Mathematical Modeling: A Tool for Material Corrosion Prediction

1 Ukoba, O.Kingsley, 2 Oke, P.K, 3 Adetoro, K, 4 Olusunle, S.O.O 5 Ebiwonjumi, B, Medupin, R.O
1,2 Federal University of Technology, Akure Nigeria
3 Federal Polythenic, Ede Osun state Nigeria
1,4 Engineering Materials Development Institute, Akure Nigeria
5 Centre for Nuclear Energy Studies, University of Port Harcourt, Rivers State, Nigeria.

ABSTRACT

This work looked at mathematical modeling as a too for material corrosion property prediction. The weight loss technique was used to carry out the corrosion rate analysis for ductile Iron and mild steel and the data produced were used to carry out the mathematical analysis. It looked at how mathematical modeling can be used to predict corrosion and help to save resources and man-hour by using mathematical modeling. At the end, it was discovered that it has over 90% efficiency and concordance.

Keywords: Corrosion, material, mathematical, modeling, Oil and Gas

1. INTRODUCTION

A mathematical model is an abstract model that uses mathematical language to describe the behavior of a system. Eykhoff (1974) defined a mathematical model as a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in usable form.

A mathematical model can further be defined as an equation or a set of equations whose solution provides (time-space evolution of the state variable) physical behavior of the system being modeled. The structure of the state equation is not and cannot be fixed in advance; it depends on the modeling method adopted.

A physical system can be observed and studied mathematically in order to have an insight of its inner structure and behavior. For this purpose experiments are often organized and suitable mathematical models are designed or developed.

In the past mathematical modeling was linked with mathematical physics but today, it can be found in almost all spheres of human activities be it sciences, engineering, management or technology.

Mathematical models are used in the natural sciences and engineering disciplines (such as physics, biology, and electric engineering) and also in the social sciences (such as economics, sociology, and political science).

Mathematical models can take many forms, including but not limited to dynamical systems, statistical models, differential equations, or game theoretic models.

These and other types of models can overlap with a given model involving variety abstract structures.

In general, mathematical model may include logic models, as far as logic is taken as a part of mathematics. In many cases, the quality of a scientific field depends on how well the mathematical models developed on the theoretical side agree with results of repeatable experiments lack of agreement between theoretical mathematical models and experimental measurements often leads to important advances as better theories are developed.

1.1 Aims and Objectives of Mathematical Model

The major aims and objectives of mathematical modeling include:

- To translate the real life problem from its physical domain to mathematical problem in a mathematical domain in order to adopt the desired goal.
- To control the errors associated with the process of analyzing the model
- To be able to solve similar problems routinely.

1.2 Why Do We Need to Study Corrosion?

Many petrol chemical plants are large-scale equipment, which could be corrosive after some time. To determine the amount of contamination arising from corrosion will have to investigate the deleterious effect of the corrosion on the process of the reaction on the product quality.

The classic example of intergranular corrosion in chemical plant is the weld delay of unsterilized stainless steel. This is caused by the precipitation of chromium carbides at the grain boundaries in a zone adjacent to the Weld, where the temperature has been between 500 C - 800 C during welding.

Corrosion rate and the form of attack can change if the material is under stress. For some combination of metal, corrosive media and temperature, the phenomenon called stress cracking can occur. This leads to premature brittle failure of the metal that constitutes the petrol chemical plant.
The conditions that cause corrosion can arise in a variety of ways. For the brief discussion on the selection of material, it is convenient to classify corrosion into the following categories:

1. General wastage of material - uniform corrosion;
2. Galvanic corrosion - dissimilar metals in contact;
3. Pitting - localized attack;
4. Intergranular corrosion;
5. Stress corrosion;
6. Corrosion fatigue;
7. Erosion - corrosion;
8. High temperature oxidation;

Metallic corrosion is essentially an electrochemical process. Fair components are necessary to set up an electrochemical cell:

1. Anode - the corroding electrode;
2. A cathode - the positive, non-corroding electrode;
3. The conducting medium - the electrolyte - the corroding fluid;
4. Completion of the electrical circuit - through the material.

