Data Mining Of Experimental Corrosion Data Using Neural Network

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Research Objectives

- Establish a data mining methodology for predicting metal/alloy life over extended periods of time
- Demonstrate the predictive capabilities of data mining by using data available for alloy materials to predict their performance and compare our predictions to the prediction of deterministic models
- Establish a methodology on data representation and analysis that can be used as a complementary tool in the laboratory to avoid time consuming capturing of additional data
- Learn and generalize material behaviors based on existing data

Data Mining

Data mining (also known as Knowledge Discovery in Databases - KDD):

- The nontrivial extraction of implicitly useful information from data
- It uses machine learning, statistical, visualization, and neural network (NN) techniques to discover and present knowledge embedded in data in a form which is easily comprehensible to humans

Activities in Data Mining

- Data collection
  - (i) Data collection and formatting
  - (ii) Data cleaning
  - (iii) Data integration
  - (iv) Data transformation
- Data analysis and model development
  - (v) Data mining or knowledge extraction
  - (vi) Pattern evaluation
- Knowledge presentation

Types of Data Analysis

- **Directed data mining**
  - Classification
  - Estimation
  - Prediction
- **Undirected data mining**
  - Affinity grouping or association rules
  - Clustering

Our focus: Prediction data mining

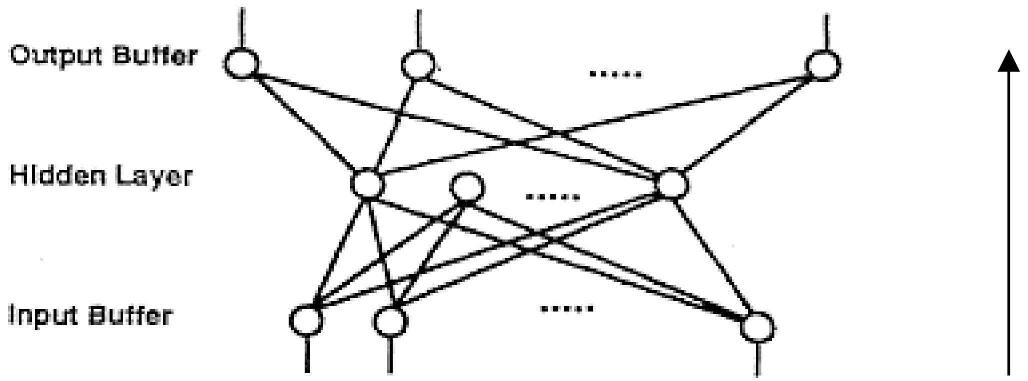
System of interest: Corrosion behavior of metals/ alloys

Method of analysis: Neural network backpropagation

Neural Network

- **Analogous to human brain activity**
  - We have neurons in our brain
  - We learn through the neuron interconnections (stronger or weaker)
- **Tasks that the brain performs well**
  - Pattern recognition
  - Classification
  - Categorization
  - Pattern reconstruction
  - Association
- **Neural network model**
  - No model is imposed
  - It learns from data

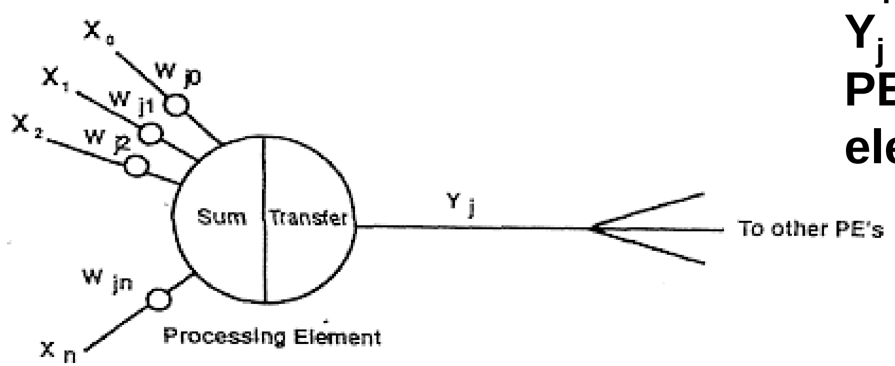
Neural Network



Direction of information flow

Typical neural network (NN)

