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The use of neural networks in understanding and predicting oxidation and corrosion behaviour in advanced energy conversion systems

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ABSTRACT

Neural networks can be a useful tool to analyse the oxidation and corrosion behaviour of materials at high temperature. Examples are given of the use of neural network models to analyse datasets of material behaviour after exposure to combustion, gasification and steam atmospheres. The use of networks to identify changes in mechanism, additional significant experimental parameters and the onset of spallation is demonstrated.

The limitations of neural network modelling are briefly discussed. Although they can be trained to fit any existing dataset, care must be taken in using the networks to predict a time sequence of events.

Keywords: neural network modelling, oxidation and corrosion behaviour, advanced energy conversion systems

1. INTRODUCTION

Oxidation and corrosion behaviour is, by its very nature, dependent on many factors including time, temperature, details of the atmosphere (composition, pressure) and alloy composition. Consequently predictive modelling of this behaviour is challenging and requires mechanistic understanding, simplification of the problem or lots of computing power.

Neural networks provide one of a range of suitable tools for analysis of this behaviour. However, in order to avoid total reliance on a 'black box' solution and potentially physically impossible or unlikely predictions, their use must be combined with materials understanding.

2. BASIS OF NEURAL NETWORKS

In 1936, the British mathematician Alan Turing developed the concept of the computer algorithm. This formed the basis of modern day computing that now enables us to use powerful, high-speed algorithm driven computers. However, for all the speed and performance of modem computers they cannot truly learn in the same sense as the brain. In the brain, neural activity passes from one neuron to another by means of electrical triggers. The passing of a signal can be to many hundreds of other neurons, thus one neuron is interconnected in a vast network. Not all of theses interconnections will be equally weighted, some will have a greater weighting than others. It is also important to note that these interconnections will have different properties, some will be exciters and others will be inhibitors, thereby serving to block the transmission. The nature of this interconnection forms the basis of artificial neural networks (ANN) [1].

McCulloch and Pitts [2] proposed the first ANN in 1943. They considered the case of a network constructed of binary decision units, and showed that such a network could perform any logical function on its inputs. Later, Rosenblatt [3] and his colleagues showed how it was possible to train a network of binary decision units; this Perceptron was shown to be able to recognise a pre-selected set of patterns. The training used what were described as connection weights. These weights were the most important objects within the neural network, and their modification, by training, enables the network to 'learn'.

The Perceptron later went on to form the basis of Rumelhart *et al.*'s [4] Back-Propagation network in 1986. Back-propagation allows the error to be transported back into the network influencing the modification of the weights enabling more complex problems to be solved. This use of multiple single neurons proved to be a popular technique.

Hopfield [5] developed a feedback ANN, the Hopfield Network, in 1982. In analysing the dynamics of networks Hopfield showed how a network of binary decision units coupled to each other and asynchronously updated, can be seen to develop with time. A further network that proved to be very attractive was the self-organising map (SOM). This had been developed by several workers in 1976 (Willshaw and von der Malsburg [6], and Grossberg [7]) and reached a very effective form for applications in terms of the self-organising feature map (SOFM) of Kohonen [8] in 1982. This allowed the weights of a single-layer network to adapt to an ensemble of inputs so as to learn the distribution of those inputs in an ordered fashion. An unsupervised network proposed by Hecht-Nielsen [9] in 1987 and titled the

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Counter-Propagation Network uses Kohonen's SOFM to allow unsupervised learning.

Cursory initial inspection of experimental data and current understanding of metal wastage in complex atmospheres shows that the task of predicting the metal wastage is too complex to be able to understand quantitatively with any precision. Approaching the task from an imprecise perspective seems to offer a greater chance of success. Fuzzy logic, originally introduced by Zadeh [10] in the 1960s, uses approximations and uncertainty to generate decisions, gives us the means to form an ANN to predict the metal wastage. Input data are assigned to sets rather than having discrete numerical values. By using fuzzy sets rather than strict memberships sets it is possible to better accommodate the experimental variability inherent in high temperature corrosion studies.

Fuzzy logic processes data sets by allowing the data to be partial members of a condition rather than a member or a non-member. In essence fuzzy logic provides a method of arriving at a definite answer based on vague, imprecise noisy or missing input data. An ANN based on this function would incorporate one or more rules based on the premise that:

If input X = 'x' and input Y = 'y' then output Z = 'z_1' with weight 'w_1' and = 'z_2' with weight 'w_2'

For the current studies neurons based on the processing units OR, AND and a complex OR/AND neuron were used to construct the neural network. This OR/AND neuron is constructed by combination of the OR and AND neurons as shown schematically in Figure 1.