Cathodes areas can arise in many ways:

(i) Dissimilar metals;
(ii) Corrosion products;
(iii) Inclusions in the metal, such as slag;
(iv) Less aerated areas;
(v) Areas of differential concentration;
(iv) Differential strained areas.

Consider the simplest corrosion problem in nature where iron is exposed to the atmospheric oxygen in the presence of moisture leading to formation of rust, iron (III) oxide as well as iron (III) chloride respectively. The chemical reaction can be summarized as follows:

\[
\begin{align*}
   4Fe + 3O_2(g) & \rightarrow 2Fe_2O_3(s) \\
   2Fe^{2+}(s) + 3Cl^-(g) & \rightarrow 2FeCl_3(s)
\end{align*}
\]

In the above equation, the Oxidation State of Fe is from 0 to +3

From the above example and some other ones found in the literature, we note that corrosion process involves molecular and electronic charge exchanges in such a way that:

- There is energy depletion as a result of redox reactions
- Synthesis of compounds formed as a result of oxidation and some compounds lost as result of reduction.
- The chemistry of corrosion involves complex interactions of compounds in form of chemical reaction activation process.
- Some basic properties of the original material before corrosion takes place such as malleability, luster, conductivity and ductility etc is lost may be after corrosion.
- Knowledge of viscosity, specific heat capacity, thermal conductivity and density of the fluid concerned and even material science of the plant, where the corrosive media is kept, need be paid special attention.
- The prediction of the life expectancy of industrial plant using equation derived need be paid attention.

2. METHODOLOGY

2.1 Model Development

Data used for this work was that by Oke and Ukoba, 2012, were they looked at the “Corrosion behavior of ductile iron in different environment”. After careful examination of the experimental data, using the graphs and tables generated, it was concluded that the data follows a non-linear trend. Also, from the Analysis of Variance (ANOVA), the R square value is less than unity confirming that the trend is non-linear. Based on this, an empirical model is hereby developed.

2.1.1 Material Cost Model:

For material cost, cost-rating equation is given by

\[
Cost\ rating = \frac{C_{X_p}}{\sigma_4}
\]

Where:

- \(C_{X_p}\) = Cost per unit mass, N/kg
- \(\sigma_4\) = density stress, N/mm²

British standard on corrosion (BS1501) resistant materials made the following classification:
Table1: Acceptable corrosion rate

<table>
<thead>
<tr>
<th>Status</th>
<th>ipy</th>
<th>mm/y</th>
</tr>
</thead>
<tbody>
<tr>
<td>Completely Satisfactory</td>
<td>&lt;0.01</td>
<td>0.25</td>
</tr>
<tr>
<td>Use with caution</td>
<td>&lt;0.03</td>
<td>0.75</td>
</tr>
<tr>
<td>Use only for short exposure</td>
<td>&lt;0.06</td>
<td>1.5</td>
</tr>
<tr>
<td>Completely unsatisfactory</td>
<td>&gt;0.06</td>
<td>1.5</td>
</tr>
</tbody>
</table>

2.1.2 The Mathematical Models

In corrosion testing, the corrosion rate is measured by the reduction in weight of a specimen of known area over a fixed period of time. This is expressed by the formula:

\[
\text{corrosion rate} = \frac{W}{TSA \times \frac{T}{365}}
\]

Where:
- \( W \) = weight loss (gram)
- \( TSA \) = total surface area (mm\(^2\))
- \( T \) = time of exposure (days)

Generally, the average values of the properties of DI can be represented as a linear function represented by:

\[
y = \alpha + \beta x + \varepsilon
\]

\( y \) represents the response variables – weight loss, while \( x \) represents the predictor variable – period (days), \( \varepsilon \) is the error term, while \( \alpha, \beta \) and \( \varepsilon \) can never be known, so the data in Table (1) are used to obtain numerical estimates, \( a \) and \( b \) of \( \alpha \) and \( \beta \), and \( Y \) becomes the estimated response variable; Younger (1985). Hence,

\[
y = a + bx
\]

By minimizing Equation (2), it leads to the solution of simultaneous linear equations called the normal equations, given by:

\[
\sum_{i=1}^{n} Y_i = na + b \sum_{i=1}^{n} X_i
\]

\[
\sum_{i=1}^{n} X_i Y_i = a \sum_{i=1}^{n} X_i + b \sum_{i=1}^{n} X_i^2
\]

Mathematica was used to solve Equations (3) and (4) and the equations are as obtained in Equations (5) and (6).

