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Development of Neural Networks to Predict General Corrosion of Duplex Stainless Steels

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Abstract

Multi-layer feed-forward (MLF) neural networks have been applied to data from the NPL Corrosion Database of Duplex Stainless Steels in order to predict the corrosion rate of DSS in sulphuric acid, formic acid and hydrochloric acid. Although the amount of data available looks at first glance to be quite significant, on more detailed examination, it is clear that the amount of data in the conditions of importance, i.e. at the boundaries between low, medium and high corrosion rates, is actually quite sparse. Nonetheless, the use of Kohonen neural networks to 'focus in' on the important data has allowed the development of predictive algorithms although the detailed validation of these is not possible, and therefore care should be taken when using them.

Analysis of the MLF neural networks has been carried out based on the network weights. These indicate the relative importance of the input parameters viz. pitting resistance equivalent number (PREn), concentration of aggressive environment and temperature. Neural-fuzzy algorithms that "mimic" the MLF neural networks have also been developed. Although the performance of these networks (in terms of distinguishing the classes of data, viz. low medium and high corrosion rates) is not as good as the MLF neural networks, they have produced some "rules" which do describe the *basic* behaviour of the duplex stainless steels.

Introduction

Continuing on from the successful development of neural network algorithms to predict the sulphide stress corrosion cracking (SSCC) behaviour of duplex stainless steels (DSS)[1], an attempt has been made to predict the general corrosion behaviour of these materials.

While the Corrosion Database of Duplex Stainless Steels can be used to identify conditions in which a low (<0.1 mm/year), medium (0.1 – 1 mm / year) or high corrosion rate (>1 mm / year) has been measured in laboratory tests, the sparse amount of data available has made it difficult to define the boundary between high and low corrosion rates.

In this work, neural networks have been developed to predict corrosion rate in

- Sulphuric acid
- Formic acid
- Hydrochloric acid

Methodology

Although the amount of data available in the DSS database looks at first glance to be quite generous, on more detailed examination, it is clear that the amount of data in the conditions of importance, i.e. at the boundaries between low and high corrosion rates, is actually quite sparse and most of the data corresponds to a low corrosion rate. Due to the imbalance of data between high, medium and low corrosion rates, it is not possible for MLF neural networks to adequately determine the conditions in which higher corrosion rates will occur. In order to deal with this problem, Kohonen neural networks were used to "focus in" on the important data as follows:

- For each environment, a Kohonen neural network was trained with all of the data (using inputs solely of concentration and temperature).
- The clusters were analysed.
- All clusters that resulted in only "low" corrosion rates were discarded.
- This was repeated until a Kohonen neural network was developed in which no clusters solely resulted in a "low" corrosion rate.

For both the formic acid and hydrochloric acid cases, this procedure was sufficient to reduce the number of datasets resulting in a low corrosion rate to levels similar to those resulting in a high rate. However, in the case of sulphuric acid, there was still a very large amount of low corrosion rate data. Therefore, the amount of the latter was reduced to a third, by discarding two out of every three datasets from a "list" of data ranked according to their Kohonen cluster. In this way, the "spread" of data was unaffected.

Table I illustrates the original and final distribution of data after this pre-processing stage. Table II highlights the maximum and minimum values that have been used in training, and consequently the boundaries within which the neural networks will be effective. The pitting resistance equivalent number (PREn) is given by:

$$PREn = \%Cr + 3.3\%Mo + 16\%N \qquad (1)$$

As can be seen from Table I, there is, after pre-processing, very little data available and consequently neural networks could not be trained, validated and tested in the normal way. Instead, a variation on cross-validation has been used whereby three neural networks have been used to "distinguish" between low and medium, medium and high, and low and high corrosion rates respectively. This procedure was carried out as follows:

- Data were split up into the three groups as classified by their result, viz. low, medium and high corrosion rates.
- A simple 3:2:1 neural network architecture (i.e. with only two hidden neurons), as shown in Figure 1, was developed for each of the following scenarios:
    - All data with low and medium corrosion rates.
    - All data with medium and high corrosion rates.
    - All data with low and high corrosion rates.
- In each case, the input parameters included the pitting resistance equivalent number (PREn) of the duplex stainless steel, the concentration of aggressive environment (%), and the temperature (°C). The outputs were always binary, i.e. 0 or 1.
- The "final" prediction was an average of the output from each of these three networks.

Since no validation data were used to halt the training (as with the SSCC algorithms), the number of training iterations was limited to 10,000 in order to prevent the neural network memorising the data. It should be noted that taking an average of all three of these networks also encourages generalisation (the prediction is general rather than simply 'remenber' the training data), although as has already been emphasised, there were not enough data to set aside from the training stage in order to test the generalising capability of these networks.

The use of a simple 3:2:1 architecture also encourages generalisation as opposed to memorisation. However, in the case of sulphuric acid, this architecture was not sufficient to "distinguish" between the classes of outputs. Therefore, a 3:3:1 architecture was employed with more success.

