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.
ukobaking@yahoo.com

ABSTRACT

This work looked at mathematical modeling as a tool 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 500^0C - 800^0C 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.

VOL. 3, NO. 4, April 2013 ISSN 2225-7217
ARPN Journal of Science and Technology

http://www.ejournalofscience.org

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;
9. Hydrogen embrittlement.

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:

i) $4Fe + 3O_2(g) \rightarrow 2Fe_2O_3(s)$

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

ii) $2Fe^{\circ}(s) + 3Cl^{\circ}(g) \rightarrow 2Fe^{-3}Cl_3^{-1}(s)$

Reducing Agent   Oxidizing agent

The processes i & ii illustrates the importance of redox reaction, i.e. oxidation and reduction processes. In these processes, iron is an oxidizing agent since it gains 3 electrons and chlorine is a reducing agent since it loses 1 election.

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

$$Cost\ rating = \frac{CX_p}{\sigma_4}$$

Where:

CX_p = Cost per unit mass, ₦/kg
ρ = density, kg/m^3
σ_4 = density stress, N/mm^2

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

Table1: Acceptable corrosion rate

Status	ipy	mm/y
Completely Satisfactory	<0.01	0.25
Use with caution	<0.03	0.75
Use only for short exposure	<0.06	1.5
Completely unsatisfactory	>0.06	1.5

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:

$$corrosion\ rate = \frac{W}{TSA \times \frac{T}{365}}$$

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:

$$Y = \alpha + \beta X + \varepsilon \quad (1)$$

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

$$Y = a + bX \quad (2)$$

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

$$\sum_{i=1}^{n} Y_i = na + b\sum_{i=1}^{n} X_i \quad (3)$$

$$\sum_{i=1}^{n} X_i Y_i = a\sum_{i=1}^{n} X_i + b\sum_{i=1}^{n} X_i^2 \quad (4)$$

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

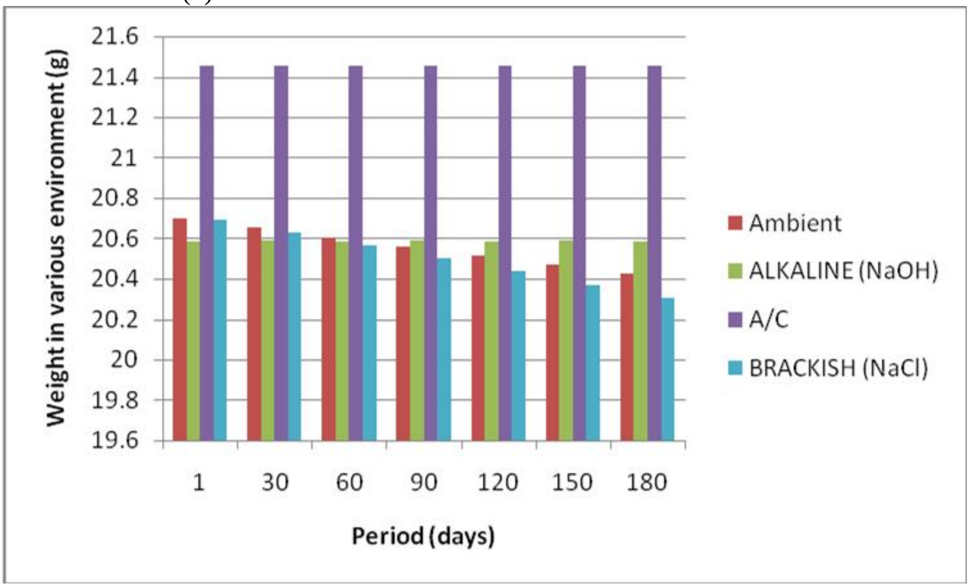

Fig 1: Weight of Ductile Iron in Various Environments

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:

ARPN Journal of Science and Technology

http://www.ejournalofscience.org

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

$\propto$ is the error

DETAIL OF THE ANALYSIS FOR AMBIENT ENVIRONMENT:

$$Y_o = 20.698 - 0.00153X_o + \alpha$$

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9997	0.9995	0.9994	0.0025

	Coefficient	Std. Error	t	P
y0	20.6945	0.0017	12332.7456	<0.0001
a	-0.0015	1.5513E-005	-96.9104	<0.0001

Parameter	Value	StdErr	CV(%)	Dependencies
y0	2.069e+1	1.678e-3	8.108e-3	0.6944987
a	-1.503e-3	1.551e-5	1.032e+0	0.6944987

Analysis of Variance:

Analysis of Variance:

	DF	SS	MS
Regression	2	2958.7680	1479.3840
Residual	5	3.0107E-005	6.0215E-006
Total	7	2958.7681	422.6812

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	1	0.0566	0.0566	9391.6216	<0.0001
Residual	5	3.0107E-005	6.0215E-006		
Total	6	0.0566	0.0094		

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:

$$Y_B = 20.585 + 0.0000863X_B + \propto$$

Where:

Y_B is the weight in the Alkaline environment

X_B is the period in days

ARPN Journal of Science and Technology

http://www.ejournalofscience.org

DETAIL OF THE ANALYSIS FOR ALKALINE ENVIRONMENT

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.0021	4.2821E-006	0.0000	0.0035

	Coefficient	Std. Error	t	P
y0	20.5866	0.0024	8542.9261	<0.0001
a	-1.0277E-007	2.2268E-005	-0.0046	0.9965

Parameter	Value	Std Err	CV (%)	Dependencies
y0	2.059e+1	2.410e-3	1.171e-2	0.6963588
a	-1.028e-7	2.227e-5	2.167e+4	0.6963588

Analysis of Variance:

Analysis of Variance:

	DF	SS	MS
Regression	2	2966.6485	1483.3242
Residual	5	6.1714E-005	1.2343E-005
Total	7	2966.6485	

423.8069

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	1	2.6427E-010	2.6427E-010	2.1411E-005	0.9965
Residual	5	6.1714E-005	1.2343E-005		
Total	6	6.1714E-005	1.0286E-005		

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:

$$Y_{Br} = 20.696 - 0.00217X_{Br} + \propto$$

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):

R	Rsqr	Adj Rsqr	Standard Error of Estimate
1.0000	1.0000	1.0000	0.0004

	Coefficient	Std. Error	t	P
y0	20.6965	0.0003	78747.5172	<0.0001
a	-0.0022	2.4298E-006	-894.8038	<0.0001

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:

	DF	SS	MS
Regression	2	2942.0282	1471.0141
Residual	5	7.3859E-007	1.4772E-007
Total	7	2942.0282	420.2897

Corrected for the mean of the observations:

	DF	SS	MS	F	P	
Regression	1	0.1183	0.1183	800673.1053	<0.0001	
Residual	5	7.3859E-007	1.4772E-007			
Total	6	0.1183	0.0197			

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.

