EXPERIMENTAL AND COMPUTATIONAL STUDIES OF FURAN DERIVATIVES IN CORROSION INHIBITION OF MILD STEEL

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To my father, mother, brothers, sisters, wife and children

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ABSTRACT

Corrosion of metals causes huge losses in resources and industrial equipment especially when they are exposed to acidic medium. One of the most practical methods to control the corrosion of a metal is the use of heterocyclic organic compounds as corrosion inhibitors. A large number of organic compounds have been investigated as corrosion inhibitors; however, only few furan derivatives have been studied. In this study, eighteen furan derivatives were investigated as corrosion inhibitors for mild steel in hydrochloric acid. Furan derivatives were chosen as promising corrosion inhibitors based on their heterocyclic structures. The inhibition performance and corrosion process were studied using several techniques, namely potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), weight loss, adsorption isotherms, field emission scanning electron microscopy (FESEM), and X-ray photoelectron spectroscopy (XPS). The results showed the ability of furan derivatives to inhibit corrosion of mild steel in acidic solution and some of them showed high inhibition efficiencies of up to 96%. In addition, quantum chemical calculations using density functional theory (DFT) were used to evaluate inhibition performances of selected inhibitors and investigate active sites on the inhibitor molecule. The results showed the ability of DFT to explain the inhibition performances and assign the active sites of the inhibitors. Furthermore, several quantitative structure–activity relationship (QSAR) procedures were applied such as genetic algorithm-partial least square (GA-PLS), interval-PLS (IPLS), penalized multiple linear regression (PMLR) using ridge, LASSO and elastic net and sparse multiple linear regression (SMLR). The results showed that PMLR based on LASSO and elastic net, and SMLR based on elastic net were useful for the regression of the inhibition efficiencies. In conclusion, the quantum calculations and QSAR procedures complement the experimental investigations and interpret experimental results.

ABSTRAK

Kakisan logam menyebabkan kerugian besar dalam sumber dan peralatan industri terutamanya apabila ia terdedah kepada medium berasid. Salah satu kaedah yang paling praktikal untuk mengawal kakisan logam ialah penggunaan sebatian organik heterosiklik sebagai perencat kakisan. Sejumlah besar sebatian organik telah dikaji sebagai perencat kakisan; walau bagaimanapun, hanya beberapa terbitan furan telah dikaji. Dalam kajian ini, lapan belas terbitan furan telah dikaji sebagai perencat kakisan keluli lembut di dalam asid hidroklorik. Terbitan furan telah dipilih sebagai perencat kakisan yang menjanjikan berdasarkan kepada struktur heterosikliknya. Prestasi perencatan dan proses kakisan telah dikaji menggunakan beberapa teknik iaitu polarisasi potentiodinamik, spektroskopi impedans elektrokimia (EIS), penurunan berat, isoterma penjerapan, mikroskopi elektron pengimbas pemancaran medan dan spektroskopi fotoelektron sinar-X. Keputusan menunjukkan keupayaan terbitan furan untuk menghalang kakisan keluli lembut di dalam larutan berasid dan sebahagian daripadanya menunjukkan kecekapan perencatan yang tinggi sehingga 96%. Tambahan lagi, pengiraan kimia kuantum menggunakan teori fungsi ketumpatan (DFT) telah digunakan untuk menilai prestasi perencat terpilih dan mengkaji tapak aktif pada molekul perencat. Keputusan menunjukkan DFT berupaya menjelaskan prestasi perencatan dan menetapkan laman aktif perencat. Tambahan pula, beberapa prosedur hubungan struktur aktiviti kuantitatif (QSAR) telah digunakan seperti genetik algoritma kuasa dua terkecil separa (GA-PLS), selang-PLS (IPLS), regresi linear berganda terhukum menggunakan rabung (PMLR), LASSO, jaringan anjal dan regresi linear berganda jarang (SMLR). Keputusan menunjukkan PMLR berdasarkan LASSO dan jaringan anjal, dan SMLR berdasarkan jaringan anjal adalah berguna untuk regresi kecekapan perencatan. Kesimpulannya, pengiraan kuantum dan prosedur QSAR melengkapkan siasatan eksperimen dan mentafsir keputusan eksperimen.