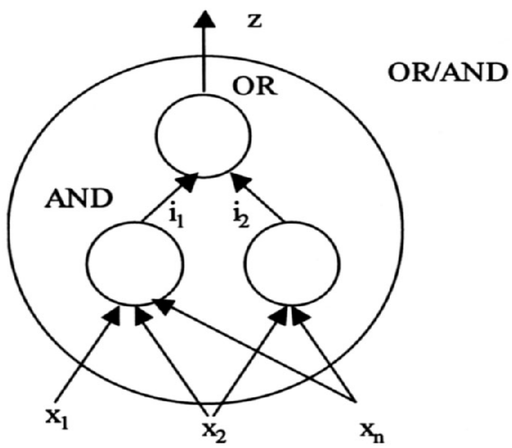

Figure 1 OR/AND neuron.

where x_1, x_2 and x_n are inputs to the neuron; i_1 and i_2 are intermediate values; and z is the output from the neuron. For the studies described in this paper a commercial neural network software package was used developed by neusciences. Within Neuframe 4 the neuro-fuzzy network is referred to as a Neufuzzy™ network.

3. EXAMPLES OF NEURAL NETWORKS IN PREDICTING OXIDATION AND CORROSION BEHAVIOUR

3.1 Metal wastage in mixed gas combustion atmospheres

The low alloy steels, T22 and T23 (compositions given in Table 1) are used in boilers were they are exposed to combustion atmospheres containing N_2, O_2, CO, CO_2, H_2, H_2S, HCl, H_2O and COS. The precise composition of the atmosphere varies with the fuel and the firing conditions in the boiler. Data from laboratory exposures at NPL [11] and from published literature were used to train a neural network to analyse metal loss within these materials. The range of exposures included temperatures from 400 to 640°C and times up to 1100 h. Inspection of the data for the two alloys showed that in identical atmospheres the two materials showed no significant difference in metal loss; thus the data for the alloys was treated as a single dataset.

During the training process the Neufuzzy network initially uses all of the input variables, but then optimises itself so that only 'key' parameters are used in the network to predict the final metal loss value. This feature potentially makes the network more useful in terms of the number of parameters needed by an end user to upgrade the model through the addition of further data. Initially the network was presented with 15 individual parameters that were derived from the gas composition, temperature and exposure time. The network constructed the necessary weighted neurons and established a set of 'rules' based on only four parameters. These were the volume % of O_2 and N_2, the temperature and the time. At first inspection the choice of N_2 content does not seem logical, however within the limited range of gas compositions investigated this can be considered to be a measure of the sum of active species in the atmosphere. The precise relationships between the four identified controlling parameters however cannot be extracted in a useable form from the neural network software.

A comparison of the predicted metal loss from the trained neural network with the experimental data showed good correlation with the exception of two datapoints which showed much lower metal loss than that predicted by the neural network (Figure 2). Detailed inspection of the dataset revealed that these two data points were at the extreme range of temperatures included in the training dataset *i.e.* they were the only tests carried out at 640°C. This observation indicates a possible change in corrosion mechanism at this temperature.

3.2 Materials behaviour in coal gasification atmospheres

The European collaborative programme, COST501 Advanced Materials for Power Engineering Components

Table 1 Composition of the T22 and T23 steels, wt%

Alloy	Fe	C	Si	S	P	Mn	Cr	Mo	V	N	Nb	W	B ppm	Al
T22	Bal.	0.10	0.5	0.025	0.025	0.6	2.25	0.54						
T23	Bal.	0.07	0.5	0.01	0.03	0.35	2.05	0.17	0.25	0.03	0.05	1.6	6	0.03

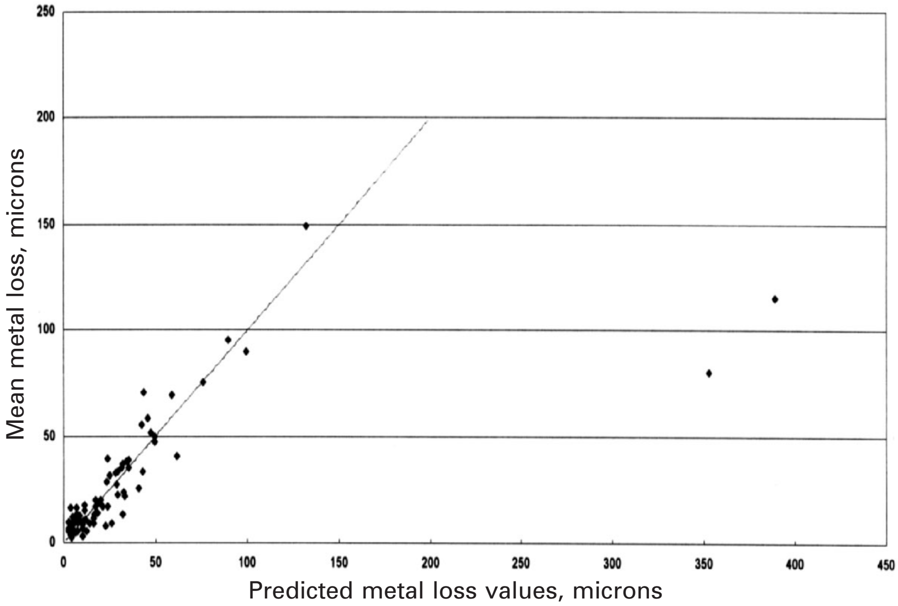

Figure 2 Comparison of trained neural network with experimental dataset for T22 and T23 exposed to mixed gas atmospheres.

