

Corrosion Inhibition and Adsorption Characteristics of API 5L X-52 Steel by an Antibiotic Drug in HCl Solution

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Authors' contributions

This work was carried out in collaboration between all authors. Author FA, performed the experimental analysis and wrote the first draft. Author MI designed the study and supervised the experimental work. Authors KU and FA carried out the computational study. Authors FA and GI did the statistical analysis. All authors read and approved the final manuscript.

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ABSTRACT

The corrosion inhibition potential of an antibiotic drug called moxifloxacin for API 5L X-52 steel in 2 M HCl solution was investigated using experimental (gravimetric and electrochemical impedance spectroscopy) and theoretical approaches. Results obtained from gravimetric and electrochemical impedance spectroscopy measurements revealed that moxifloxacin inhibit the corrosion of steel, and recorded instantaneous maximum inhibition efficiency of 88% and 82.7% respectively at 303 ± 1 K. Statistical consideration revealed that there was no significant difference between the two methods employed. The adsorption behavior of the inhibitor was best described by the Langmuir adsorption isotherm. Dipole moment calculated from quantum chemical calculation method was found to be in good agreement with those reported for some good corrosion inhibitors. The sites for nucleophilic and electrophilic attacks correspond to the atom N3, C12, C15, C22, C24, C27, O28 and N3, N8, C11, C13, C15, O28 respectively.

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1. INTRODUCTION

The application of API 5L X-52 steel pipes as means of transporting industrial and domestic fluids, crude petroleum and sewage has been an extensive practice. The problem of internal corrosion of these pipes is equally a giant industrial and scientific challenge. The internal walls of pipelines in crude oil pipes is more susceptible to internal corrosion because of the presence of water which is denser than oil. The existence of corrosive agent such as Cl^- , SO_4^{2-} , CO_2 , H_2S and Sulphur reducing bacterial contributes to the internal corrosion of API 5L X-52 steel pipe [1]. An estimate of losses to corrosion indicates that cost of corrosion is huge. The consequence of pipeline corrosion leakage includes: resultant causalities, ecological impact, contamination and shut down. The adverse effect of corrosion can be reduced significantly by understanding the mechanism and subsequent application of corrosion control measure through injection of chemical inhibitors, pigging operations [1]. The use of chemical inhibitors such as plant extracts, synthetic compounds and drugs are convenient and cheap [2-5]. Organic compounds containing heteroatoms like P, S, N, and O have been reported to be efficient corrosion inhibitors [6]. The application of pharmaceutical drugs as corrosion inhibitors has been widely reported by several authors [5-12].

As a contribution to the current interest on environmentally friendly corrosion inhibitors, the present study aims at broadening the application of antibiotics drug for API 5L X-52 steel pipeline corrosion inhibition and adsorption behaviour in HCl solution using Gravimetric, electrochemical impedance spectroscopy (EIS) techniques and theoretical approaches

2. EXPERIMENTAL DETAILS

2.1 Materials

API 5L X-52 steel used in this work were obtained from Chemistry Department, University of Calabar, Calabar-Nigeria, through Dr. (Mrs.) M. E. Ikpi. API 5L X-52 steel has the composition given in Table 1.

Gravimetric experiments were conducted on the steel with dimension 1.0 cm x 1.0 cm x 1.0 cm and with a surface area of 6.0 cm^2 , whereas 1.0 cm^2 exposed surface area isolated with commercially available epoxy resin were used in electrochemical impedance spectroscopy (EIS) technique as a working electrode. Before used for the corrosion test, the steel samples were polished using emery paper up to 800 grit, degreased with absolute ethanol, and dried using acetone in gravimetric experiment. All chemicals used were of Analar grade.

2.2 Inhibitor Preparation

Moxifloxacin is the antibiotic drug used in the study, the tablets of it were used without further purification. Different concentrations were prepared by dissolving appropriate quantities of the tablets from the mass of the drug sample. The stock solution of the drug was prepared by digesting 500 mg in 1000 ml of 2 M HCl solution to obtain 500 ppm concentration of stock solution. The stock solution was allowed to stand for 24 hours. From the stock solution after filtering, inhibitor test solution was prepared for different concentration using the dilution formula $C_1V_1 = C_2V_2$. The concentrations of the inhibitor used were 50 ppm, 100 ppm, 200 ppm, 300 ppm and 500 ppm for EIS and 50 ppm, 200 ppm and 500 ppm for gravimetric experiment.