Given that in general, there was shown to be a clear distinction between the data that resulted in a low and a high corrosion rate, it has been possible to demarcate the transition between the two groups. Consequently it has also been possible to estimate corrosion rates in this region. This has been carried out as follows:

- By analysing graphs of performance of the neural network algorithms, "boundaries" were allocated where almost all (if not all) of the data for which the MLF predictions fell below one limit resulted in a low corrosion rate, and all of the data for which the MLF predictions were greater than another limit resulted in a "high" corrosion rate.
- The range of predictions falling between these two boundaries were taken to be the full range between which corrosion rates would vary between 0.1 mm/year and 1 mm/ year.
- The corrosion rate was linearly correlated to the MLF predictions in this range.

Results and Analyses

Figures 2 – 4 illustrate the predictive capability of each of the algorithms developed. The performance graph (a) in each case shows how the average of the MLF predictions correlates to the actual corrosion rates. The "boundaries" within which the corrosion rate has been assumed to vary between 0.1 and 1 mm/year have also been shown. Examples of corrosion maps that were generated by querying the neural networks with an array of data are also shown in part (b) of the figures. Superimposed onto these figures are labels that highlight the corrosion rate (high, medium, or low) of actual data from the database (used to train the neural networks).

As stated earlier, no database data could be set aside to test the generalisation capability of the neural networks, and therefore caution should be exercised when using predictions. This is particularly true when querying the neural networks with scenarios in which the PREn is different to those that were used to train the neural networks.

Some further analysis of the MLF networks was achievable by viewing the weights attributed to each connection, although it was not possible to establish any equations as such using these weights. It was however possible to establish the relative importance of each parameter for the networks created. The average importance of each input parameter is shown in Figure 5 for the three environments.

Further exploration of the neural network algorithms has been possible with the use of neural-fuzzy technology. Models have been generated which "mimic" the MLF algorithms by the using the corrosion rates (converted from the MLF network predictions) as the output data in training. These rules, together with the performance of the neural-fuzzy networks are shown in Figures 6-8.

Discussion

It can be seen from Figures 2-4 that the neural networks are quite effective in modelling the boundaries between low and high corrosion rates, despite the lack of the data. However, this lack of data does pose problems with regards to validating the neural networks, and consequently caution should be exercised when using the predictions. Although the neural networks can in theory be used to interpolate between different PREn values, there has been no way to assess the accuracy or the generalisation capability for other grades of DSS (i.e. those not used in training) and therefore extreme caution should be exercised in this case.

The network weights did not produce much additional information, which is not surprising since only three parameters were used. The neural-fuzzy "rules" reinforced established knowledge of DSS performance in these environments, i.e.:

- Duplex stainless steels with a higher PREn are generally more resistant to general corrosion in sulphuric acid, formic acid and hydrochloric acid.
- Corrosion rates in these environments are generally higher at higher temperatures.
- For both sulphuric and hydrochloric acid environments, the corrosion rates are at their highest between a medium and high concentration.
- For the narrow concentration of HCl for which data were available (i.e. up to 5%), higher concentrations are shown to lead to higher corrosion rates.

It must be noted that these rules only basically describe the nature of the duplex stainless steels in these environments, and consequently these neural-fuzzy networks do not perform as well as their respective MLF counterparts.

Conclusions

- Neural network algorithms have been developed which distinguish between low and high corrosion rates in sulphuric acid, formic acid and hydrochloric acid. Using these algorithms, corrosion rates in the interim region have also been estimated.
- Due to the lack of data, it is not possible to thoroughly validate the algorithms and consequently caution should be exercised in using these predictions.

Table I. Distribution of data before and after pre-processing.

	Frequency of data					
	Before pre-processing			After pre-processing		
	Low	Medium	High	Low	Medium	High
Sulphuric acid	568	25	32	47	25	32
Formic acid	168	9	6	8	9	6
Hydrochloric acid	44	4	18	18	14	18

Table II. Maximum and minimum values of input parameters used in MLF neural network training.

	PREn		Concentration (%)		Temperature (°C)	
	Min	Max	Min	Max	Min	Max
Sulphuric acid	25.26	47.68	0.5	98	20	102
Formic acid	25.26	42.52	10	100	100	107
Hydrochloric acid	25.26	42.52	0.2	5	20	102

Reference

1. Zhou, S., Coleman, D., and Turnbull, A., “Application of Neural Networks to Predict Sulphide Stress Corrosion Cracking of Duplex Stainless Steels ”, NPL Report MATC (A) 21, May 2001.

