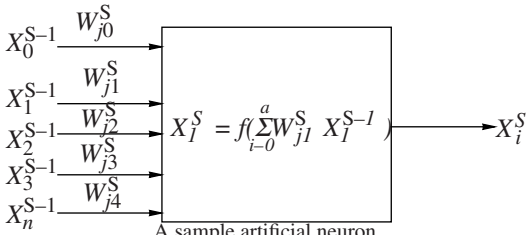
Jianping Cai, R.A. Cottis, and S.B. Lyon [4] developed a NN model to predict the atmospheric corrosion of steel and zinc. The network estimated the corrosion depth as a function of temperature, time of wetness, sulphur dioxide concentration, chloride concentration and exposure time. Multiple correlation coefficient (R) showed that the neural network could account for about 70% of the variance in the corrosion data for steel and zinc. This result was better than that of the previous linear regression studies. Sensitivity analysis also demonstrated the effects of sulphur dioxide, chloride and exposure time on atmospheric corrosion in specific environments. Sensitivity analysis was a useful technique to demonstrate the effects of affecting variables and suggest corrosion mechanism as well.

In this study, the time to failure due to chloride SCC on stainless steel AISI 304 in hot aqueous chloride media and sensitivity analysis have been estimated by ANN technique. The database used for training the NNs was chosen by collecting data of many reliable references.

ARTIFICIAL NEURAL NETWORKS (ANNS)

There are different types of ANNs that have been applied to a number of situations [5–7]. The foundations of all of them are the processing elements, also called neurons, which are interconnected and operate in parallel [1]. These elements are constructed so that they combine a number of inputs by a simple summation, modify them by some type of transfer function (usually a Sigmond function), and then send the result as output either to another processing element or out of network (Fig. 1) [1, 3]. Each of the input value is multiplied by a weight prior to being summed and then the transfer function is applied.

Although, there are different types of ANNs, feed-forward multilayer perception is probably the most widely used due to its powerful modeling capability. It consists of three layers: the input, the hidden and the output layers. The input layer contains the properly scaled input observables upon which the network is trained. In this case, the input layer contains some of important experimental parameters in SCC researches, e.g. Temperature, Chloride ions concentrations and



X_j^S	Current output slate of jtn neuron in layer S
W_{j-1}^S	Weight on connection joining ith neuron in layer (S–1) to jth neuron in layer S
$f(x)$	Transfer function

Fig. 1. Back-propagation processing element. The weights are multiplied by each of the inputs, summed together, and passed through the sigmoid to produce the output

Applied stress. The summation of the inputs time's weights is performed in each of the processing elements in the hidden layer, and the output is sent on either another hidden layer or directly to the output layer. In this case, the output layer contains the time of failure due to SCC.

A neural network is not programmed but trained [1]. The algorithm used for supervised learning of the neural network in this paper is based on the mostly used back-propagation method. In this algorithm attempts to find a set of weights such that the sum of the square of the differences between the actual outputs and those calculated from the neural network for the training set are minimized.

To evaluate the test result, the multiple correlation coefficient (R) is used in this study:

$$R = \frac{\sum_k (\hat{y}_k - \bar{y})(y_k - \bar{y})}{\sqrt{\sum_k (\hat{y}_k - \bar{y})^2 \sum_k (y_k - \bar{y})^2}}, \quad (1)$$

where y is the average of the time to failure which observed, y_k is the predicted value of the k^{th} y and y_k is the actual value of the k^{th} y, N is the number of y.

DATABASE

All of data in database were extracted of references [8–31] and they divided to two sets: first set contains 80% of database to train the network and another set that contains 20% of database to test the trained network. Variables used include temperature, chloride ions concentration, applied stress and time of the failure. Table 1 lists the range of the variables data used in this work.

PROCESS OF TRAINING AND TESTING

This section presents an Artificial Neural Network (ANN) model for the prediction of the time to failure of

Table 1. Characteristics of the database used to train the neural networks

Variable	Min. Value	Max. Value
Temperature (°C)	300	300
Chloride ions (ppm)	0.1	4000
Applied stress (MPa)	500	500

Table 2. Features of neural networks in this study

ANN characteristic	Feature
No. of neuron in Input layer	3
No. of neuron in Hidden Layer	8 (4–4)
No. of neuron in Output Layer	1
Transfer function	Sigmoid
Minimization algorithm	Gradient

AISI 304 due to SCC as a function of relevant experimental variables (T, Cr, a) in this study. The ANN topology in this study showed in Fig. 2.

The fundamental characteristics of the ANN model used in the present work are listed in Table 2.