2.3 Gravimetric Experiments

The steel sample used for gravimetric experiment were previously weighed and completely immersed and suspended with the help of a nylon thread and rod in 250 ml of the test solution of 2 M HCl alone, and with different concentration of the inhibitors at (303 ± 1) K. The specimen was retrieved separately after 5 days, 10 days, 15 days, 20 days and 25 days of immersion. The corrosion products were removed by washing each specimen with distilled water using a bristle brush. The washed specimen was rinsed in acetone and dried before reweighing. The difference in weights for each period of immersion were taken and recorded as weight loss. From the weight loss results, the inhibition efficiency, surface coverage (θ) and

Table 1. Chemical composition of API 5L X-52 steel

Element	C	Mn	P	S	Si	V	Nb	Ti	Fe
Wt %	0.24	1.40	0.05	0.015	0.45	0.01	0.05	0.04	98.28

the corrosion rate of the steel were calculated using equation 1a, 1b and 2 respectively.

$$IE \% = (W_{\text{blank}} - W_{\text{inh}}/W_{\text{blank}}) \times 100 \quad (1a)$$

$$\theta = (W_{\text{blank}} - W_{\text{inh}}/W_{\text{blank}}) \quad (1b)$$

$$CR = (WL/At) \times 100 \quad (2)$$

where W_{blank} is the weight loss for the blank, W_{inh} is the weight loss in the presence of inhibitor, WL is the weight loss in mg, A is the specimen surface area, t is immersion time and θ is the surface coverage.

2.4 Electrochemical Impedance Spectroscopy (EIS)

Before EIS measurement, the working electrode was introduced into the test solution and left for 30 minutes to attain the open circuit potential (OCP) at which the change of OCP with time is 5 mV/s. During this stage, the system had been stabilized. The model of the EIS and the principle used for this research has been documented in [7].

2.5 Theoretical Consideration

The Fukui indices, bond length and dipole moment were observed with a view to establish the active sites as well as local reactivity of the molecule. The simulations were performed by means of density functional theory (DFT) electronic program using the Dmol³ module present in the Material studio 4.0 software.

3. RESULTS AND DISCUSSION

3.1 Gravimetric Results

Table 2 shows the variation of weight loss, average corrosion rate and inhibition efficiency of

API 5L X-52 steel in 2 M HCl solution in absence and presence of inhibitor at different time interval at (303 ± 1) K. The weight loss increased with exposure time and decreased by the addition of inhibitor. The percentage inhibition efficiency (IE %) was calculated based on equation.1.

Table 2 and Fig. 1a shows that the inhibition efficiency of the inhibitor at a definite fixed time of immersion increases with increasing the concentration of the inhibitor, except for day 5 and 10. The dependency of the inhibition efficiency of the MOX on the immersion time in presence of certain concentration of the inhibitor shows an increased in the efficiency with increasing in the immersion, this behaviour is probably due to the interaction of the inhibitor with the corrosion products [13].

Fig. 1b shows the trend of the average corrosion rate for MOX in API 5L X-52 steel. The results of the experiment show a decrease in corrosion rate of the steel in the presence of the inhibitor. The increase in corrosion rate of API 5L X-52 steel in the blank solution within the five weeks of immersion period shows that the rate of corrosion of the API 5L X-52 steel is higher in the blank than in acid-inhibitor solution. The corrosion rate decreases as the inhibition efficiency increases, signifying that the surface coverage of the API 5L X-52 steel is been saturated with high concentration of moxifloxacin.

3.1.1 Kinetic studies

In order to study the kinetics of corrosion inhibition of API 5L X-52 steel in HCl solution, the data obtained from gravimetric measurement were used to fit curve for different order of reaction kinetics. The results obtained revealed that the data fitted first order reaction kinetics. This implies that the rate of corrosion of API 5L X-52 steel in HCl solution could be related to the weight loss of API 5L X-52 steel based on equ. 3

Table 2. Weight loss, inhibition efficiency and average corrosion rate values calculated for API 5L X-52 steel in 2 M HCl solution in absence and presence of various concentration of the studied inhibitor at (303 ± 1) K

Conc.	Immersion period										CR (mgcm ⁻² day ⁻¹)
	5 days		10 days		15 days		20 days		25 days		
gcm ⁻²	IE %	gcm ⁻²	IE %	gcm ⁻²	IE %	gcm ⁻²	IE %	gcm ⁻²	IE %	gcm ⁻²	IE %
Blank	1.317		2.864		4.181		5.698		6.430		1.546
50ppm	1.011	23	2.134	25	2.145	48	2.231	60	2.326	63	1.061
200ppm	0.481	63	0.918	67	1.148	72	1.108	80	0.931	85	0.496
500ppm	0.794	39	1.026	64	1.170	72	0.719	87	0.741	88	0.563