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LIST OF ABBREVIATIONS

AD	-	Applicability domain
BE	-	Binding energy
BFA	-	5-Bromo-2-furoic acid
IE	-	Corrosion inhibition efficiency
CR	-	Corrosion rate
CE	-	Counter electrode
DFT	-	Density functional theory
DMFA	-	5-(Dimethylaminomethyl)furfuryl alcohol hydrochloride
EIS	-	Electrochemical impedance spectroscopy
ECMF	-	Ethyl 5-(chloromethyl)-2-furoate
EF	-	2-Ethylfuran
FESEM	-	Field emission scanning electron microscope
3-fold CV	-	3-Fold cross-validation
FMT	-	2-Furanmethanethiol
FFA	-	Furfuryl alcohol
FAM	-	Furfurylamine
FA	-	2-Furoic acid
FN	-	2-Furonitrile
FC	-	2-Furoyl chloride
FCH	-	5-(2-Furyl)-1,3-cyclohexanedione
GA	-	Genetic algorithm
GA-PLS	-	Genetic algorithm-partial least square
GNP	-	Gross national product
IPLS	-	Interval partial least square
LASSO	-	Least absolute shrinkage and selection operator
MSE	-	Mean squared error

MF	-	Methyl 2-furoate
MMF	-	Methyl 2-methyl-3-furoate
MNF	-	Methyl 5-nitro-2-furoate
MFF	-	5-Methylfurfural
MFA	-	5-Methylfurfurylamine
MM2	-	Molecular mechanics
MOPAC	-	Molecular orbital package
MLR	-	Multiple linear regression
NVF	-	2-(2-Nitrovinyl)furan
OCP	-	Open circuit potential
OLS	-	Ordinary least squares
PLS	-	Partial least squares
PMLR	-	Penalized multiple linear regression
QSAR	-	Quantitative structure activity relationship
QSIR	-	Quantitative structure inhibition relationship
RE	-	Reference electrode
RSS	-	Residual sum of squares
RR	-	Ridge regression
RMSECV	-	Root-mean-square error of cross-validation
SCE	-	Saturated calomel electrode
SEM	-	Scanning electron microscope
SCAD	-	Smoothly clipped absolute deviation
SMLR	-	Sparse multiple linear regression
SMLRE	-	Sparse multiple linear regression using elastic net
SMLRR	-	Sparse multiple linear regression using ridge penalty
SIS	-	Sure independence screening
FAA	-	trans-3-Furanacrylic acid
WE	-	Working electrode
XPS	-	X-ray photoelectron spectroscopy

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CHAPTER 1

INTRODUCTION

1.1 Overview

"*The cost of corrosion works out to much higher than any of the calamities the nation has faced over the years."* – NACE International India [1]**.** Verink [2] stated that the lost to corrosion in the United States is over $220 billion each year, which is equivalent to 3 or 4% of the gross national product (GNP). There are huge losses due to corrosion such as waste of materials and energy, economical loss, and environmental impact. Therefore, corrosion is an economic and environmental problem which leads to serious consequences. The consequences of corrosion are many such as loss of mechanical strength of metals in industry, structural failure or breakdown that causes hazards or injuries to people, fluids contamination in pipes and vessels, harms to the surrounding environment due to pipes and vessels leakage, mechanical damages and loss of surface properties of metals [1]. Therefore, awareness and huge efforts are required to reduce damages and losses to corrosion.

Metals corrosion is a destructive attack of metals by reaction with their environment [3]. A metal corrosion happens when a metal reacts chemically or electrochemically with a corrosive medium forming corrosion products. As a result, this metal loses weight and becomes corroded. The mechanism of corrosion process of an exposed metal to a corrosive solution follows the steps of an electrochemical reaction. The corrosive solution performs as an electrolyte and the metal acts as

anode. The steps of reaction involve the transfer of electrons from the metal to the cathode, and moving of metal ions to the electrolyte [3, 4].