Before the neural network is trained, all data in the database are scaled to fit within the interval 0 to 1, which is a fundamental operation prior to training known as data ho-mogenization. Input variables were scaled to be as closed to the range of 0 to 1 as possible. For example, the chloride ions concentration was changed to their base 10 algorithm. Such scaling was used in output layer to change in the range of 0 and 1. These arrangements aids in successful convergence of the regression. Most of the analysis was done using a network containing one output and variable hidden layers and related nodes. The network was first trained with all three input variables using one, two, three or four nodes in one and two hidden layers. The normal procedure is to start with a single hidden layer and few processing elements and then choose the network which gives acceptable performance and training time. Therefore, sixteen training topology were repeated to achieve a lowest error. The database was divided into three data sets: training set (No. 1), validation set (No. 2), and test set (No. 3) containing 80%, 10%, and 10% data of database respectively.

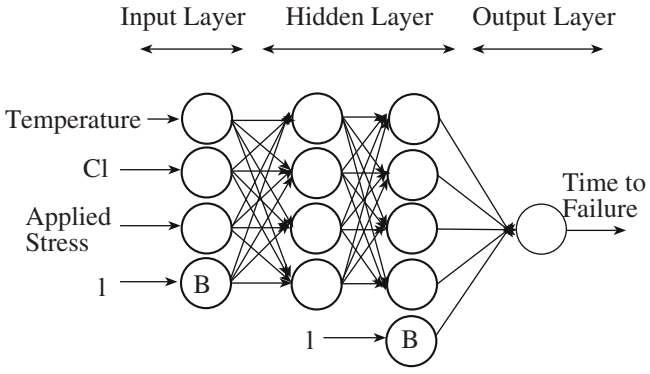


Fig. 2. Artificial neural network topology.

The learning process was conducted using as optimization procedure the standard Back-propagation algorithm, with weight updates each time the complete learning data set was considered. The initial sets of weights were obtained using Montecarlo optimization, hence reducing the possibility of getting trapped in local optima. For a given set of initial weights, the learning process was stopped when the mean square error in the validation data set started to grow for additional number of iterations in the optimization procedure. The best set of weights was selected as the one with the lowest possible mean square error and relative good performance on the validation data test.

RESULTS AND DISCUSSION

5. 1. Training and Test

The final weights matrix between any two layers (sub-layer) is shown as follows:

The matrix between the input layer and the first hidden layer:

$$W^1 = \begin{bmatrix} 0.1425 & -0.0031 & 1.8102 & 2.0834 \\ 3.2680 & 0.7787 & -1.9911 & 0.4114 \\ 2.6003 & 0.0855 & 1.3763 & -0.0006 \\ -1.9333 & 0.6431 & -3.0598 & 1.2481 \end{bmatrix}.$$

The matrix between the first and the second hidden layer:

$$W^2 = \begin{bmatrix} 0.4203 & 1.4195 & -3.5519 & 0.0003 \\ 1.5377 & 0.6231 & -0.0041 & 2.5108 \\ -2.116 & 1.9862 & -2.5117 & 0.4287 \\ 1.6662 & -3.1028 & 0.0023 & 0.9286 \end{bmatrix}.$$

The matrix between the second hidden layer and the output layer:

$$W^3 = \begin{bmatrix} 0.0224 & -0.6149 & 1.9732 & -3.3349 & 2.0001 \end{bmatrix}.$$

The trained network was evaluated by multiple correlation coefficients (R). The results show that the average correlation coefficient for the designed ANN model is approximately 74%. Therefore, the ANN model can account for more than 70% of the variance of the experimental value in estimation of time to failure (Table 3).

Figure 3 illustrate the predicted data from ANN and the actual time of failure data.

5.2. Sensitivity Analysis

In aqueous chloride environments, applied stress, chloride ions concentration, and temperature have significant effects on SCC of AISI 304. Sensitivity analysis conducted on the trained neural network shows the effects of all parameters in Figs. 4–6. In these figures, the neural network separates the effects of any parameter from other variables and simulates the effects of each individual factor.

Figure. 4 shows that, in the specified condition, the relation between temperature and time to failure on SCC of AISI 304 is almost polynomial grade two. On the other hand, this demonstrates the time to failure is strongly decreased at a critical temperature. The austenitic stainless steel, type 304, that is ductile material, has a brittle fracture appearance, whenever transgranular stress corrosion cracking (TGSCC) and intergranular stress corrosion cracking (IGSCC) take place. In order for the brittle fracture to take place, a dislocation movement in the grains, which can occur over several grains and more, needs to be inhibited by an obstacle. It seems up to 180°C (critical temperature) the time to failure decreased due to increasing in corrosion rate, and then decreased due to collapse of dislocations.