2.3 Empirical Models Developed

Using the experimental values of material properties in Table 1 and Mat Lab, the constants ‘\( a \)’ and ‘\( b \)’ in equations (2), (3), and (4) were determined, and equations were obtained as:
a. Ambient environment:

\[ Y_o = 20.698 - 0.00153X_o + \alpha \]

Where:

- \( Y_o \) is the weight for the ambient environment
- \( X_o \) is the period (days) for the ambient environment
- \( \alpha \) is the error

**DETAIL OF THE ANALYSIS FOR AMBIENT ENVIRONMENT:**

\[ Y_o = 20.698 - 0.00153X_o + \alpha \]

<table>
<thead>
<tr>
<th>R</th>
<th>Rsqr</th>
<th>Adj Rsqr</th>
<th>Standard Error of Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9997</td>
<td>0.9995</td>
<td>0.9994</td>
<td>0.0025</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Std. Error</th>
<th>t</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y0 )</td>
<td>20.6945</td>
<td>0.0017</td>
<td>12332.7456</td>
</tr>
<tr>
<td>( a )</td>
<td>-0.0015</td>
<td>1.5513E-005</td>
<td>-96.9104</td>
</tr>
</tbody>
</table>

**Parameter** | **Value** | **StdErr** | **CV(%)** | **Dependencies**
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( y0 )</td>
<td>2.069e+1</td>
<td>1.678e-3</td>
<td>8.108e-3</td>
<td>0.6944987</td>
</tr>
<tr>
<td>( a )</td>
<td>-1.503e-3</td>
<td>1.551e-5</td>
<td>1.032e+0</td>
<td>0.6944987</td>
</tr>
</tbody>
</table>

**Analysis of Variance:**

<table>
<thead>
<tr>
<th><strong>DF</strong></th>
<th><strong>SS</strong></th>
<th><strong>MS</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>2</td>
<td>2958.7680</td>
</tr>
<tr>
<td>Residual</td>
<td>5</td>
<td>3.0107E-005</td>
</tr>
<tr>
<td>Total</td>
<td>7</td>
<td>2958.7681</td>
</tr>
</tbody>
</table>

Corrected for the mean of the observations:

<table>
<thead>
<tr>
<th><strong>DF</strong></th>
<th><strong>SS</strong></th>
<th><strong>MS</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>1</td>
<td>0.0566</td>
</tr>
<tr>
<td>Residual</td>
<td>5</td>
<td>3.0107E-005</td>
</tr>
<tr>
<td>Total</td>
<td>6</td>
<td>0.0566</td>
</tr>
</tbody>
</table>

**Statistical Tests:**

- **Normality Test (Shapiro-Wilk)**
  Passed (P = 0.7896)
  W Statistic = 0.9567
  Significance Level = 0.0500

- **Constant Variance Test**
  Failed (P = 0.0384)

b. Alkaline environment:

\[ Y_B = 20.585 + 0.0000863X_B + \alpha \]

Where:

- \( Y_B \) is the weight in the Alkaline environment
- \( X_B \) is the period in days
DETAILED ANALYSIS FOR ALKALINE ENVIRONMENT

<table>
<thead>
<tr>
<th>R</th>
<th>Rsqr</th>
<th>Adj Rsqr</th>
<th>Standard Error of Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0021</td>
<td>4.2821E-006</td>
<td>0.0000</td>
<td>0.0035</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Std. Error</th>
<th>t</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>y0</td>
<td>20.5866</td>
<td>0.0024</td>
<td>8542.9261</td>
</tr>
<tr>
<td>a</td>
<td>-1.0277E-007</td>
<td>2.2268E-005</td>
<td>-0.0046</td>
</tr>
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</table>