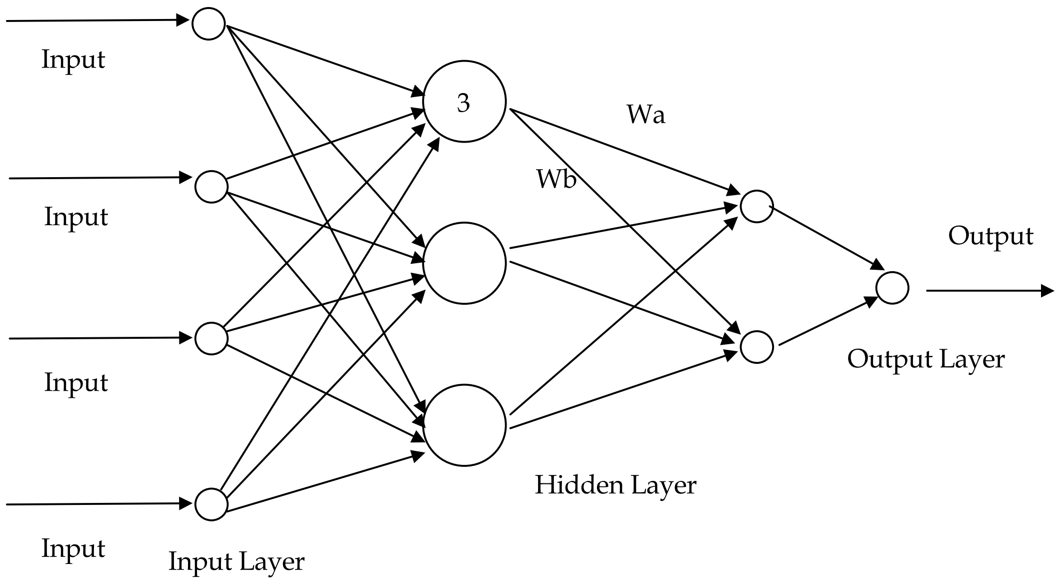
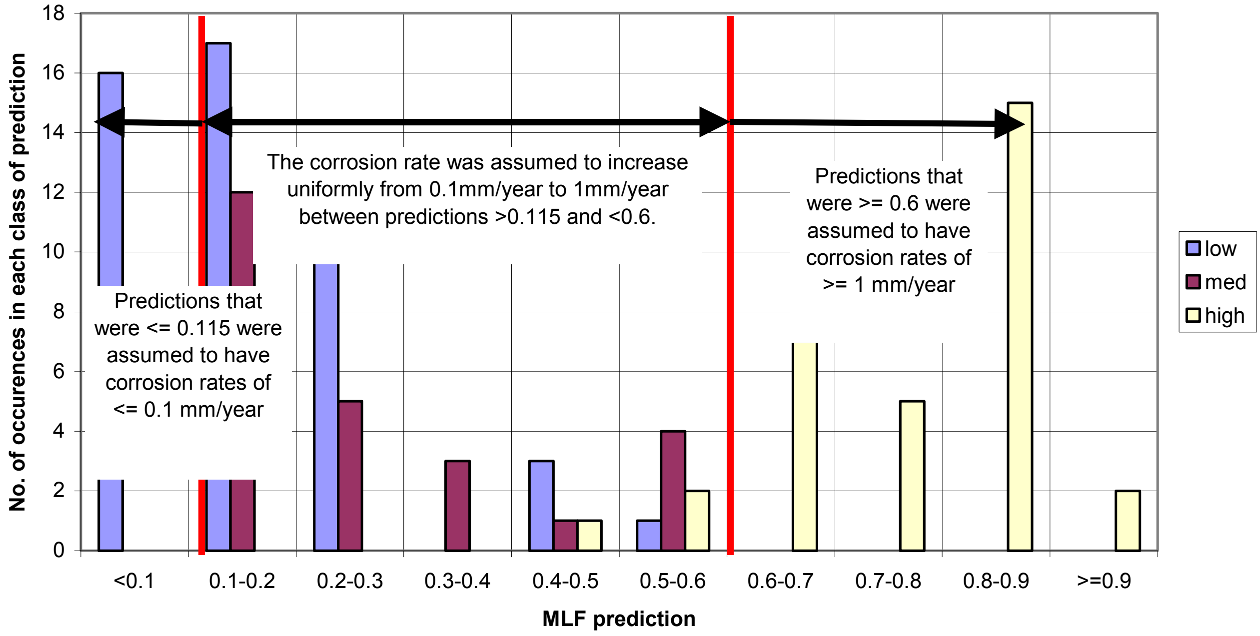
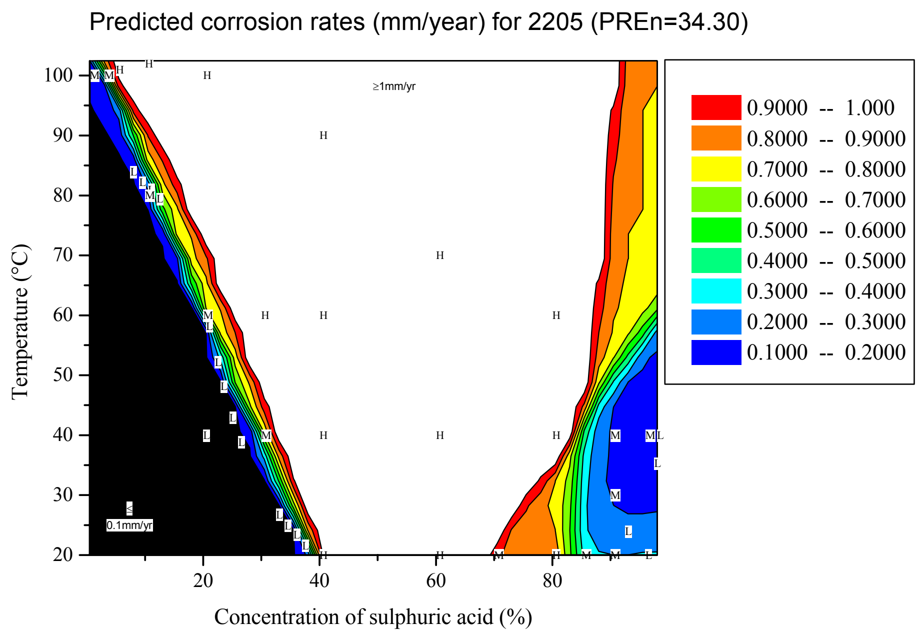


Figure 1. A 3 : 2 : 1 neural network architecture.