x_i -- Inputs
w_i -- Weights
Y_j -- Outputs
PE -- Processing element



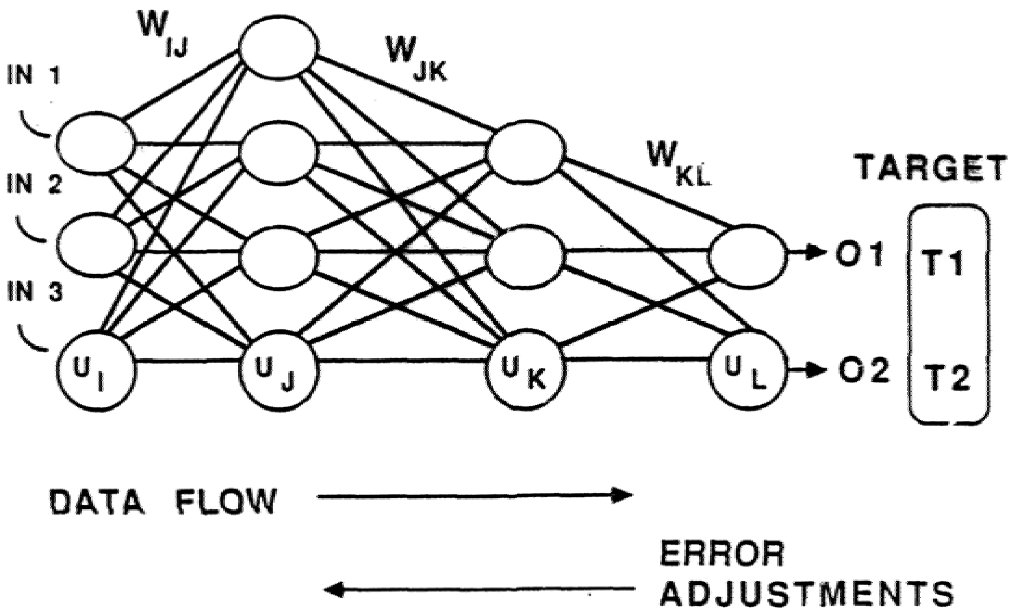
Processing element

BackPropagation Neural Network

- BackPropagation (BP) Neural Network (NN) is a learning algorithm that learns by example where the user provides a set of inputs and known outputs
- The BP learning process works in iterative steps:
  - The network initially starts with one example of inputs and some random weights and produces outputs based on the current state of the inputs and weights
  - The outputs are compared to the known outputs
  - The error (mean-squared) between the network outputs and the known outputs is propagated backwards through the network and small changes are made to the weights in each layer to reduce the error for the case in questions
  - The whole process is repeated for each of the example cases and back to the first case again and so on
  - The cycle is repeated until the overall error value drops below some pre-specified error threshold
  - The network is then said to have learned the mapping functions between the inputs and outputs and the final weights are calculated

Neural Network

To extrapolate and establish relationships to categorize importance of input parameters (pH, T, [Cl$^-$], etc.) on output parameters (general corrosion rate, localized damage, etc.), neurons and neuron layers can be simulated mathematically: supervised learning with backpropagation.



Typical backpropagation layout

Our Approach

- Data collection on generalized and localized corrosion of several metals in contact with several environments
- Data reprocessing, that includes data filtering (for bias information), data transformation (to accentuate certain data features) and data normalization (to give all variables the same order of importance)
- Statistical data “cleaning” used to identify outliers
- Data representation in different spaces using mathematical transformations; it is a very important step to identify contrasting data features
- Data analysis
  - Identify hidden functions that relate measured parameters to alloy corrosion rates. The discovered function (supervised backpropagation in neural network) is used to make extrapolations