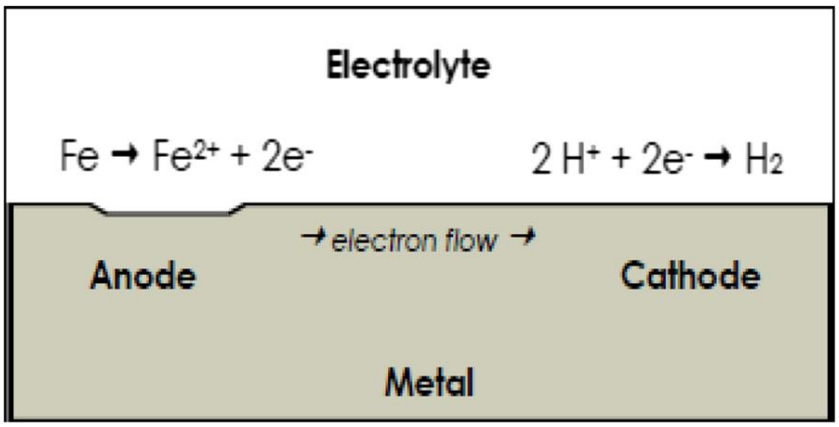

Figure 1.1: Schematic representation of metal electrochemical corrosion process [3]

The anodic and cathodic reactions of iron and steel are shown by the following chemical equations. The anodic reaction is as follows:

$$\mathrm{Fe} \rightarrow \mathrm{Fe}^{2+} + 2e^{-} \qquad (1.1)$$

After the release of electrons at the anode site of metal atoms, cathode reaction takes place. Four common reactions at the cathode site as follows [3]:

- oxygen reduction in acidic medium

$$\mathrm{O_2} + 4\mathrm{H}^{+} + 4e^{-} \rightarrow 2\mathrm{H_2O} \qquad (1.2)$$

- oxygen reduction in neutral or basic medium

$$\frac{1}{2}\mathrm{O_2} + \mathrm{H_2O} + 2e^{-} \rightarrow 2\mathrm{OH}^{-} \qquad (1.3)$$

- production of hydrogen in acidic medium

$$2\mathrm{H}^{+} + 2e^{-} \rightarrow \mathrm{H_2} \qquad (1.4)$$

- production of hydrogen in neutral water

$$2\mathrm{H_2O} + 2e^{-} \rightarrow \mathrm{H_2} + 2\mathrm{OH}^{-} \qquad (1.5)$$

Steel is a valuable material due to its wide applications in construction, domestic, transportation means, hospital equipment, etc [5]. It is the main material of instrumentation and industries equipment; however, it is reactive and prone to corrosion especially in acidic solutions. In industrial processes, acid solutions are

essential for cleaning, descaling, pickling of steel structures, and for well acidification to enhance oil/gas recovery. These processes are accompanied by considerable dissolution of the steel because of the aggressiveness of acid solutions [6-9]. Therefore, steel corrosion is a serious issue which result in waste of resources, decrease the equipment's lifetime and harms the environment [10]. Prevention of corrosion or reduction in the corrosion rate has been widely studied. Considerable effort has been given to studying iron and mild steel corrosion in acid solutions [11-13]. Therefore, it is necessary to increase the efforts given to steel corrosion due to the following reasons:

- Increasing the use of steel in industries, machinery, constructing, long water and oil/gas pipelines, and in wide aspect of daily life.
- The increase of air and water pollution which cause more corrosive environment.
- Corrosion may cause fail in tragic way for the strict safety standards of operating equipment in industries such as electrochemical and chemical industries, power, nuclear, petroleum, and food industry.

Various methodologies are used to prevent and control corrosion such as the use of a proper design, selection of suitable materials, coatings and linings, cathodic protection, and corrosion inhibitors [2]. The use of corrosion inhibitors is the most practical technique to prevent and control steel corrosion in chemical and electrochemical industries, nuclear, power, petroleum, food industry, and oil/gas pipelines [14].