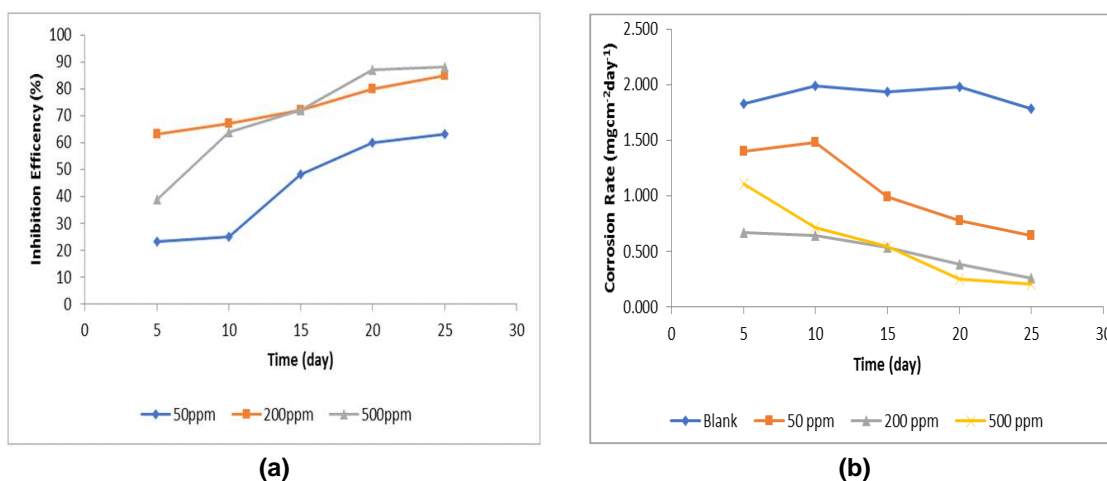


Fig. 1. (a) Variation of inhibition efficiency with time for API 5L X-52 steel in 2 M HCl solution containing different concentrations of moxifloxacin (MOXI) at 303 K. (b) Variation of corrosion rate with time for the corrosion of API 5L X-52 steel in 2 M HCl containing various concentration of moxifloxacin (MOXI).

$$d[Fe]_o / dt = K_1[Fe]_t \quad (3)$$

where $[Fe]$ is the concentration of API 5L X-52 steel that has reacted. Rearranging and integrating equ. 3 within the limits $[Fe]_t$ and $[Fe]_o$ at time t and $t=0$ respectively, equ. 3 becomes;

$$\text{Log } [Fe]_t - [Fe]_o = -K_1 t / 2.303 \quad (4)$$

Equ. 4 can also be expressed as equ. 5

$$\ln([Fe]_t/[Fe]_o) = -K_1 t \quad (5)$$

where $[Fe]_o$ and $[Fe]_t$ are the weights of initial and final concentration of API 5L X-52 steel. Therefore, the plot of $\ln([Fe]_t/[Fe]_o)$ versus time (t) gives a straight line with slope is equal to K_1 [14,15]. Fig. 2 show the kinetics plots for the corrosion of API 5L X-52 steel in the absence and presence of different concentrations of MOX at 303 K. From the slopes of the plots, the values of K_1 were computed and used to obtained the half-life of the corrosion of API 5L X-52 steel according to equ. 6

$$t_{1/2} = 0.693/K_1 \quad (6)$$

Values of K_1 and $t_{1/2}$ are listed in Table 3. The rate constant decreases with increasing concentration of the inhibitors. It was also observed that the half-life of API 5L X-52 steel in 2 M HCl solution containing various concentrations of the inhibitors are higher than

the half-life of API 5L X-52 steel in the blank solution indicating that the compounds MOX increase the half-life of API 5L X-52 steel in HCl solution, thereby reducing the rate of dissolution of API 5L X-52 steel at 303 K. The results obtained for the rate constant and half-life exhibit similar trends to works reported by [14,16-19].

3.2 Electrochemical Impedance Spectroscopy (EIS)

Fig. 3 shows the Nyquist impedance plot of API 5L X-52 steel in 2 M HCl solution in absence and presence of different concentration of MOX. The Nyquist plots contain depressed semicircle in high frequency region with center under the real axis. The size of the semicircle increases with increase in the concentration of the inhibitor, indicating that the corrosion of API 5L X-52 steel is controlled by a charge transfer process [20,21]. The impedance spectra of the Nyquist plots were appropriately analyzed by fitting the data into the equivalent circuit model shown in Fig. 4. The model is consisted of solution resistance (R_s), charge transfer resistance of the interfacial corrosion (R_{ct}) and constant phase element representing double layer capacitance (C_{dl}). The capacitance double layer (C_{dl}) is defined in equ.7 [22-24].