Data Mining Tasks

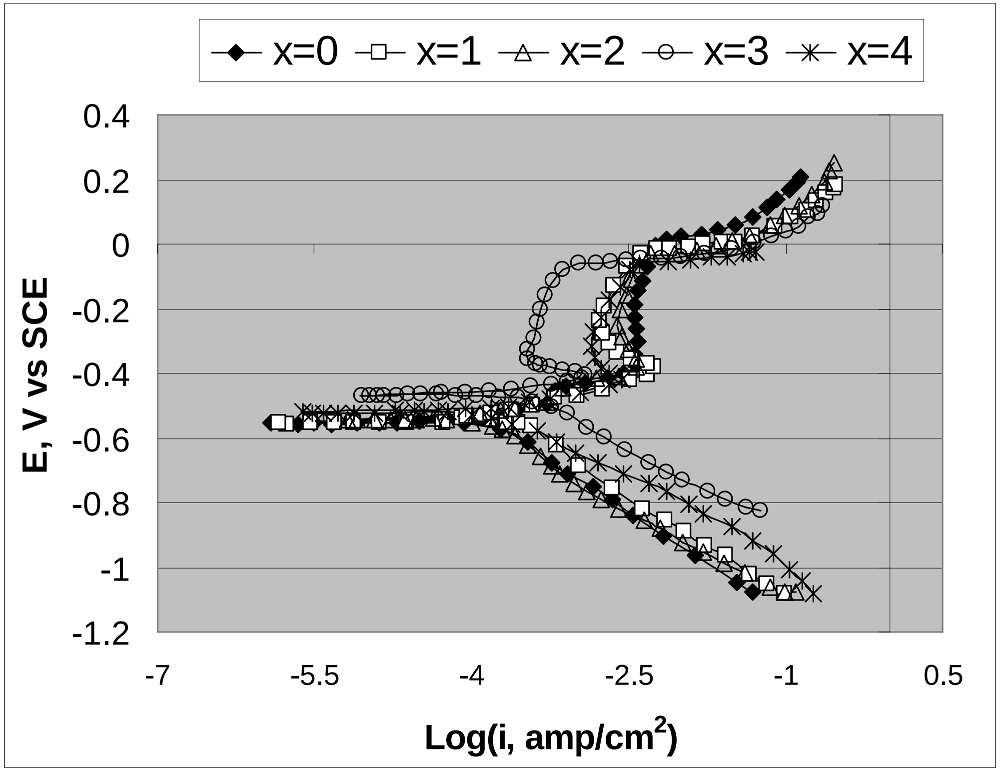
- Data collection
  - General corrosion data on Iron-alloy ($Fe_{68}Ni_{14-x}Mo_xSi_2B_{16}$ metallic glasses for different x values) (source: article available publicly [1])
  - Crevice corrosion on Ti-alloy (grade-2 Titanium) (source: article available publicly [2])
- Data processing and model development
  - Backpropagation designed for predicting the polarization behavior for metalic glasses
  - Backpropagation developed for predicting localized corrosion behavior for grade-2 Titanium

Ref:

[1] B. Seshu, A.K. Bhatnagar, A.Venugopal and V.S.Raja, *Journal of Materials Science*, 32, 2071 (1997).

[2] X. He, J.J. Nöel and D.W. Shoesmith, *Corrosion Science*, 47, 1177 (2005).

Polarization Data on Iron-alloy



Polarization curves for $Fe_{68}Ni_{14-x}Mo_xSi_2B_{16}$ metallic glasses with x=0, 1, 2, 3, 4 in 1N HCl [1].

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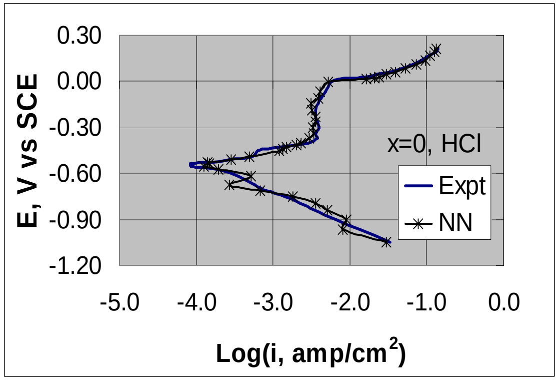
Polarization Data on Iron-alloy

Kinetic parameters for $Fe_{68}Ni_{14-x}Mo_xSi_2B_{16}$ metallic glasses with x=0, 1, 2, 3, 4 in 1 N HCl [1]. βa and βc are Tafel constants and Rp is polarization resistance.