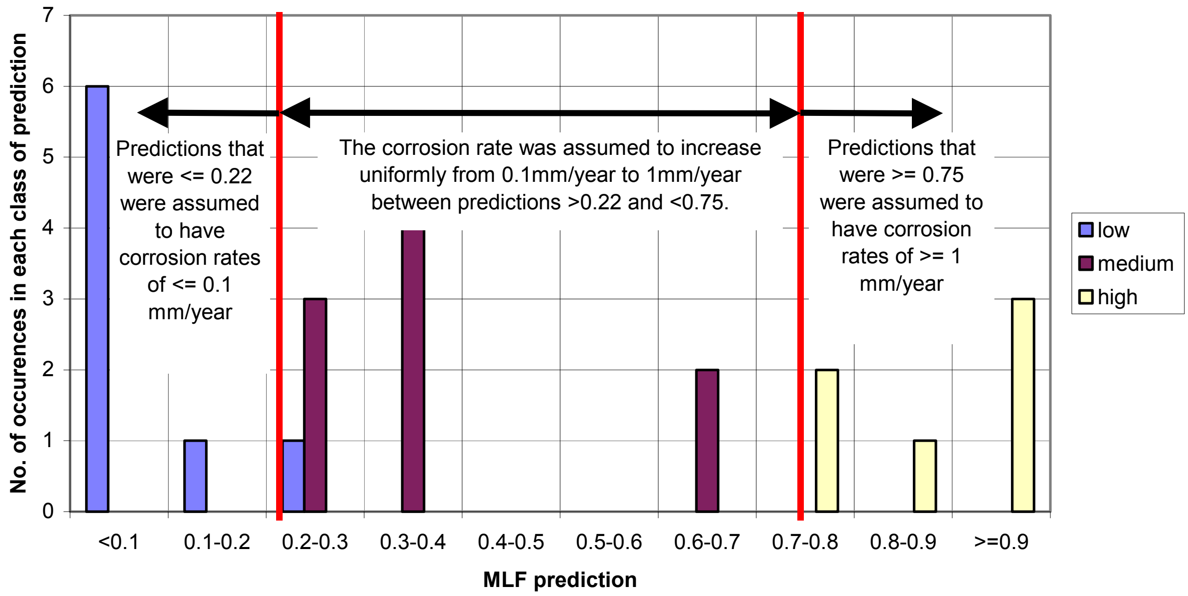


(a)

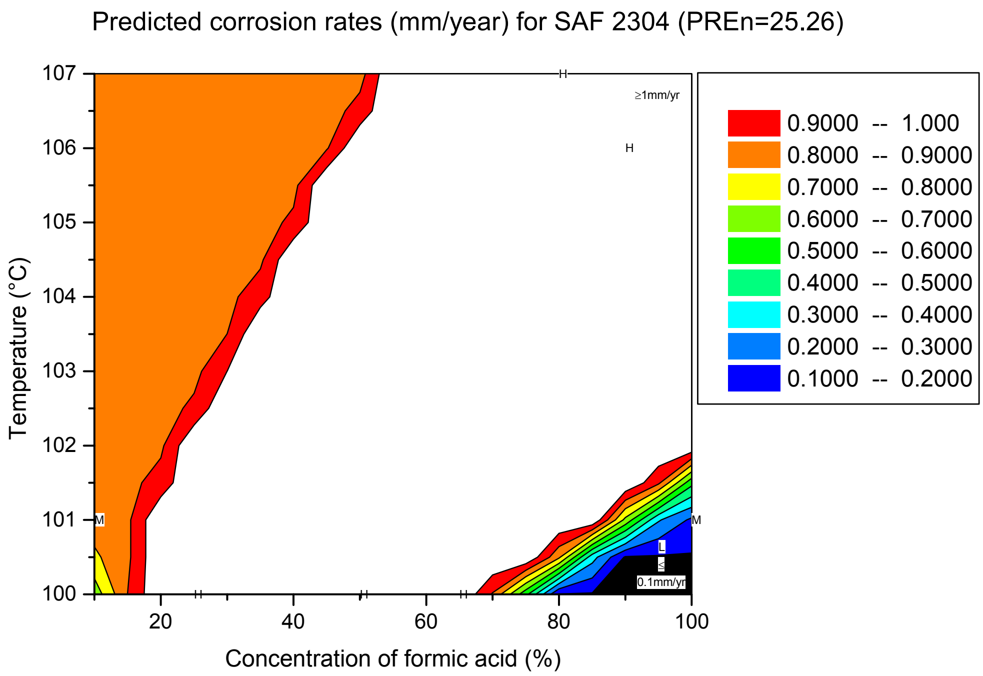


(b)

Figure 2. **(a) Performance of MLF neural network algorithms for prediction of corrosion of DSS in sulphuric acid.**
(b) Example map of predicted corrosion rates for a 2205 DSS, together with labels denoting the severity of corrosion that has been shown to actually occur (from the DSS Database), where H = high (≥ 1 mm/year,) M = medium (0.1-1 mm/year) and L = low (≤ 0.1 mm/year).

