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Prediction of primary water stress corrosion crack growth rates in Alloy 600 using artificial neural networks

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ABSTRACT

After reviewing of the data for primary water stress corrosion cracking (PWSCC) for Alloy 600 in the literature, a crack growth rate (CGR) database was assembled, and an ANN model was developed and trained upon the data, in order to model PWSCC in Alloy 600. The dependence of PWSCC CGR on each of the principal independent variables of the system has been predicted. Sensitivity analyses were conducted via "fuzzy logic" and the importance of each variable was analyzed and show that IGSCC in Alloy 600 is primarily mechanical in character with the electrochemistry being a significant contributor.

1. Introduction

Ni-based Alloy 600 has been used widely for steam generator (SG) tubing and penetration nozzles for the control rod driving mechanism (CRDM), and for other pressure boundary components, in pressurized water reactors (PWR), because of its good corrosion resistance. However, there have been many reports of intergranular stress corrosion cracking (IGSCC) in "mill-annealed" Alloy 600 resulting in component failure after long-term operation in PWR primary environments. The first such corrosion mechanism to cause concern in PWRs was IGSCC from the primary side of "hot leg" steam generator tubes in contact with the primary coolant ($LiOH/H_3BO_3$ at 290–330 °C), which has become known in the nuclear power industry as primary water stress corrosion cracking (PWSCC). This phenomenon is of great importance, considering the safety issues involved and the costs to the consumer and operator, alike. The problem could be significantly alleviated if a model was available that could precisely predict the crack growth rate (CGR), because then repairs might be affected during scheduled outages, so as to avoid costly, unscheduled outages, the cost of which is not built into the price of the product. However, it is well known that CGR in Alloy 600 is controlled by many properties of the system, reflecting a complex combination of stress, environment, and a susceptible material. It is extremely difficult to study the influences of all possible parameters by independent experiment, due to the difficulty in controlling or even measuring a large number of independent variables simultaneously in the high pressure, high temperature aqueous environment. Many studies have focused on the establishment of PWSCC models and their use in predicting CGR. Empirical/phenomenological models, including the Scott model [1]; the similar Materials Reliability Program, MRP-55, model [2]; and the MRP-115 model for weld metal [3] have been developed for this alloy/environment system. Recently, a theoretical model known as the Fracture Research Institute (FRI) model has been proposed by Shoji and other researchers from Tohoku University [4]. The FRI model incorporates both electrochemistry and fracture mechanics considerations, although the inclusion of electrochemical factors is somewhat inadvertent in that the model is calibrated on CGR data that are clearly affected by the electrochemistry of the system. The FRI model does not incorporate the electrochemistry of the system explicitly. Thus, none of these models incorporate explicitly electrochemical mechanisms, such as that embodied in the Mixed Potential Model (MPM) for estimating the electrochemical corrosion potential (ECP), or for the purpose of describing ion transport down a crack or within the external environment. However, the coupled-environment fracture model (CEFM), which was developed by Macdonald et al. [5,6] for calculating CGR in sensitized Type 304SS in light water reactor (LWR) coolant environments, does incorporate physico-electrochemical–mechanical factors with emphasis on both the mechanics and electrochemistry of the system. This model, which is based on the differential aeration hypothesis, takes into account both electrochemical and mechanical processes, with crack advance being assumed to occur through the slip/dissolution/repassivation mechanism augmented by hydrogen-induced fracture (HIF), and the basis of this model is a statement of charge conservation and Faraday's law of charge-mass equivalency. These

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constraints render the model deterministic, due to the fact that the predictions are constrained to "physical reality" by the relevant natural laws.

A major problem in qualifying models for predicting CGR in Alloy 600 (and other alloys) is that CGR data, when shown in two-dimensional plots (e.g., CGR versus extent of cold work or CGR versus temperature), display a dispersion of several orders of magnitude (in some cases up to 3–4 orders of magnitude). This uncertainty arises partly from the failure of many researchers to measure, control, or even report environmental parameters that may have an obvious impact on CGR, such that the matrix containing all the independent variables information is almost always "sparse". As some of the missing information can be calculated [e.g., conductivity can be calculated from the composition of solution [7] and ECP can be estimated from $[H_2]$, $[H_2O_2]$, $[H^+]$, $[O_2]$, temperature, and flow velocity (if known)] using the Mixed Potential Model (MPM) [8], it is postulated that the measured CGR is usually much more accurate than the two-dimensional plots demonstrate. Another issue that needs to be considered is that the apparent dispersion is always so large that it is almost always possible to find data in excellent agreement with any model predictions, so as to "prove" the efficacy of a particular model.