provided a large body of data for the corrosion of alloys in coal gasification atmospheres [12]. Metal loss data for Alloy 800 (composition range given in Table 2) at temperatures between 400 and 800°C were summarised. Atmospheres were defined in terms of the partial pressure of oxygen and sulphur and also by an oxygen excess parameter. Interestingly the dataset included several exposures at high pressure.

The network was trained using data from exposures at ambient pressure using time, temperature and the three descriptors for the atmosphere as input parameters. The correlation between predicted metal loss and data is shown in Figure 3.

The trained network was then run to predict metal wastage in exposures at high pressures. These results are shown as the open symbols (◇) in Figure 3. It can be seen that in almost every case the network over estimates the metal loss in the high pressure exposures thereby showing conclusively that pressure is an important control variable. The network was thus re-trained using pressure as an additional input variable. The results are shown in Figure 4 where in can be seen that there is now good correlation at all pressures.

Table 2 Composition of Alloy 800, wt%

	Fe	C	Ni	Cr	Al	Ti
Min.	Bal.		30.0	19.0	0.15	0.15
Max.	Bal.	0.10	35.0	23.0	0.60	0.60

3.3 Scale growth and spallation of scales formed under steam environments

The growth and spallation of oxide scales grown on 9–12%Cr martensitic steels has been studied extensively [13]

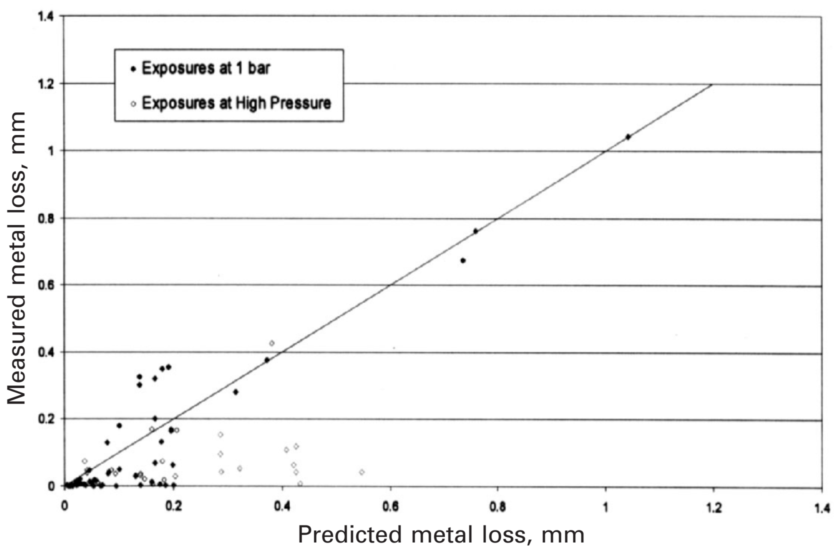

Figure 3 Comparison of trained neural network with experimental dataset for Alloy 800 exposed to coal gasification atmospheres.

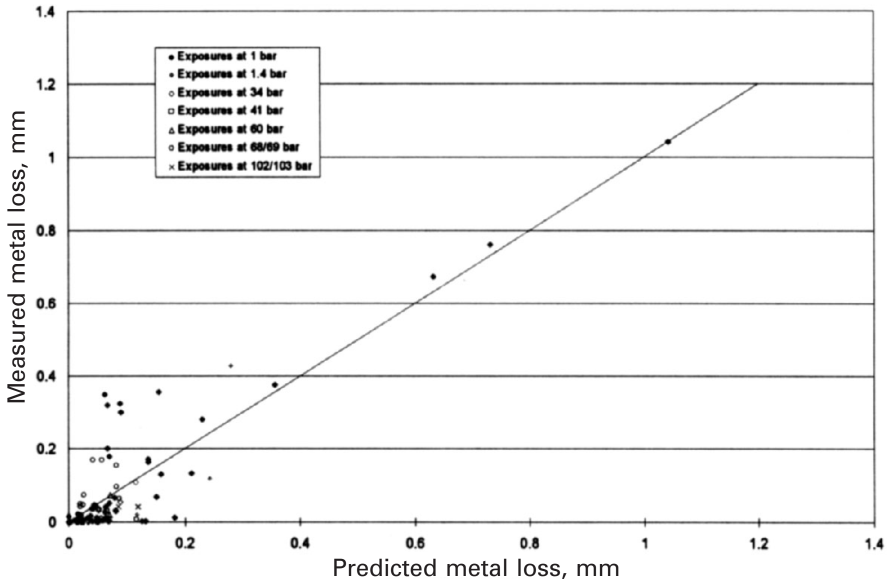

Figure 4 Comparison of trained neural network (including pressure as input parameter) with experimental dataset for Alloy 800 exposed to coal gasification atmospheres.