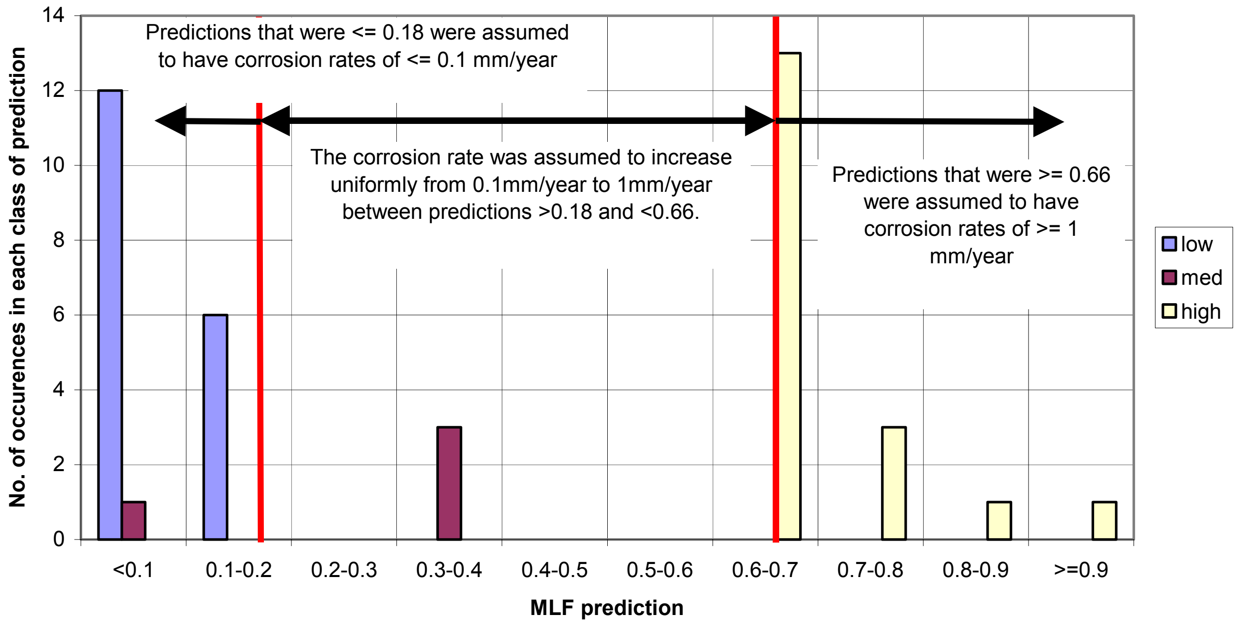


(a)

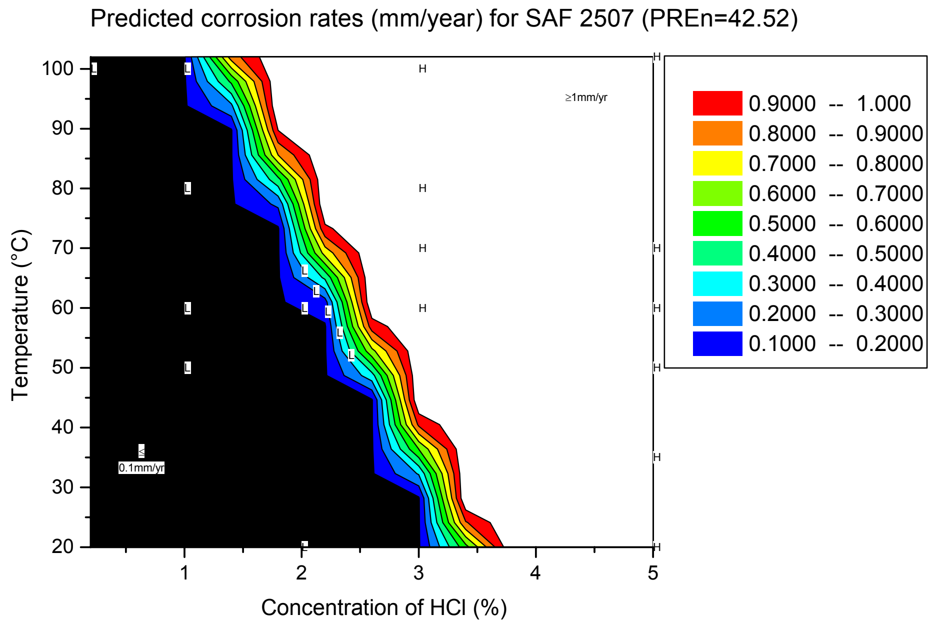


(b)

Figure 3. **(a) Performance of MLF neural network algorithms for prediction of corrosion of DSS in formic acid.**
(b) Example map of predicted corrosion rates for a SAF 2304 DSS, together with labels denoting the severity of corrosion that has been shown to actually occur (from the DSS Database), where H = high (≥ 1 mm/year,) M = medium (0.1-1 mm/year) and L = low (≤ 0.1 mm/year).