Sample	E_{corr} mV	i_{corr} μA/cm²	βa mV/decade	βc mV/decade	Rp ohm.cm²
1	-571	153	109	203	201
2	-540	226	71	223	103
3	-567	153	79	237	167
4	-506	271	31	154	41
5	-554	141	70	134	142

Analysis of Polarization Data on Iron-alloy



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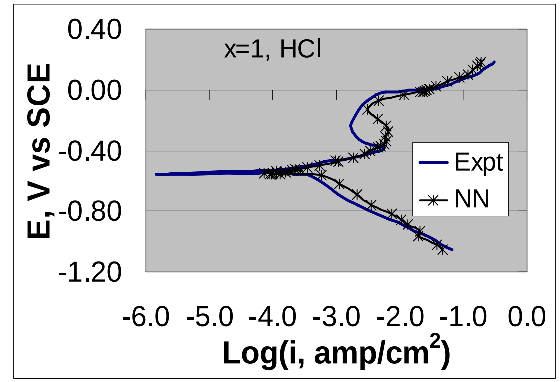
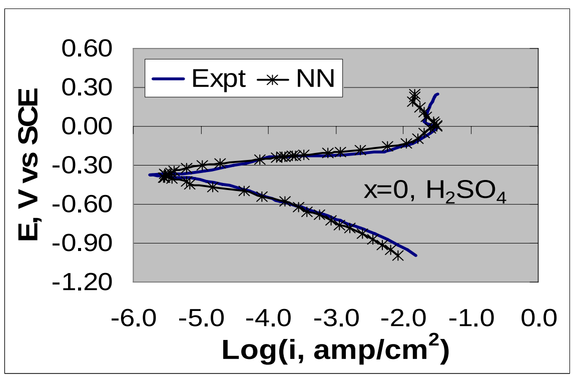


(b)



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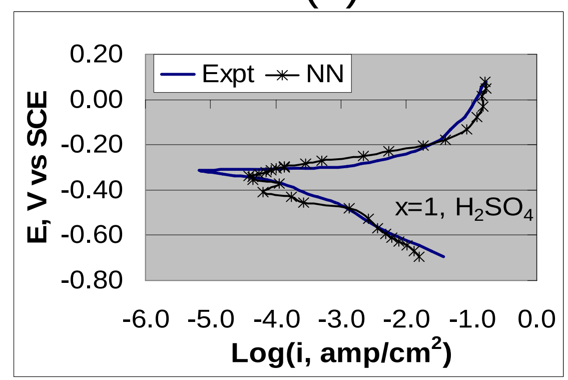
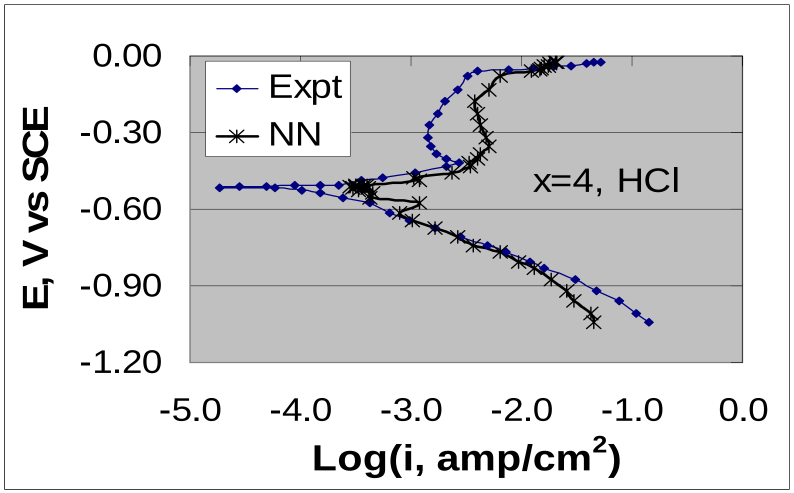