1.2 Corrosion inhibitors

Corrosion inhibitors are one of the economic techniques to protect metals from corrosion. Inhibitors are substances that are added to corrosive media in order to decrease or prevent metal corrosion [4, 15-17]. A large number of inorganic and organic compounds have been tested as corrosion inhibitors [17]. Many organic compounds are found to be effective inhibitors against metal corrosion. According

to Raja, Qureshi, Abdul Rahim, Osman and Awang [13] most reported corrosion inhibitors in acidic media are organic compounds with heteroatoms at their functional groups such as sulfur, nitrogen, oxygen, phosphorus, or compounds containing multiple bonds, give them the ability to be adsorbed onto the surface of different metals. The adsorption of the heteroatoms compounds onto metal surface forms a protective film, blocks active sites and thus decreases the corrosion rate. The mechanism of adsorption is by the overlap of p-electrons of heterocyclic molecules to vacant d-orbital of metal atoms [16, 18-21]. Thus, corrosion inhibitors play two roles, prevention metal dissolution and minimizing acid consumption [22].

The corrosion inhibition performance of organic inhibitors depends on their electronic structures, electron density at the donor sites, molecular area, aromaticity and steric factor. The higher number of lone pair and π-electrons on the inhibitor molecule increases its electron density and causes a strong interaction with metal surface [23, 24]. Furan derivatives are heterocyclic five-membered aromatic compounds. The aromatic characteristic of furan derivatives and the presence of oxygen atom with two pairs of unshared electrons in their molecules give them ability to perform as efficient corrosion inhibitors [25].

1.3 Methods of Measurements

The investigation of corrosion inhibition performance of the inhibitors can be conducted experimentally and/or using computational chemistry. Experimental measurements of the corrosion inhibition efficiency and monitoring the inhibition process are usually conducted using various techniques such as weight loss, linear polarization, potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), UV−visible spectroscopy, scanning electron microscope (SEM), X-ray spectroscopy (EDX) [26], and cyclic voltammetry [27]. However, applying experimental procedures only is expensive, time consuming and harmful to the environment [28]. Therefore, computational chemistry has been a field of interest for many researchers [29].

Besides the experimental measurements, theoretical tools are useful and powerful means in corrosion inhibition studies [30]. The use of theoretical and computational means in corrosion inhibition studies has become increasingly desirable [29]. Computational methods have been applied to study, design and develop organic corrosion inhibitors [31]. Many theoretical techniques such as quantum chemical calculations and quantitative structure–activity relationship (QSAR) have attracted great attention of many researchers in the studies of corrosion inhibitors [32].

Quantum chemical calculations are useful techniques to study reaction mechanisms in a molecule, electronic structure level and electronic parameters of a molecule using quantum chemistry methodologies [32]. Quantum chemical calculations are applied to calculate structural properties of organic corrosion inhibitors, which are related to corrosion inhibition properties [29]. Density functional theory (DFT) is one of the quantum chemical methods which is considered as a powerful theoretical tool with reasonable accuracy in calculating molecule's electronic parameters, and analyzing inhibitor/surface interaction in corrosion inhibition studies. Various electronic parameters, which are obtained by quantum chemistry methodologies, are used for theoretical investigations of corrosion inhibition properties and to support experimental measurements [31-33]. Among these parameters are the highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital energy (E_{LUMO}), energy gap (ΔE), dipole moment (μ), ionization potential (I), electron affinity (A), softness (S), the fraction of electrons transferred from the inhibitor to the metal surface (ΔN), Mulliken atomic charges, and Fukui indices can be calculated using DFT. Besides the usefulness of those parameters to explain the relationship between molecular properties of the corrosion inhibitors and their inhibition efficiencies [21, 34, 35], they can be used to explain the experimental findings and to design new inhibitors.

QSAR is a computational technique that has been widely applied in the field of medicinal chemistry for estimation of molecular behavior, electronic structure and activity [35, 36]. The principle of QSAR is to model a physicochemical activity or biological activity of collected chemical compounds based on their structural