Figure 5 demonstrates the effect of applied stress on the time to failure. For 304 stainless steel passive film formed at crack tips and on the other surface, serves as the obstacle of the dislocation movement. In the case of the sensitized specimens, Cr carbides formed along the grain boundaries also serve as the obstacle as well as the film and hence the dislocation movement would be limited within one grain. For that reason, grain boundary sliding (GBS) would, therefore, be significantly predominant for the sensitized specimens instead of the dislocation movement in the grains. It seems that applied stress is the most effective parameter on passive film rupture for 304 stainless steel and in high applied stress value, the time to failure will dramatically decrease.

Table 3. ANN efficiency in this work

Training sets	Correlation coefficient (R)
Training Set No. 1	0.788
Training Set No. 2	0.712
Training Set No. 3	0.724
Average of Sets	0.741

In Fig. 6, the relation between chloride ions concentration and time to failure due to SCC in 304 stainless steel is shown. Unfortunately the trend of this figure is more complex and result extraction of that is impossible.

Thus, sensitivity analysis can demonstrate the effect of variables and suggest possible mechanisms or future research direction. Furthermore, this analysis makes a view of other related parameter which is not considered.

5.3. Errors and Variations

There are still considerable unexplained variances in the neural network prediction. Such unexplained variances are mainly attributable to three reasons:

a) Ignorance of other affecting variables

b) scattered data

c) Different ways of estimation or extraction of data

Although applied stress, temperature and chloride ions concentration are the most important parameters but some other parameters such as pH and cations in the solution might have some effects but these were not

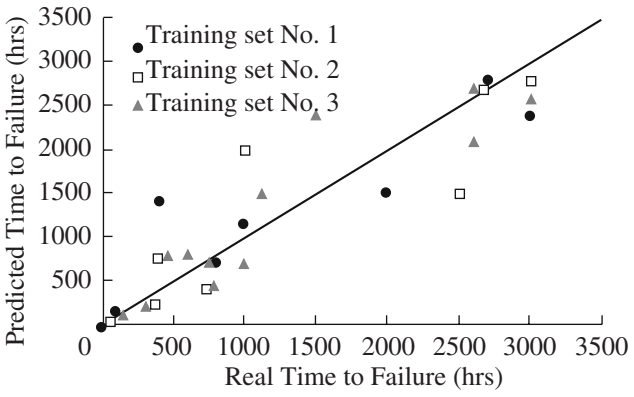


Fig. 3. Real time to failure in SCC versus the predicted amounts by designed ANN model.

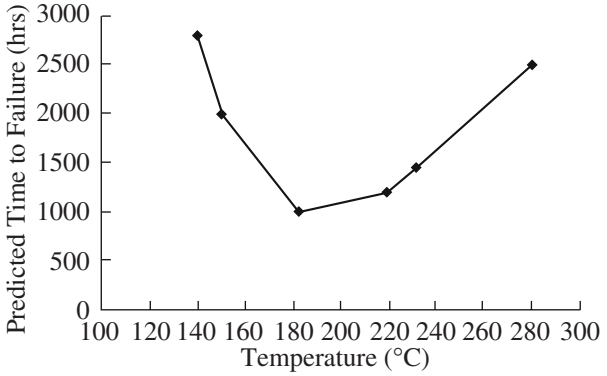


Fig. 4. Effect of temperature on time to failure (Cl^- = 2500 ppm and a = 100 MPa.)

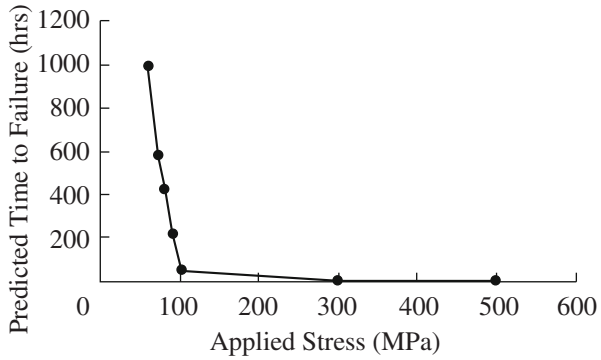


Fig. 5. Effect of applied stress on time to failure (Cl^- = 2100 ppm and a = 130 MPa).

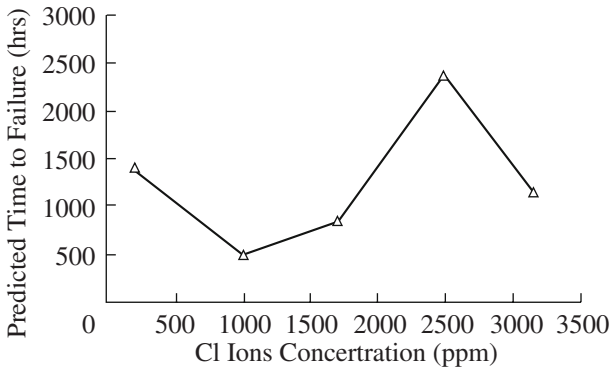


Fig. 6. Effect of chloride ions concentration on time to failure (T = 150°C and o = 150 MPa).

considered in this work because of the shortage of reliable data. Furthermore, other sources of errors in this study are as follows:

d) Some data were not very exact and accurate

e) The range of data extraction was not uniform

f) Test specimens have not been exactly the same in all the experiments. Nevertheless, the neural network has a strong capability of fault-tolerance and it is expected that the modeling capability of the neural network will increase with the consideration of the more affecting factors and the availability of the more accurate data.