Analysis of Variance:

<table>
<thead>
<tr>
<th>DF</th>
<th>SS</th>
<th>MS</th>
<th>F</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
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<td>2966.6485</td>
<td>1483.3242</td>
<td>2.1411E-005</td>
</tr>
<tr>
<td>Residual</td>
<td>5</td>
<td>6.1714E-005</td>
<td>1.2343E-005</td>
<td>1.0286E-005</td>
</tr>
<tr>
<td>Total</td>
<td>7</td>
<td>2966.6485</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Corrected for the mean of the observations:

<table>
<thead>
<tr>
<th>DF</th>
<th>SS</th>
<th>MS</th>
<th>F</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
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<td>2.6427E-010</td>
<td>2.6427E-010</td>
<td>2.1411E-005</td>
</tr>
<tr>
<td>Residual</td>
<td>5</td>
<td>6.1714E-005</td>
<td>1.2343E-005</td>
<td>1.0286E-005</td>
</tr>
<tr>
<td>Total</td>
<td>6</td>
<td>6.1714E-005</td>
<td>1.0286E-005</td>
<td></td>
</tr>
</tbody>
</table>

Statistical Tests:

Normality Test (Shapiro-Wilk) Failed (P = 0.0016)
W Statistic= 0.6663 Significance Level = 0.0500

Constant Variance Test Passed (P = 0.6019)

c. Brackish environment:

\[ Y_{br} = 20.696 - 0.00217X_{br} + \alpha \]

Where:

\( Y_{br} \) is the weight in the brackish environment
\( X_{br} \) is the period in days for the brackish environment

DETAILS OF THE ANALYSIS FOR BRACKISH (NaCl):

<table>
<thead>
<tr>
<th>R</th>
<th>Rsqr</th>
<th>Adj Rsqr</th>
<th>Standard Error of Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>0.0004</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Std. Error</th>
<th>t</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>y0</td>
<td>20.6965</td>
<td>0.0003</td>
<td>78747.5172</td>
</tr>
<tr>
<td>a</td>
<td>-0.0022</td>
<td>2.4298E-006</td>
<td>-894.8038</td>
</tr>
</tbody>
</table>
Parameter | Value | StdErr | CV(%) | Dependencies
--- | --- | --- | --- | ---
y0 | 2.070e+1 | 2.628e-4 | 1.270e-3 | 0.6944985
a | -2.174e-3 | 2.430e-6 | 1.118e-1 | 0.6944985

Analysis of Variance:

<table>
<thead>
<tr>
<th></th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
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<td>2942.0282</td>
<td>1471.0141</td>
</tr>
<tr>
<td>Residual</td>
<td>5</td>
<td>7.3859E-007</td>
<td>1.4772E-007</td>
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<tr>
<td>Total</td>
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<td>2942.0282</td>
<td>420.2897</td>
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Corrected for the mean of the observations:

<table>
<thead>
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<th></th>
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<th>SS</th>
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<th>F</th>
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</tr>
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<tbody>
<tr>
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<td>0.1183</td>
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<td>&lt;0.0001</td>
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<td>Residual</td>
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<td>7.3859E-007</td>
<td>1.4772E-007</td>
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<tr>
<td>Total</td>
<td>6</td>
<td>0.1183</td>
<td>0.0197</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Statistical Tests:

**Normality Test (Shapiro-Wilk)**
Passed (P = 0.7896)

W Statistic= 0.9567 Significance Level = 0.0500

**Constant Variance Test**
Failed (P = 0.0384)

d. We did not have for air condition because it was the same.

Using the above empirical model, the predicted weight of the DI was developed. And it is shown below in table 2 as the predicted value.

![Fig 2: Predicted weight of Ductile Iron in various environments](image-url)
3. CONCLUSION

A lot of investment in terms of resources and man-hour goes into determining the corrosion property of a material. This work has shown that a lot can be saved in terms of resources and man-hour by using mathematical modeling after collecting a set of data that are consistent within a given period.

ACKNOWLEDGEMENT

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REFERENCES