(a)



(b)

Figure 4. **(a) Performance of MLF neural network algorithms for prediction of corrosion of DSS in hydrochloric acid.**
(b) Example map of predicted corrosion rates for a SAF 2507 DSS, together with labels denoting the severity of corrosion that has been shown to actually occur (from the DSS Database), where H = high (≥ 1 mm/year,) M = medium (0.1-1 mm/year) and L = low (≤ 0.1 mm/year).

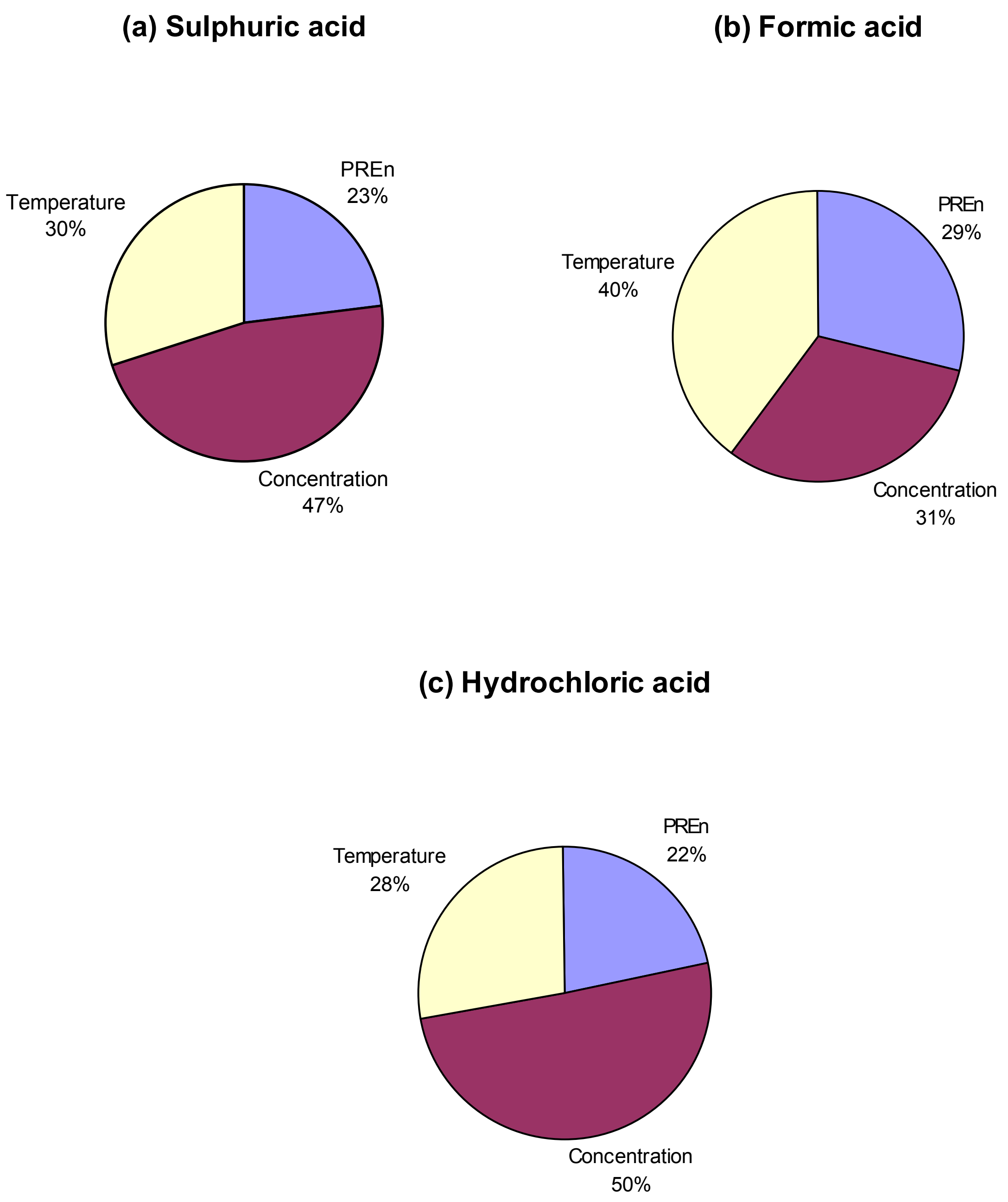
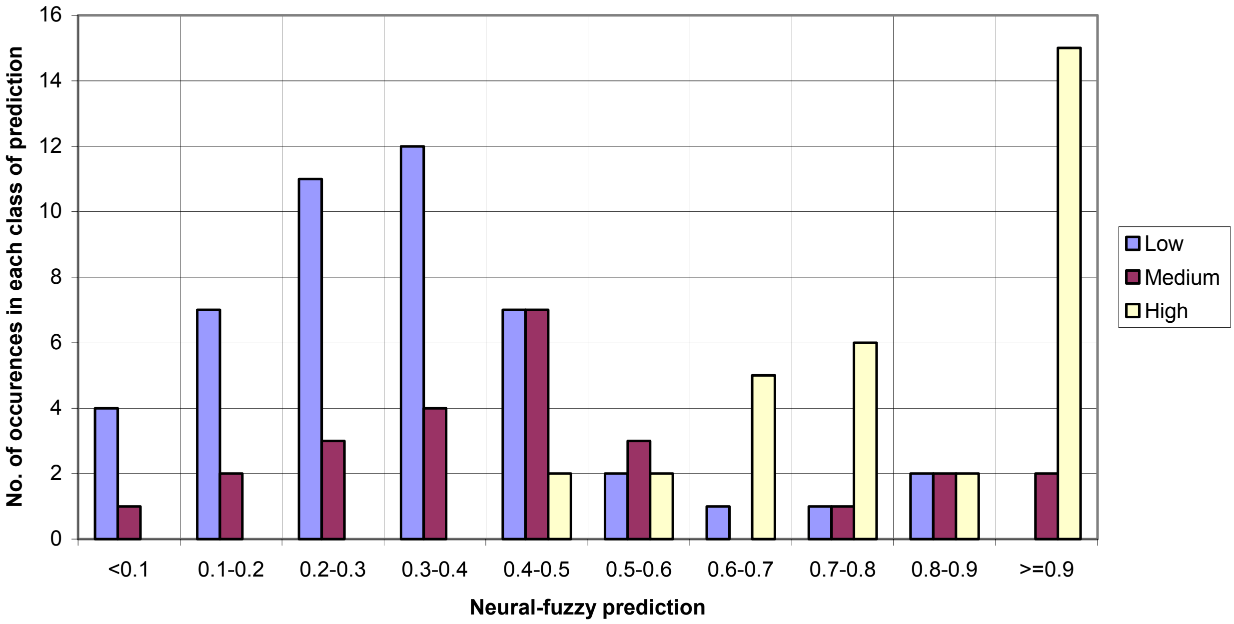