However, unlike the models mentioned above, an ANN model contains no pre-conceived, physico-electrochemical model, but instead seeks to identify and quantify hidden relationships between the dependent and independent variables; in other words an ANN "tells it the way it is". The main benefits are that prediction results are based purely on data and not on preconceptions, and that the network can extrapolate effects from learned relationships without a mathematical model for extrapolation being specified.

2. Artificial neural network model

2.1. Introduction of artificial neural networks

Artificial neural networks (ANNs) are computational tools inspired by an animal's central nervous systems (in particular the brain) that are capable of machine learning and pattern recognition. They are usually presented as systems of interconnected "neurons" that can compute values from inputs by feeding information through the network. ANNs have been applied successfully by a number of researchers in the field of corrosion prediction and a few of these prior works are as follows. P.-C. Lu, et al. were the first to use artificial neural networks to study stress corrosion cracking [9,10], in which they applied an ANN to the study of IGSCC in sensitized Type 304 SS in high temperature water at 288 °C. Cai et al. [11], Pintos et al. [12], and Halama et al. [13] studied atmospheric corrosion using ANNs, and through sensitivity analysis, the effects of various factors were demonstrated. Smets and Bogaerts [14] successfully used ANNs for predicting SCC risk in austenitic stainless steels, and for defining the combined effects of three parameters (temperature, chloride concentration, and oxygen content) on the occurrence of SCC in austenitic chromium-nickel stainless steels in high-temperature water. Benhaim and Macdonald [15] applied an ANN to the study of the effect of various parameters on the acidity of simulated geological salt repositories, which contain brine inclusions, and predicted that the pH of the saturated brine inclusions would lie between 3.2 and 5, as the temperature of the repository decayed over thousands of years. All of these studies demonstrated that an ANN is an efficient computational tool for analyzing complex systems, especially when conventional modeling by analyzing specific reactions and processes may be difficult or unfeasible.

2.1.1. Basic elements

As noted above, an artificial neural network (ANN) is a computational tool based on biological neural networks and comprises an interconnected group of artificial neurons. The schematic of a three-layer neural network is shown in Fig. 1(a). Each layer consists of one or more neurons, as defined in Fig. 1(b). Each neuron in the first layer (also known as the input layer) receives a user specified input vector, processes the input vector and generates an output value. The output values from this layer are then passed on as inputs to each neuron in the next layer. The output values from the last layer (known as the output layer) correspond to the quantities that we need. The layers between the input and the output layers are termed "hidden layers".

Mathematically, the output of the k_{th} neuron in the l_{th} layer receiving a n-dimensional input vector is expressed as the following equation:

$$y_k^{(l)} = f\left(b_k^{(l)} + \sum_{i=1}^{n} w_{k,i}^{(l)} x_i^{(l)}\right) \tag{1}$$

where y_k is the output of the k_{th} neuron from an input vector $x = (x_1, \ldots, x_n)$, with x_i representing the input parameters. The $w_{k,i}^{(l)}$ values are the weights, which are used for scaling the respective input value to the neuron. Thus, within each layer, these weights indicate the relative importance of the parameters. The parameter b_k is termed the bias, which is used to account for the contribution of the unknown, but influential parameters, that have not been included in the analysis, most likely because of the lack of relevant data. The bias is much like a weight, except that its value is determined during the training of the net and is independent of the weighted inputs from the neurons from the previous layer (see Fig. 1). Its function is to modify the output, as indicated in Eq. (1). The weighted sum of the inputs and the bias value are passed through the transfer function f, which produces the scalar output. The establishment of the weights essentially imbues the net with "memory" and enables the relationships between the output (CGR) and each of the independent input variables (temperature, ECP, K_I, conductivity, pH, boron content, lithium content and extent of cold work) to be defined. In this study, a hyperbolic tan (tanh) function has been used as the transfer function in the hidden layers, while a linear function, rather than a sigmoid function, as used for the hidden layers, has been used for output layer.

2.1.2. Architecture

The number neurons in the input and output layer effectively represents the number of variables used in the prediction and the number of variables to be predicted, respectively. The hidden layers act as feature detectors and, in theory and practice, there is generally more than one hidden layer. However, universal approximation theory suggests that a network with a single hidden layer with a sufficiently large number of neurons can interpret any input–output structure [16]. The critical aspect is the choice of the number of neurons in the hidden layer. More hidden neurons result in a longer training period, while fewer hidden neurons provide faster training at the cost of having fewer feature detectors.

2.1.3. Training

Once the architecture of an artificial neural network and the network weights and biases are initialized, the network is ready for training. The training process of an ANN involves tuning the values of the weights and biases of the network to optimize the performance of network, which is judged by the mean squared error (σ) defined below. The general objective is to make output t_i and input a_i identical for $i = 1,2,\ldots,n$.

$$\sigma = \frac{1}{N}\sum_{i=1}^{N}(e_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(t_i - a_i)^2 \tag{2}$$