$$C_{dl} = 1/2\pi f_{\max} R_{ct} \quad (7)$$

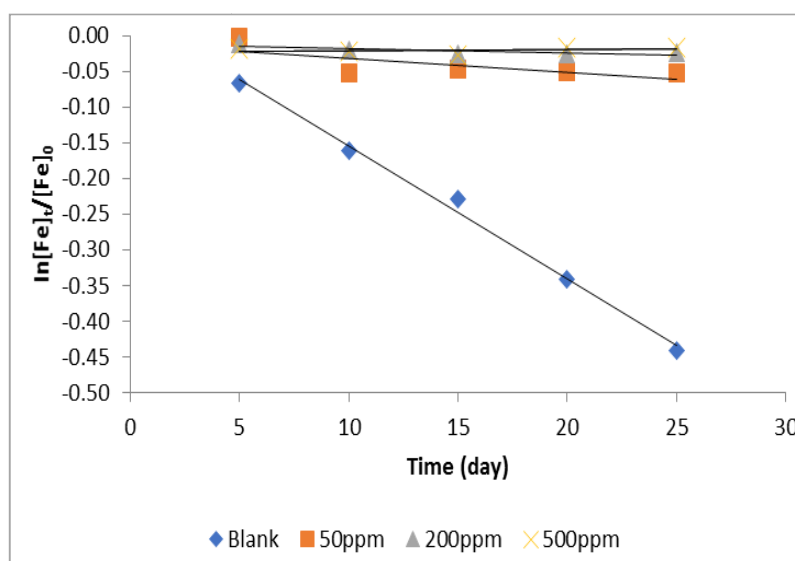


Fig. 2. Plot of $\ln([Fe]_t/[Fe]_o)$ against time t , for API 5L X-52 steel in 2 M HCl solution containing moxifloxacin at different concentrations

Table 3. Calculated values of rate constant and half-life for API 5L X-52 steel in 2 M HCl solution containing various concentration of MOX at 303 K.

System	Rate constant $\times 10^{-3} \text{ day}^{-1}$	Half-life(days)	R^2
Blank (2 M HCl)	0.018	39	0.999
50 ppm MOX + 2 M HCl	0.002	347	0.994
200 ppm MOX + 2 M HCl	0.001	693	0.902
500 ppm MOX + 2 M HCl	0.001	693	0.986

where f_{max} is the frequency at which the imaginary component of the impedance (Z_{max}) is maximal. The charge transfer resistance (R_{ct}), constant phase element (CPE), surface coverage (θ), inhibition efficiency (IE %) were calculated and are Tabulated in Table 4. The R_{ct} values increases in the inhibited system with a corresponding decrease in the double layer capacitance (C_{dl}) as the concentration of the inhibiting compounds increases. The increasing R_{ct} values were in agreement with the increasing diameters of the Nyquist semicircles. The observed decrease in C_{dl} values corresponds to alteration of the double layer thickness, due to the covering or blockage of large surface of the steel by the inhibitors which protected the metal from the corrosive effect of the aggressive acids. Charge transfer resistance (R_{ct}) values increased with increasing concentration of the inhibitors, this confirmed the inhibiting properties of the compounds. Similar report has been documented previously [20,21]. Inhibition efficiency from impedance data was estimated by comparing the values of the charge transfer resistance in the absence $R_{ct_{blank}}$ and presence of inhibitors $R_{ct_{inh}}$

according to equ. 8a, and the surface coverage (θ) was also calculated using equ. 8b and the results were presented in Table 4.

$$IE \% = (R_{ct_{inh}} - R_{ct_{blank}} / R_{ct_{inh}}) \times 100 \quad (8a)$$

$$\theta = (R_{ct_{inh}} - R_{ct_{blank}} / R_{ct_{inh}}) \quad (8b)$$

where $R_{ct_{inh}}$ is the charge transfer resistance of the inhibited solution, $R_{ct_{blank}}$ is the charge transfer resistance of the uninhibited solution and θ is the surface coverage. Base on the Figure 5 and the statistical analysis, it is observed that inhibition efficiency results obtained from both methods were in good agreement.