Figure 5. Relative importance of input parameters for each set of algorithms.



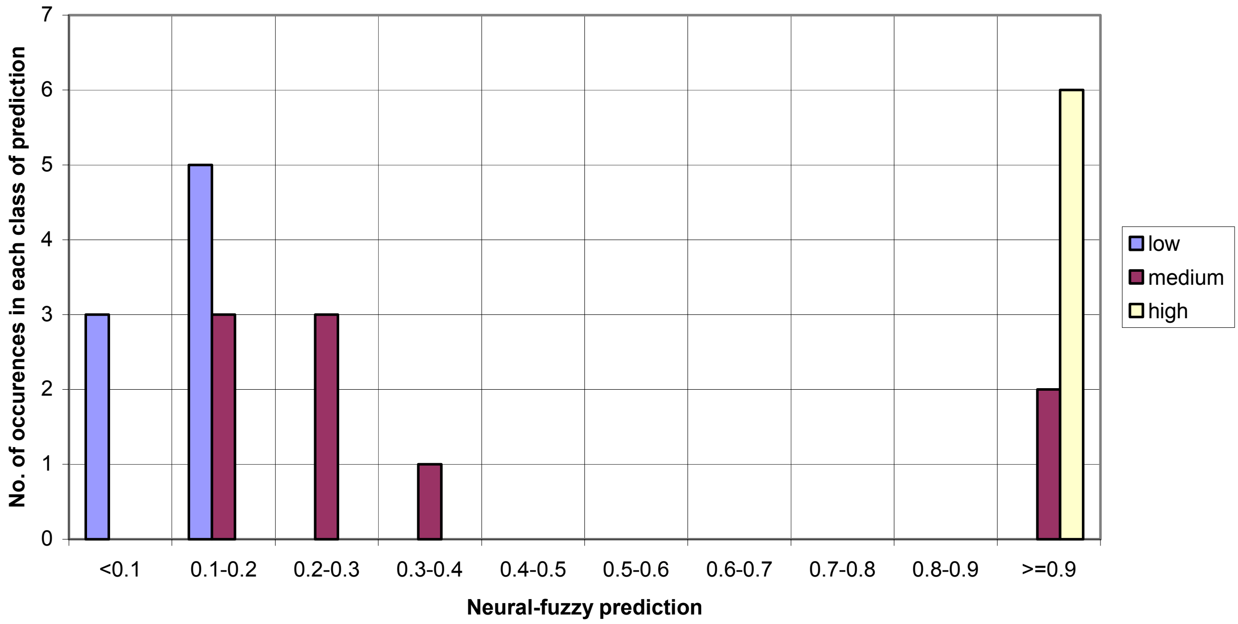
Rules:

1: IF Concentration is very low THEN Corrosion rate is low (1.00)
2: IF Concentration is low THEN Corrosion rate is low (0.18) OR Corrosion rate is medium (0.82)
3: IF Concentration is medium THEN Corrosion rate is medium (0.48) OR Corrosion rate is high (0.52)
4: IF Concentration is high THEN Corrosion rate is high (1.00)
5: IF Concentration is very high THEN Corrosion rate is low (0.38) OR Corrosion rate is medium (0.62)

6: IF PREn is low THEN Corrosion rate is medium (0.69) OR Corrosion rate is high (0.31)
7: IF PREn is high THEN Corrosion rate is low (0.72) OR Corrosion rate is medium (0.28)

8: IF Temperature is low THEN Corrosion rate is low (0.66) OR Corrosion rate is medium (0.34)
9: IF Temperature is high THEN Corrosion rate is medium (0.26) OR Corrosion rate is high (0.74)

Figure 6. Performance of sulphuric acid neural-fuzzy network and "rules" generated.