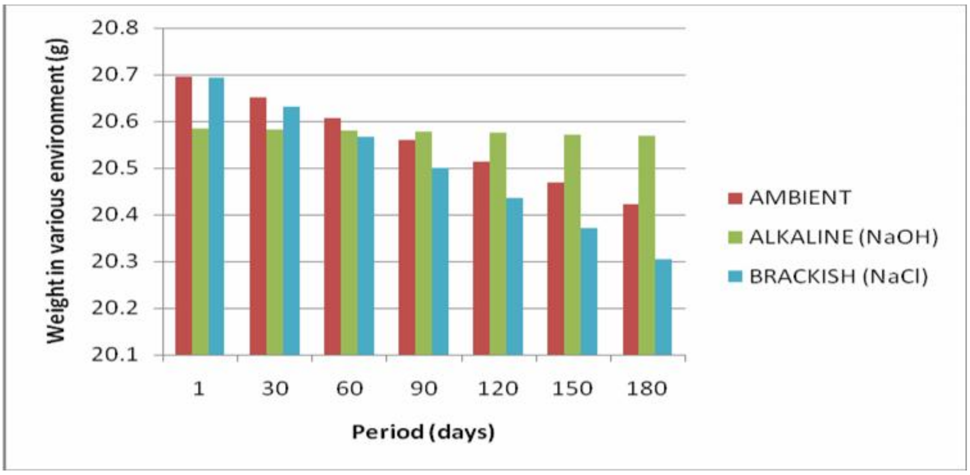

Fig 2: Predicted weight of Ductile Iron in various environments

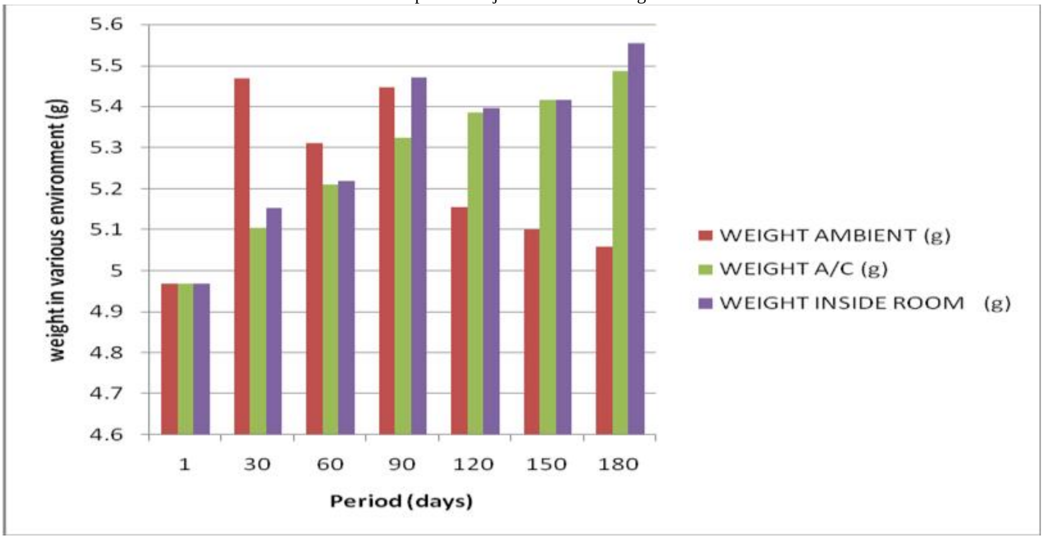

Fig 3: Weight of Mild steel in different environment

3. CONCLUSION

Alot of investment in terms of resources and man-hour goes into determining the corrosion property of a material. This work has shown that alot 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

The authors wish to acknowledge everyone whose work was cited, EMDI Akure management and staffs that aided in the research work especially Engr. Alasoluyi and others too numerous to mention, your effort and contributions are well appreciated.

REFERENCES

[1] Alan O. Sykes (2010). The Inaugural Coarse Lecture "An Introduction to Regression Analysis" Chicago Working Paper in Law & Economics.

[2] Ale S.O. (1981) "Curriculum development in modeling process". Trieste, Italy, International Centre for Theoretical Physics occasional publication,1981 ,SMR/99 - 42.

[3] Ale S.O. (1986). "Encouraging the Teaching of mathematical modeling in Nigerian schools." Nigerian Education Forum 9(2), 185 – 191,

[4] Oke, P.K and Ukoba, O.K (2012). "Corrosion behavior of ductile iron in different environment". 4th International Conference on Engineering Research and Development, ICERD2012, UniBen, Edo state Nigeria.

[5] Olokode, O.S. (2011). "Empirical Model for Estimating the Physical/Mechanical properties of Clay/Cement Steel". Pacific Journal of Science and Technology. 12(1):81-88.

[6] Oyelami, B and Asere, A (2010). "Mathematical modelling: an application to corrosion in a petroleum industry". National Mathematical Centre Abuja, Nigeria

[7] Morton Daniel (1980). "Mathematically Speaking". New York: Harcourt Brace, Jovanovich, Inc,

[8] Younger, M.S. (1985). A First Course in Linear Regression, 2nd Edition. Duxbury Press: Boston. MA.