3.2.1 Statistical consideration

Quotient test was used to test whether the corrosion rate and inhibition efficiency results of MOXI at the concentration of 500 ppm after 5 days and 10 days of immersion should be retained or rejected. The Q_{exp} (Quotient experimental test) values were obtained using equ. 9 or 10.

$$Q_{exp} = \frac{\text{Difference between the Questionable value and the closer value}}{\text{Range between the set of values}} \quad (9)$$

$$Q_{exp} = x_n - x_i / x_2 - x_1 \quad (10)$$

In the average corrosion rate, $x_n = 1.10$, $x_i = 0.66$, $x_2 = 1.40$ and $x_1 = 0.66$, while in average inhibition efficiency, $x_n = 63$, $x_i = 39$, $x_2 = 63$ and $x_1 = 23$. From the calculated Q_{exp} values, it was observed that the results of average corrosion rate and average inhibition efficiency at 5 days and 10 days of 500 ppm MOXI are to be retained, because the $Q_{critical}$ value at 90 % confident limit is greater than Q_{exp} value that is (at 5 days $Q_{exp} = 0.59 < Q_{crit} = 0.94$ and at 10 days $Q_{exp} = 0.094 < Q_{crit} = 0.94$, while for average inhibition efficiency at 5 days $Q_{exp} = 0.6 < Q_{crit} = 0.94$ and at 10 days $Q_{exp} = 0.07 < Q_{crit} = 0.94$). T_{test} statistical analysis was used to compare the results obtained between the two methods at concentration of 50 ppm, 200 ppm and 500 ppm at 303 K. T_{test} experimental calculated values were obtained using equ. 11.

$$T_{test} = \frac{x_2 - x_1 \sqrt{\frac{MN}{M+N}}}{Sp} \quad (11)$$

where M is the number of set of values in the first method and N is the number of set of values in the second method, x_2 is the mean of result of the first method while x_1 is the mean of result of the second method obtained from Table 5 and Sp is pulled standard deviation which can be calculated using equ 12.

$$Sp = \sqrt{\frac{\sum(x_2 - x_1)^2 + \sum(x_2 - x_1)^2}{M+N-2}} \quad (12)$$

Where x_2 is the set of individual values, x_1 is the mean of the set of data, $M + N - 2$ is the degree of freedom. The T_{test} experimental and critical values were listed in Table 6. The results obtained indicates that T_{test} experimental value in the two methods compared was found to have a lesser T_{test} experimental value than the critical value at 0.05 significant level, which means there is no significant difference between Gravimetric and Electrochemical impedance spectroscopy

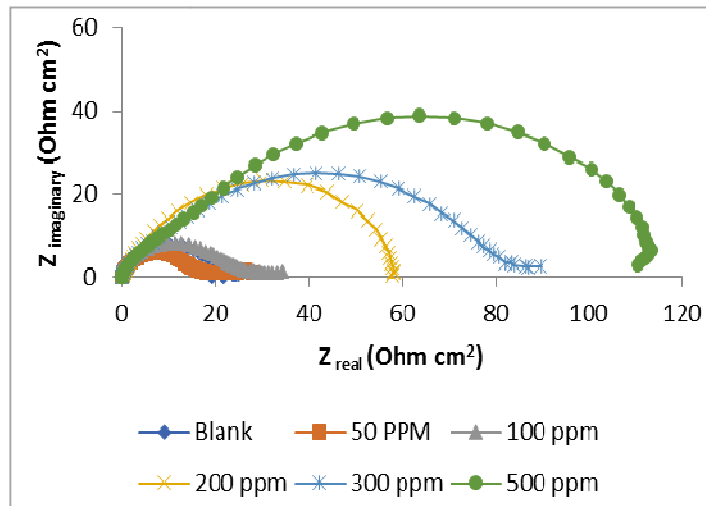


Fig. 3. Impedance spectra of the corrosion of API 5LX-52 Steel in 2 M HCl solution in the absence and presence of moxifloxacin at 303 K

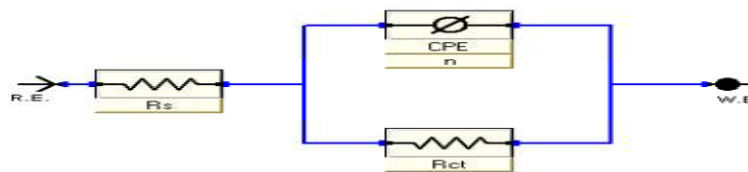


Fig. 4. Electrical equivalent circuit model to the impedance data in the absence and presence of moxifloxacin at 303 K

Table 4. Electrochemical and kinetic parameters obtained from EIS technique for the corrosion of API 5 L X-52 steel at different concentration of the investigated inhibitor at 303 K

Conc. (ppm)	$R_{ct} \Omega cm^{-2}$	$CPE \times 10^{-3} F cm^{-2}$	Surface coverage θ	IE %
Blank 2 M HCl	19.24	207		
50 ppm MOX + 2 M HCl	25.70	155	0.3296	33.0
100 ppm MOX + 2M HCl	32.46	58	0.4410	44.1
200 ppm MOX + 2M HCl	58.36	68	0.6703	67.0
300 ppm MOX + 2M HCl	89.56	44	0.7851	78.5
500 ppm MOX + 2M HCl	111.40	36	0.8257	82.7