properties. Therefore, QSAR is a mathematical model that can be used to predict the biological activity or physicochemical properties such as corrosion inhibition efficiency (IE) of new compounds [36-38]. The use of QSAR models to predict corrosion inhibition efficiencies of potential organic compounds has become increasingly desirable [35]. Therefore, the number of organic compounds to be experimentally tested can be reduced to only those suggested compounds by QSAR models. Accordingly, a large number of non-effective compounds will be excluded from experimental measurements which lead to save both time and money [28]. In the area of QSAR modeling, chemical compounds are often treated as observations, molecular descriptors are treated as predictor variables, and the response variable is represented by physicochemical properties such as biological activity or corrosion inhibition efficiency. Typically, a good QSAR model should possess high predictability and be easily interpretive [39]. Molecular descriptors are calculated based on the molecular structures of chemical compounds. Quantum chemical calculations are the most traditional methods for molecular descriptors calculations. In addition, other techniques such as Molconn-Z, CODESSA and Dragon software are used to calculate molecular descriptors [40]. A number of 4885 molecular descriptors can be calculated using Dragon software [41]. Different approaches are used as regression methods such as partial least squares (PLS) [42] and multiple linear regression (MLR) [43].

PLS regression is an effective approach for finding the correlation between a molecule structure and its properties. Mathematically, PLS relates dependent variables matrix (Y) to molecular structure descriptors matrix (X). The objectives of PLS are to achieve several steps. First, PLS approximate the X and Y data matrices, and maximize the correlation between them. A regression equation relating each Y variable with the X matrix is created during the stepwise extraction of PLS components and the independently assessment of the importance of each component. PLS splits the X matrix into several latent variables with best correlation with the molecules activities [42].

The analysis of MLR is one of the most important approaches for constructing QSAR models. It is used for analyzing the relationship between many

predictor and response variables. In addition, MLR is considered as the traditional and standard method for multivariate data analysis. Multivariate analysis is conducted using statistical methods to analyze multidimensional data metrics. It relates the dependent variable, a desired chemical property such as biological activity or corrosion inhibition efficiency, to a number of independent variables (molecular descriptors) based on linear equations. This regression method estimates the regression coefficients values based on least square curve fitting method [43].

1.4 Problem Statement

The inhibition of steel corrosion in acidic solutions using organic compounds as corrosion inhibitors is the most practical technique. Large number of organic compounds has been investigated as corrosion inhibitors. However, only few furan derivatives have been investigated as corrosion inhibitors. Therefore, this research focuses to search new efficient furan derivatives as inhibitors for steel corrosion in acidic solutions. In addition, the use of experimental measures only for investigating new corrosion inhibitors is costly, time consuming and harmful to the environment. Therefore, it is economic, fast, and eco-friendly to apply computational techniques as predictive techniques such as quantum chemical calculations and QSAR modeling approach. Computational methods can complement the experimental investigations and be effective tools to propose the best corrosion inhibitors among a group of organic inhibitors. In this study, quantum chemical calculations and QSAR modeling are used to overcome the experimental disadvantages. Furthermore, most of computational modeling studies were conducted based on quantum chemical parameters (descriptors); however, limited studies have used electronic properties-based descriptors in corrosion inhibition studies. Therefore, in this study, besides the quantum chemical parameters, electronic properties-based descriptors (calculated by Dragon software) are effectively used.

1.5 Research Objectives

The objectives of the study are:

1. To evaluate the inhibition performance of selected furan derivatives (18 compounds) as corrosion inhibitors for mild steel in acidic medium (1M HCl) experimentally at room temperature using potentiodynamic polarization measurements at two concentrations 0.002M and 0.005M, and to study the detailed inhibition performance for one selected inhibitor using potentiodynamic polarization, EIS, and weight loss at various concentrations, i.e. 0.0005M, 0.001M, 0.002M and 0.005M.
2. To investigate the adsorption mechanism of a selected inhibitor on the surface of mild steel using adsorption isotherms, field emission scanning electron microscope (FESEM), and X-ray photoelectron spectroscopy (XPS) analyses.
3. To conduct quantum chemical calculations on selected inhibitors using DFT method by calculating different quantum chemical parameters to be used for theoretical evaluations of the inhibitors performance.
4. To develop QSAR modeling procedures based on electronic properties-based descriptors (calculated by Dragon software) and the experimental corrosion inhibition efficiencies of the studied inhibitors.