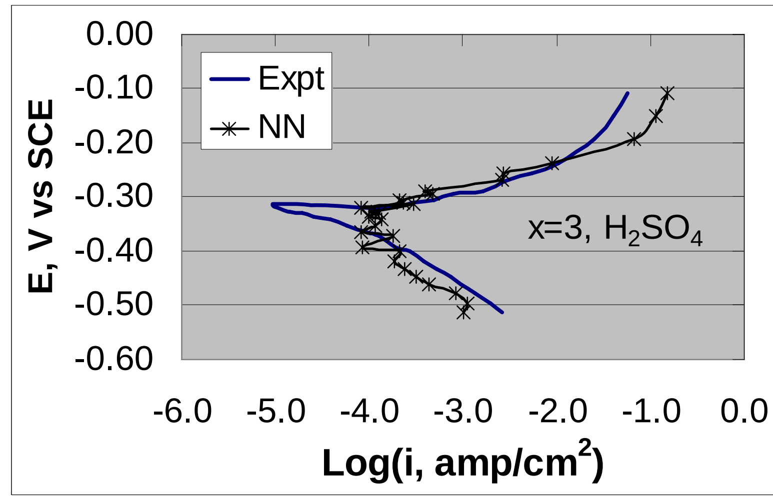
(d)

Polarization curves for $Fe_{68}Ni_{14-x}Mo_xSi_2B_{16}$ metallic glasses with (a) x=0 in 1N HCl, (b) x=1 in 1N HCl, (c) x=0 in 1N H_2SO_4, and (d) x=1 in 1N H_2SO_4. The NN is validated with the same data sets as the model was trained with.

Analysis of Polarization Data on Iron-alloy



(a)



(b)

Polarization curves for $Fe_{68}Ni_{14-x}Mo_xSi_2B_{16}$ metallic glasses with (a) x=4 in 1N HCl, and (b) x=3 in 1N H_2SO_4. The NN is validated with test data sets that were <u>not seen</u> by the model during training.

Localized Corrosion Data on Ti-2

Data used to develop a damage function for crevice corrosion of Ti-2 in 0.27 mol/dm^3 NaCl solution at 95°C [2]. Q refers to the charge in coulombs; W is the weight loss expressed in coulombs.

Incubation period (days)	Duration (days)	Maximum penetration depth, Dmax (μm)	Q (C)	Weight change (g)	Q/W	O_2 consumed (%)
1.19	**3.02**	**140**	**9.03**	**0.0525**	**0.0143**	**0.5**
2.42	**9.78**	**604**	**106**	**0.0773**	**0.114**	**5**
0.54	**15.13**	**938**	**371**	**0.1595**	**0.193**	**19**
0.76	**15.5**	**969**	**333**	**0.2728**	**0.101**	**17**
1.31	**23.15**	**1265**	**578**	**0.2333**	**0.206**	**29**
1.22	**31.07**	**1645**	**899**	**0.321**	**0.232**	**45**
1.26	**53.14**	**1611**	**1189**	**0.6508**	**0.152**	**60**
0.95	**64.26**	**1694**	**1269**	**0.6603**	**0.159**	**64**

Analysis of Localized Corrosion Data on Ti-2

Models for localized corrosion analysis:

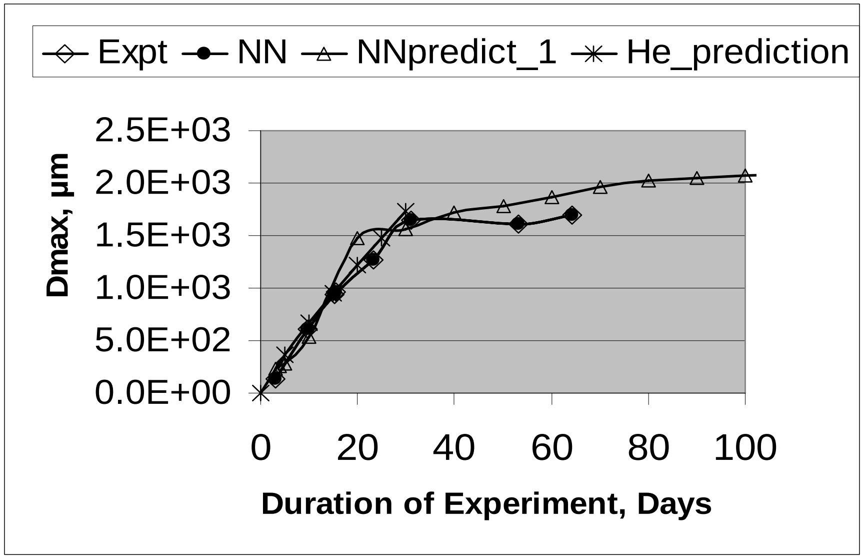
- **Empirical model**
  - Requires a significant database to develop a reliable model
  - Requires a functional relationship to be specified
  - Typical model for damage function: $D = kt^m$
- **Deterministic model**
  - Good for future prediction
  - Decreases the requirement of large databases
  - Requires that the mechanism of damage functions be known for the specific operating conditions

NN Model for Localized Corrosion Analysis

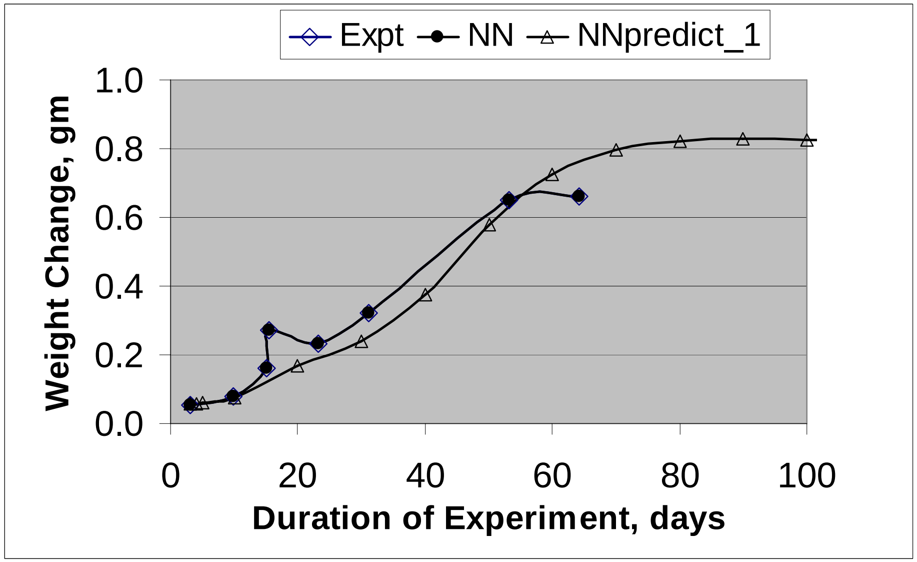
Supervised NN (backpropagation) model:

- Requires an extensive data base (as empirical model)
- Helps to perform non linear mapping between the inputs and outputs that can be used to establish relationships between input and output parameters/variables
- NN learns the "underlying functions" that relate those mappings and once trained, they can be used to make "smart predictions" or extrapolations over extended parameter range (unlike the ability of empirical models)
- NN backpropagation for the He et al. data
  - 3 layers, 20 neurons/layer, hyperbolic tangent function
  - Inputs: incubation time, duration of experiments
  - Outputs: weight change, Q, Q/W, % O_2 consumed and their logarithms
  - RMS error <0.001%

Analysis of Localized Corrosion Data on Ti-2



(a)



(b)

NN results in the study of crevice corrosion of grade-2 Ti in 0.27mol/dm^3 NaCl solution at 95^{o}C [2]. (a) Prediction of maximum penetration depth, Dmax, and (b) Prediction of sample weight change, Expt: experimental data, NN: model prediction using the same input data that was used for training, NNpredict_1: prediction for 100 days, He_prediction: predicted Dmax by He et al. $D\max = 89.74t^{0.87}$.