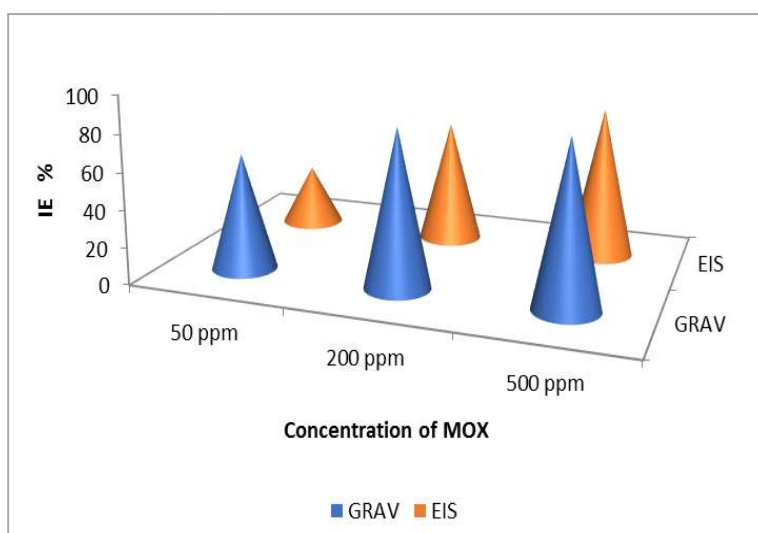


Fig. 5. Comparative results between gravimetric and electrochemical impedance spectroscopy

Table 5. Statistical data analysis for the comparative study between Gravimetric and Electrochemical impedance spectroscopy methods

	GRAV			EIS		
Concentration of MOX	X	$X-X_2$	$(X-X_2)^2$	X	$X-X_2$	$(X-X_2)^2$
50 ppm MOX + 2 M HCl	63.0	-15.6	243.4	33.0	-27.9	780.6
200 ppm MOX + 2 M HCl	85.0	6.4	41.0	67.0	6.1	37.6
500 ppm MOX + 2 M HCl	88.0	9.4	88.4	82.7	21.8	476.1
X_2	78.6		372.7	60.9		1294.3

where X_2 is the mean of the set of data

methods. The results obtained in the two techniques shows that there are in good agreement and that have also be confirmed in Fig. 5.

Table 6. Statistical T_{test} result for the comparative between the two methods employed

METHODS	$T_{test exp.}$	Sp	$T_{test critical}$
GRAV. AND EIS	1.06	20	2.78

3.2.2 Adsorption isotherms

The perceptive of the nature of the adsorption of the process of MOX on metal surface is necessary to our knowledge of inhibition achievement on corrosion. To explain the adsorption behaviour of MOX, various adsorption isotherms were tested and Langmuir kinetic adsorption isotherm fits the experimental data well. The expression of Langmuir isotherm is given in equ. 13

$$C/\theta = 1/K_{\text{ads}} + C \quad (13)$$

where θ is the degree of surface coverage, C is the concentration of the inhibitor and K_{ads} is the equilibrium constant of the adsorption process. The plot shown in Fig. 6 assume adsorption of the molecule of MOX as monolayer over the metallic surface. The Langmuir isotherm is applied to both GRAV and EIS data and the equilibrium constant of adsorption K_{ads} is obtained from the intercept of the plot, then related to the free energy of adsorption ΔG_{ads} given as equ. 14 [7].

$$\Delta G_{\text{ads}} = -2.303 RT \log (55.5) K_{\text{ads}} \quad (14)$$

where R is the universal gas constant, T is the absolute temperature and 55.5 is the molar concentration of water in solution. The values of ΔG_{ads} and K_{ads} are given in Table 7. And this value is in the interval of physical adsorption. It is well known from the study of adsorption that values of ΔG_{ads} ranging from -40 kJmol^{-1} and above reflect a chemical adsorption and below -40 kJmol^{-1} shows physical adsorption [7]. The negative sign of ΔG_{ads} revealed that the adsorption process of MOX over API 5L X-52 steel is spontaneous. The active centers for the adsorption of the compound MOX is described using some of the quantum chemical parameters such as dipole moment, bond length and Fukui function.