1.6 Significance of the Study

The wide uses of steel in every aspect of our lives reflect the huge loss in economy because of its corrosion. Therefore, this study contributes significantly to propose new corrosion inhibitors as one of the most effective, practical and economical techniques to control steel corrosion. The use of quantum chemical calculations in this study complements the experimental measurements and provides theoretical descriptions for the inhibition behavior of the proposed corrosion inhibitors. QSAR modeling aims to produce new mathematical models to be derived from the high dimensional molecular descriptors obtained by Dragon software.

Since the use of Dragon software for the calculations of molecular descriptors is very limited; therefore, the calculations of molecular descriptors using Dragon software will introduce new descriptors, which, in turn, contribute to enrich the description of inhibitors' corrosion inhibition properties. These modeling procedures will serve as effective tools for building predictive, robust and reliable QSAR models. The implementation of these procedures is useful to predict potential efficient corrosion inhibitors, and thus will reduce the cost and time of testing inefficient organic compounds.

1.7 Scope of the Research

The research is designed to study the corrosion inhibition efficiencies of 18 furan derivatives at room temperature and also to investigate the inhibition mechanism based on experimental measurements and theoretical studies. The used experimental measurements are potentiodynamic polarization measurements, EIS, weight loss (gravimetric), adsorption isotherms, FESEM, and XPS analyses. Potentiodynamic polarization measurements will be used to investigate corrosion inhibition efficiencies of the studied furan derivatives (18 compounds) at 0.002M and 0.005M concentrations of the furan derivatives in 1M HCl. Besides the potentiodynamic polarization measurements, the EIS and weight loss measurements will be used to test the inhibition efficiencies of one selected inhibitor, i.e. 2-Furanmethanethiol (FMT) at 0.0005M, 0.001M, 0.002M and 0.005M concentrations of furan derivatives in 1M HCl. The data obtained from weight loss measurements will be used to carry out adsorption isotherms study. The adsorption isotherms calculations will be carried out to investigate the adsorption mechanism of the selected inhibitor onto mild steel surface. The FESEM will be used to explore the surface morphology of polished surface without immersion in corrosive solutions, uninhibited specimens (immersed in 1M HCl), and inhibited specimens by the selected inhibitor in 1M HCl. The XPS analyses will be used to confirm the adsorption of the selected furan derivative as a corrosion inhibitor onto mild steel

surface, and also to elucidate the nature of the organic thin layer formed on the mild steel surface.

Theoretically, two computational approaches are performed, i.e. quantum chemical calculations and QSAR. Quantum chemical calculations using DFT will be conducted to calculate quantum parameters and discuss the relationship with the experimental inhibition efficiencies. The results of the quantum chemical calculations can be served as a theoretical confirmation for the experimental data based on the quantum chemistry of the inhibitors molecules. QSAR studies will be carried out to model the experimental corrosion inhibition efficiencies of the studied inhibitors based on their structural properties (molecular descriptors). Molecular descriptors will be calculated using Dragon software. Various regression methods, i.e. PLS, MLR using ordinary least squares (OLS), and penalized multiple linear regression (PMLR) will be used in this study to develop robust and reliable QSAR models.

1.8 Outline of the Thesis

The thesis is divided into six chapters. Chapter 1 gives an overview of the study, brief background to corrosion inhibitors, experimental methods of measurements, and theoretical approaches. It includes also the problem statement, objectives, significant and scope of the present study. Chapter 2 reviews the relevant literature of the present study. The literature was reviewed under three main topics, i.e. organic compounds as corrosion inhibitors, quantum chemical calculations on corrosion inhibitors, and QSAR studies on corrosion inhibition of mild steel by organic corrosion inhibitors. Chapter 3 gives the details of the experimental work. It includes a description of the main experimental procedures used to investigate the corrosion inhibition of mild steel in 1M HCl. The results obtained from the experimental work, discussion, and derived conclusions are presented. Chapter 4 provides the details of the quantum chemical calculation. The description of the used procedures and calculated quantum parameters are presented. Chapter 5 presents the

chemometrics study. It gives the details of several procedures and methods of developing QSAR models. It discusses the evaluation and validation criteria of the developed QSAR models. Chapter 6 gives a brief summary of this study and main conclusions of the present work, and provides some suggestions for future work.

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