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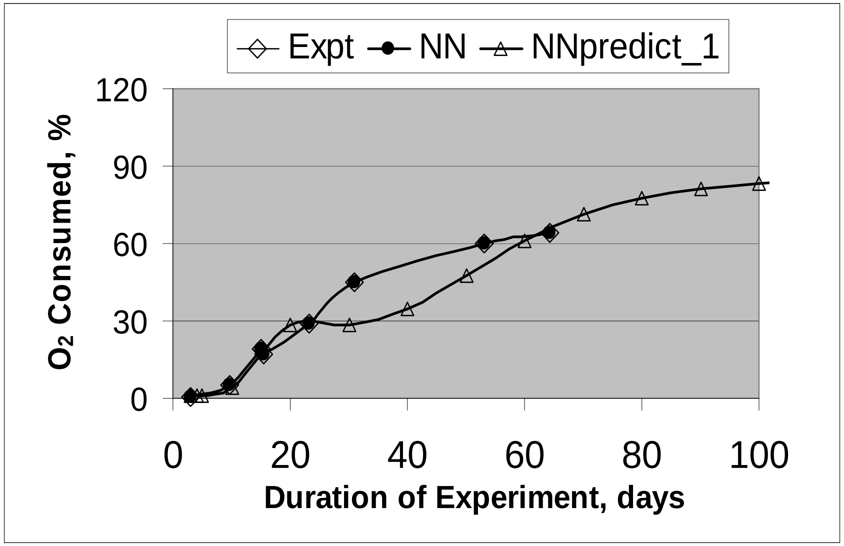
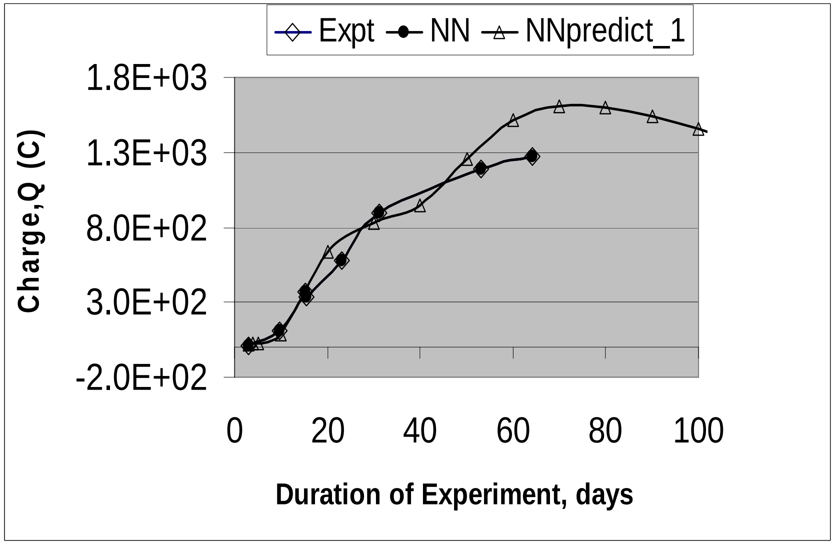
Analysis of Localized Corrosion Data on Ti-2



(c)



(d)

NN results in the study of crevice corrosion of grade-2 Ti in 0.27mol/dm^3 NaCl solution at 95^{o}C [2]. (c) Prediction of O_2 consumption, and (d) Prediction of electronic charge difference, Q. Expt: experimental data, NN: model prediction using the same input data that was used for training, NNpredict_1: prediction for 100 days.

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Summary

- Two examples of NN backpropagation are presented
- We demonstrated that this type of technique or tool can represent a useful complement to empirical or deterministic models
- NN model developed using polarization data for general corrosion of metallic glasses shows good agreement with experimental data at the specified operating conditions
- NN model developed using crevice corrosion data on grade-2 Titanium was validated against experimental data to show good agreement. The model was then used to predict future maximum penetration depth and other variables of interest under similar operating conditions