3.2.3 Computational consideration

The concept of modelling nucleophilic f^+ and electrophilic f^- behaviour of corrosion inhibitor

are packaged in the Fukui function. Thus, the preferred sites for an attack by an electrophile and nucleophile were observed at the position where the values of Fukui f^- and f^+ is maximum. Corrosion inhibition involve electron donation and electron acceptance which involve nucleophilic and electrophilic attack, usually inhibitor donates electrons (that is acting as nucleophile) while metal accepting electron thus acting as an electrophile. However, it has been found that apart from donating electron, the inhibitor can also accept electron from the d-orbital of the metal leading to the formation of a feedback bond [12]. The f^+ measure the change of density when a molecule gains electrons and it corresponds to reactivity with respect to nucleophilic attack, on the other hand f^- correspond to reactivity with respect to electrophilic attack or when the molecule loss electrons. It can be deduced from Table 8 that the sites for nucleophilic attack are on the N3, C12, C15, C22, C24, C27 and O28 atoms. Though, the sites for electrophilic attack are on the N3, N8, C11, C13, C15 and O28 atoms. The Fukui function can be illustrated in Fig. 7.

Shorter bond lengths are less reactive than longer bond lengths and also multiple bonds are reactive than single bond. The bond lengths of the molecule were also calculated. The bond length between C1-C2, C4-C53, C5-C6, C5-C7, C9-C10, C19-C20 C20- C18. were 1.547 Å, 1.539 Å, 1.545 Å, 1.529 Å, 1.528 Å, 1.524 Å, and 1.520 Å. These values reflected good inhibition efficiency, Dipole moment is the measure of polarity in a bond, therefore inhibitor

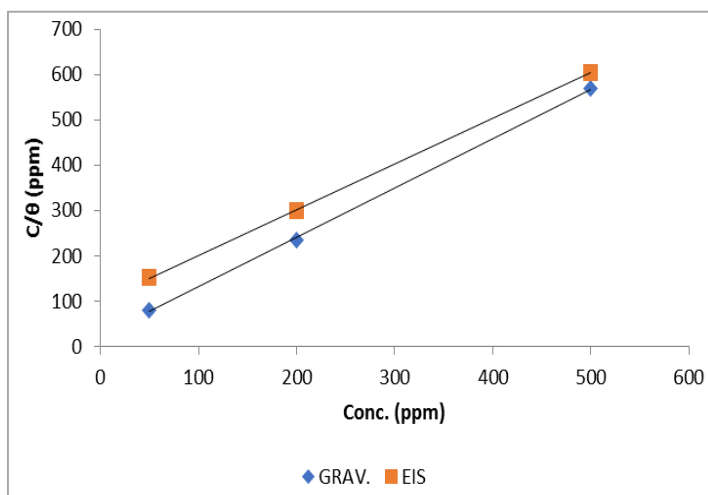


Fig. 6. Langmuir adsorption isotherm plot for the adsorption of MOX on the API 5L X-52 steel in 2 M HCl solution

Table 7. Adsorption parameters obtained from Langmuir isotherm for the adsorption of MOX on API 5L X-52 steel in 2 M HCl solution at 303 K

Method	Equilibrium constant $K_{ads}(M^{-1})$	$\Delta G_{ads}(kJmol^{-1})$	R^2
Gravimetric	4.5×10^{-2}	- 0.46	0.999
Electrochemical impedance spectroscopy	1.0×10^{-2}	- 0.10	0.999

Table 8. Calculated values of bond lengths, DFT Fukui (f) indices and Fukui (f^+) indices for Moxifloxacin compound

Atom	Bond	Length	Fukui (f)	Fukui (f^+)
C1	C1-C2	1.547	-0.012	-0.007
C2	C2-N3	1.475	-0.017	-0.009
N3	N3-C4	1.473	0.029	0.049
C4	C4-C5	1.539	-0.007	-0.003
C5	C5-C6	1.545	-0.013	-0.006
C6	C5-C7	1.529	-0.016	-0.007
C7	C7-N8	1.460	-0.031	-0.018
N8	N8-C9	1.461	0.026	0.022
C9	C9-C4	1.528	-0.029	-0.016
C10	N8-C10	1.467	0.005	0.029
C11	C10=C12	1.420	0.035	0.033
C12	C11-C12	1.387	0.016	0.046
C13	C12-C13	1.397	0.035	-0.007
C14	C13-C14	1.401	0.018	0.007
C15	C14=C15	1.425	0.047	0.047
O16	C15-O16	1.408	0.01	0.012
C17	O16-C17	1.433	-0.026	-0.02
C18	C14-N21	1.454	-0.005	0.001
C19	N21-C19	1.467	0.005	-0.005
C20	C19-C20	1.524	-0.02	-0.029
N21	C20-C18	1.520	0.002	0.01
C22	N21-C22	1.442	0.016	0.114
C23	C22=C23	1.342	0.008	0.019
C24	C23-C24	1.478	0.019	0.049
C25	C24-C13	1.478	0.018	0.032
O26	C23-C25	1.479	0.013	0.017
O27	C25-O26	1.393	0.029	0.057
O28	C25=O27	1.217	0.085	0.082
F29	C24=O28	1.219	0.03	0.033