6. CONCLUSIONS

The application of an artificial neural network for modeling of the occurrence of stress corrosion cracking is promising. In this work, ANN can be applied for the estimation of the time to failure of AISI 304 in aqueous chloride solutions.

Using the proposed solution methodology an ANN model was constructed and evaluated using the collection of experimental data associated with the SCC of AISI 304 as a function of temperature, chloride ions concentration and applied stress.

Artificial neural network accounts for about 74% of the variance of the SCC real data. This result is better than previous studies.

Sensitivity analysis is a useful technique to demonstrate the effects of the important variables and shows the probable effects of the other affecting variables.

REFERENCES

1. Smets, M.G, Bogaerts W.F.L., *Corrosion*, 1992, v. 48, p. 618.
2. Lu, P.C., Urquidi-Macdonald, M., *Corrosion'94*, NACE, Baltimore, MD, USA, 1994, February–March, no. 151.
3. Rosen, E.M. and Silverman, D.C., *Corrosion*, 1992, v. 48, p. 734.
4. Cai, J., Cottis, R.A., and Lyon, S.B., *Corrosion Sci.*, 1998, v. 1, p. 2001.
5. Karmer, M.A. and Leonard, J.A., *Computers Chem. Eng.*, 1990, v. 14, p. 1323.
6. Lippmann, R.P., *IEEE ASSAP Magazine*, 1987, v. 4, p. 46.
7. Rumelhart, D.E. and McClelland, J.L., MIT press, 1986, v. 84.
8. Shreir, L.L., Jarman, R.A., and Burstein, G.T., *Corrosion*, Bodmin: Great Britain by Hartnolls, 1993, v. 1, p. 52.

9. Stachle, R.W., Hochman, J., McCright, R.D., and Slater, J.E., NACE, Houston, USA, 1977, p. 380.
10. Sprowls Donald, O., *Stress Corrosion Cracking*, ASTM, 1998, ch. 17, p. 365.
11. Uhlig, H.H., NACE, Houston, USA, 1969, p. 86.
12. Blackburn, M.J., Symrl, W.H., and Feency, J.A., NRL, Washington DC, USA, 1972, p. 271.
13. McMinn, A., Burghard, H.C., Lyle, F.F., and Leverant, G.R., NACE, Houston, USA, 1984, p. 243.
14. Bursle, A.J. and Pugh, E.N., TMS-ALME, Warrendale, USA, 1977.
15. Cottis, R.A. and Tagi, E.A., HMSO, London, UK, 1987, no. 483.
16. Tamaki, K., Tsujikawa, S., and Hisamatsu, Y., NACE (in press), Houston, USA.
17. Logan, H.I., N.Y.: John Wiley & Sons, 1966.
18. Trumn, J.E., Stainless Steel, ISI publication 117, Iron and Steel Institute, 1969, p. 101.
19. Denhard, E.E. and Gaugh, R.R., STP 425, American Society for Testing and Materials, 1967, p. 41.
20. Stress Corrosion Testing, American Society for Testing and Materials, 1967.
21. Sedriks, A.J., Office of Naval Research, ASTM, 1990.
22. Latanision, R.M. and Staehle, R.W., NACE, Houston, USA, 1969.
23. Copson, H.R., N.Y.: Interscience Publishers, 1959, p. 247.
24. Hoar, T.P., NACE, Houston, USA, 1969, p. 98.
25. Boyd, W.K., NACE, Houston, USA, 1969, p. 593.
26. Scully, J.C., NATO, Brussels, Belgium, 1971.
27. Kawashima, A., Agrawal, A.K., and Staehle, R.W., STP 665, ASTM, Philadelphia, USA, 1979, p. 266.
28. Trumn, J.E., British Nuclear Energy Society Symposium on Effects of Environment on Material Properties in Nuclear Systems, Institute of Civil Engineers, July 1971, paper no. 10.
29. Copson, H.R., Interscience, 1959, p. 247.
30. Shreir, L.L., Jarman, R.A., and Burstein, G.T., *Corrosion*, Bodmin: Great Britain by Hartnolls, 1993, v. 1, p. 3.
31. Betts, A J. and Boulton, L.H., *British Corrosion Journal*, 1993, v. 28, p. 279.