but is still not completely understood. It is well known that the chromium content of the alloy affects the scale growth rate but other elements also have a significant influence [14]. A neural network approach was thus used to try and rationalise the problem.

Initially the network was presented with 18 individual input parameters that were derived from the exposure technique, temperature, exposure time and alloy composition. The network constructed the necessary weighted neurons and established a set of 'rules' based on only six of these parameters. These were the exposure technique, temperature, time, and the wt% content of Mn, Cr and N. Using these relationships the neural network was able to predict the specific mass change, the results of this are presented in Figure 5, which shows a plot of the specific mass change as predicted by the network compared with the actual experimental value, this figure illustrates the good agreement between the neural network and observed data.

An approach to predict spallation of the oxide scale was then developed. Further networks were trained to predict the thickness of the individual oxide layers in the scale *i.e.* the outward growing magnetite and inward growing spinel.

Table 3 Prediction of spallation based on the thickness of the outward growing scale

Network Prediction,	Experimental observation	
	Spallation	Intact oxide scale
Spallation	**11**	0
Possible spallation	43	32
Intact scale	87	**1164**
Success Rate	88%	

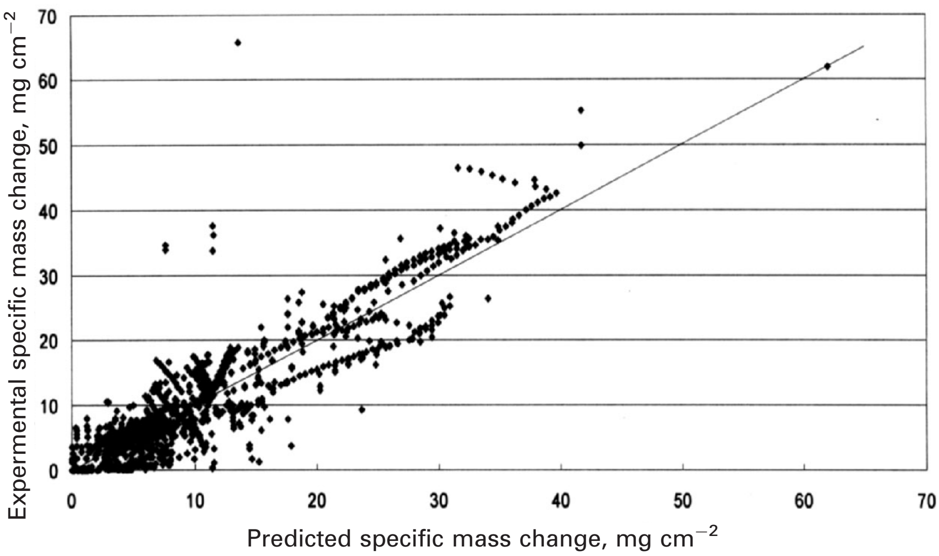

Figure 5 Comparison of predicted specific mass change of 9–12%Cr steels with the observed experimental value.

The thickness of these layers was then used as an additional input parameter to predict whether the scale would spall. Table 3 shows a comparison of network prediction with reported spallation events. The success rate of the neural networks is 88% when it uses the thickness of the outward growing oxide layer to predict spallation. However some caution should be exercised as in this study non-reporting of spallation was taken as data for the scale remaining intact – this may not necessarily have been the case. It should also be noted that the predictions are non-conservative; in 87 cases within the dataset spallation having occurred without being predicted. Further refinement of the model is clearly necessary.

4. DISCUSSION AND CONCLUSIONS

It has been demonstrated that neural networks can be a useful tool to analyse the oxidation and corrosion behaviour of materials at high temperature. The networks can be used to provide guidance on

- changes in corrosion mechanism
- the significance of specific experimental variables
- the onset of scale spallation

Although the networks can be trained to fit any existing dataset, care must be taken in using the networks to predict a time sequence of events. Even within the envelope of conditions used to train the network the precise algorithm developed may not be consistent with known mechanisms. In no circumstances must the neural network model be used to predict behaviour significantly beyond the envelope of conditions in the training database.

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