with high dipole moment form strong dipole-dipole interaction with the metal which result in strong adsorption on the metal surface, thus leading to greater inhibition efficiency. The value for the dipole moment of the studied molecule is ($\mu = 10.35$ debyes). This value confirmed the accumulation of the inhibitor on the surface layer [6]. The adsorption of the inhibitor on the steel surface takes nearly parallel to the surface so as

to maximize its contact with the surface shown in Fig. 8a.

The relationship between the electron donating properties (E_{HOMO}) of the inhibitor and inhibition efficiency of moxifloxacin can be explain using Fig. 8b. The plot revealed a strong correlation $R^2 \approx 1$ between the experimental inhibition efficiency and energy of occupied molecular orbital.

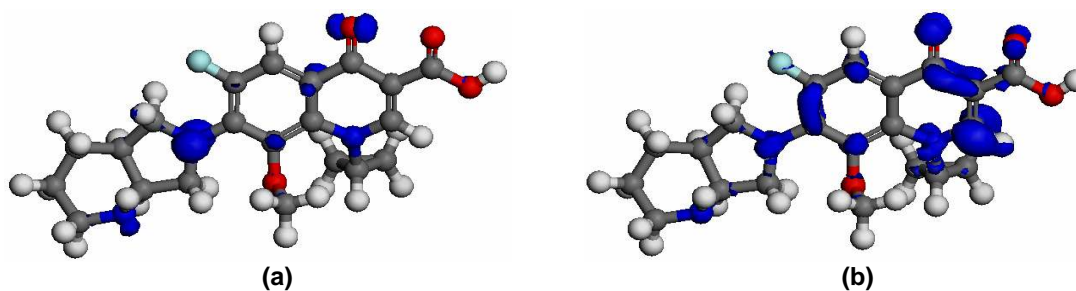


Fig. 7. (a) Electrophilic (f) Fukui indices plot and (b) Nucleophilic (f^+) Fukui indices plot for MOX

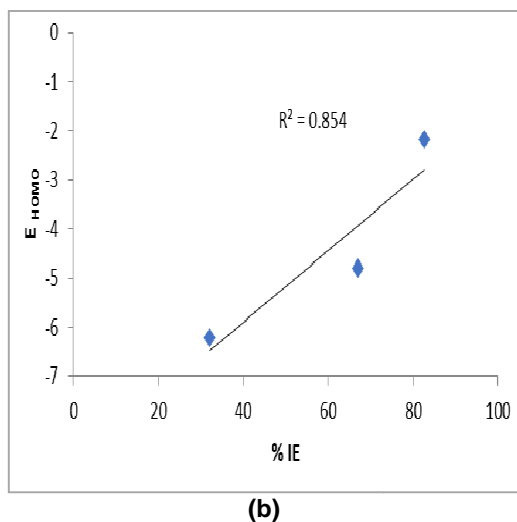
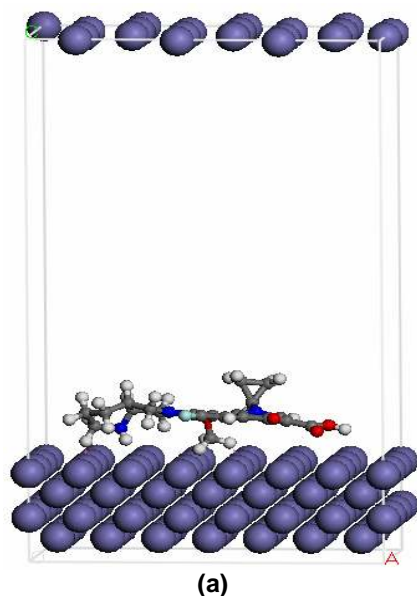


Fig. 8. (a) The adsorption of the inhibitors on the steel surface (b) Variation of experimental inhibition efficiency with the energy of the HOMO for moxifloxacin

4. CONCLUSION

From the studies, the following are concluded

- i. The gravimetric and electrochemical impedance spectroscopy results revealed that the studied antibiotic drug (moxifloxacin) act as excellent corrosion inhibitor.
- ii. The results obtained from both methods shows that there was no significant difference between Grav and EIS methods.
- iii. The corrosion inhibition of moxifloxacin can be ascribed to physical adsorption at the steel surface supported by the results of isotherm model
- iv. The inhibiting potential of the drug were theoretically confirmed with quantum chemical computation

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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