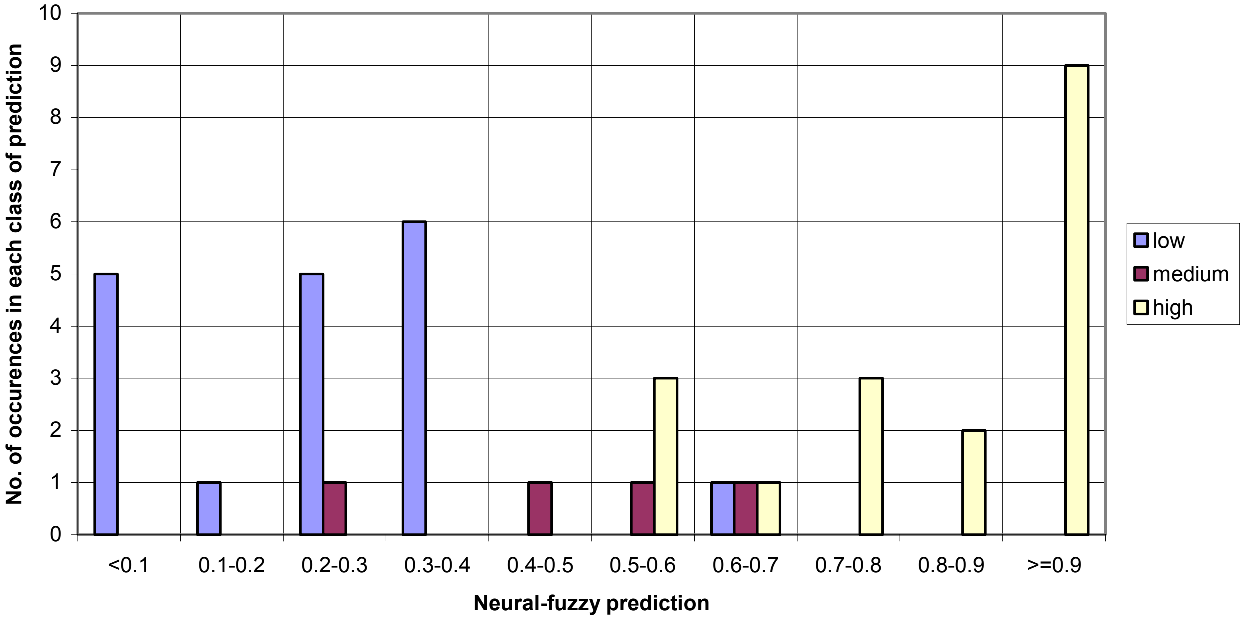


Rules:

1: IF PREn is low AND Concentration is low THEN Corrosion rate is low (0.31) OR Corrosion rate is high (0.69)
2: IF PREn is medium AND Concentration is low THEN Corrosion rate is low (0.83) OR Corrosion rate is high (0.17)
3: IF PREn is high AND Concentration is low THEN Corrosion rate is low (0.93) OR Corrosion rate is high (0.07)
4: IF PREn is low AND Concentration is medium THEN Corrosion rate is high (1.00)
5: IF PREn is medium AND Concentration is medium THEN Corrosion rate is low (0.84) OR Corrosion rate is high (0.16)
6: IF PREn is high AND Concentration is medium THEN Corrosion rate is low (0.94) OR Corrosion rate is high (0.06)
7: IF PREn is low AND Concentration is high THEN Corrosion rate is low (0.97) OR Corrosion rate is high (0.03)
8: IF PREn is medium AND Concentration is high THEN Corrosion rate is low (0.69) OR Corrosion rate is high (0.31)
9: IF PREn is high AND Concentration is high THEN Corrosion rate is low (0.86) OR Corrosion rate is high (0.14)

10: IF PREn is low AND Temperature is low THEN Corrosion rate is low (0.81) OR Corrosion rate is high (0.19)
11: IF PREn is medium AND Temperature is low THEN Corrosion rate is low (1.00)
12: IF PREn is high AND Temperature is low THEN Corrosion rate is low (0.92) OR Corrosion rate is high (0.08)
13: IF PREn is low AND Temperature is high THEN Corrosion rate is low (0.12) OR Corrosion rate is high (0.88)
14: IF PREn is medium AND Temperature is high THEN Corrosion rate is low (0.29) OR Corrosion rate is high (0.71)
15: IF PREn is high AND Temperature is high THEN Corrosion rate is low (0.83) OR Corrosion rate is high (0.17)

Figure 7. Performance of formic acid neural-fuzzy network and "rules" generated.



Rules:

1: IF Temperature is low THEN Corrosion rate is low (0.91) OR Corrosion rate is high (0.09)
2: IF Temperature is high THEN Corrosion rate is low (0.51) OR Corrosion rate is high (0.49)

3: IF PREn is low THEN Corrosion rate is low (0.37) OR Corrosion rate is high (0.63)
4: IF PREn is high THEN Corrosion rate is low (0.80) OR Corrosion rate is high (0.20)

5: IF Concentration is low THEN Corrosion rate is low (1.00)
6: IF Concentration is high THEN Corrosion rate is high (1.00)

Figure 8. Performance of hydrochloric acid neural-fuzzy network and "rules" generated.