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Corrosion Inhibition of Low Carbon Steel in 1 M HCl Solution by Cephalexin Monohydrate Drug and Synergistic Iodide Additives

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Abstract: The effect of Cephalexin monohydrate drug on the corrosion performance of low carbon steel (LCS) in 1 M HCl solution has been examined by weight reduction (WR), potentiodynamic polarization (PP) and AC impedance spectroscopy (EIS) tests. The inhibition efficiency (IE) raised with increasing the cephalexin monohydrate drug dose but lowered with higher temperatures. The adsorption of the Cephalexin monohydrate drug established to follow Temkin isotherm. The PP tests designated that the cephalexin monohydrate drug is of mixed type. Synergism among iodide ion and cephalexin monohydrate drug was suggested. The outcome data gotten from the three altered tests were in excellent agreement. Theoretical relationships have been utilized to examine the influence of molecular structure on IE of the Cephalexin monohydrate drug.

Keywords: Corrosion inhibition; LCS; HCl; Cephalexin monohydrate drug; Synergistic effect.

1. Introduction

Low carbon steel is a material frequently utilized because of its properties of protection to corrosion in both the maritime field and the industrial domain. LCS has been selected in this paper because of its frequently utilized, and ’it’s weak relatively resistant to dissolution, allowing to assess more easily the effect of the environment. It is probable to decrease the rate of dissolution to a safe level by appending inhibitors. Several heterocyclic composites containing N, O, and S either in the aromatic or long carbon chain system have been described to be productive inhibitors [1-4]. These compounds have including functional groups (such as –OR, -C=C-, -OH, -NR_2, -NH_2 and –SR). These groups afford electrons that enable the inhibitor adsorbed of on the metal superficial [5-10]. Most of the organic inhibitors are cost, poisonous, and have a side influence on the atmosphere this property restricts ’ it’s utilized to protect the metal dissolution. Therefore, it is significant and essential to improving small price and eco-friendly corrosion protection [11, 13]. As of late specialists have focused on the improvement of medications as drugs for metallic dissolution. In the review, numerous writers have described the impact of drugs on the corrosion of metals in a corrosive environment [14-26]. The choice of this drug Cephalexin monohydrate as a corrosion inhibitor is based on the resulting:(a) can be simply obtained (b) including active atom such as (O, N and S) (c) has solubility higher in a corrosive environment (d) non-hazardous and (e) low cost.

The current study aimed to utilized cephalexin monohydrate drug has studied the hindering effect on the dissolution of LCS in 1 M HCl. Also, the association among deliberate quantum parameters and %IE of the cephalexin monohydrate drug was debated.

2. Materials and Methods

2.1. Materials.

The tests were achieved with LCS samples with the composition shown in Table 1.

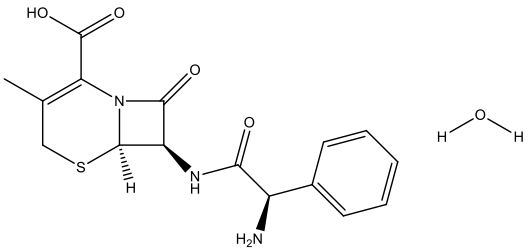
Table 1. The LCS weight percentage.

Elements	C	Cr	Ni	Si	Mn	P	S	Fe
Wt %	0.14	0.1	0.01	0.024	0.5	0.05	0.05	Reset

All chemicals and reagents utilized are with investigative grade and utilized deprived of further purification (utilized as received).

2.2. Materials and Solutions.

The corrosive environment utilized was 37% HCl (AR grade). "Appropriate doses of acid were ready utilized distilled water. 1000 ppm stock solutions from the examined cephalexin monohydrate drug were ready by liquefying the suitable weight of the utilized chemically pure solid drug in second distilled water. The cephalexin monohydrate drug stock solution 10^3 ppm was used to prepare (100, 200, 300, 400, 500, and 600 ppm)". The structure of the cephalexin monohydrate drug was utilized as a corrosion hindrance for LCS in 1 M HCl.



Scheme 1. Cephalexin monohydrate drug.

2.3. Techniques used for corrosion measurements.

2.3.1. Weight loss method (WL).

Three parallel LCS sheets of 2 x 2 x 0.2 cm were abraded with emery paper up to 1200 grit and then washed with bidistilled water and acetone. "Pre-treatment and pre-weighed carbon steel specimens were immersed in the aggressive media in the absence and presence of studied additives with the concentration range of (100–600 ppm). The maximum duration of immersion was 180 min. After equal time intervals (30 min), the specimens were taken out, rinsed with distilled water, air-dried, and accurately weighed. All the experiments were achieved in triplicate in order to ensure reproducibility. Then the tests were ready at altered temperatures. The (%IE) and the grade of surface coating (θ) of cephalexin monohydrate drug on the dissolution of LCS were measured from the next balances" [27]:

$$IE\ \% = [(W^{\circ} - W)/ W^{\circ}] \times 100 \quad (1)$$

$$\theta = [(W^{\circ} - W)/ W^{\circ}] \quad (2)$$

where W° and W are the data of the WL attendance and lack of appending of the cephalexin monohydrate drug, correspondingly.

2.3.2. Electrochemical methods.

2.3.2.1. i-PP tests.

Further corrosion tests were analyzed electrochemically in a three-compartment glass cell consisted of the working electrode "(LCS electrode) with an uncovered area of 1 cm^2, the reference electrode (saturated calomel electrode) and the counter electrode (a platinum foil). Electrochemical tests were carried out under the static conditions in a naturally aerated solution of 1 M HCl in the attendance and lack of varied doses of additives (cephalexin monohydrate drug) at 25± 1 ^{0}C. Polarization curves were started from cathodic to the anodic direction and were approved by sweeping the electrode potential mechanically from -300 to +700 mV segment to OCP at a scan rate of 0.5 mV s^{-1}. Current corrosion density (i_{corr}) magnitudes were verified from the acquired polarization bends utilizing Tafel extrapolation". IE% and the (θ) were defined as:

$$IE\ \% = \theta \times 100 \quad (3)$$

$$\theta = [(i_{corr} - i_{corr(inh)}) / i_{corr}] \quad (4)$$

where i_{corr} and $i_{corr(inh)}$ are the current unprotected and protected, individually.

The EIS tests were achieved at "OCP by analyzing a frequency response of the electrochemical system with the range extended from 0.01 Hz at minimum to 100,000 Hz at maximum frequency, and the excitation signal is 5 mV sine wave. Gamry PCI4-G750 Potentiostat/Galvanostat/ ZRA. Echem Analyst V6.30" Software was applied for electrochemical data bends, fitting and graphing.

3. Results and Discussion

3.1. (WL) tests.

The WL of LCS specimen in 1.0M HCl solution, without and with altered cephalexin monohydrate drug doses (100-600 ppm), "were measured at altered times of dipping (30 to 180 min) at 25 ^{o}C. Fig. 1 signifies the WL of LCS in aggressive solution, without and with various cephalexin monohydrate drug doses. The attendance of the cephalexin monohydrate drug diminishes the corrosion rate (CR) of LCS in HCl. Table 2 demonstrates the results obtained from WL tests for LCS in HCl attendance and lack of altered doses of the utilized cephalexin monohydrate drug as can see from Table 2 that IE % raised and CR lowered with improving cephalexin monohydrate drug dose. This is due to the improving adsorption and raising coverage of cephalexin monohydrate drug on the surface of LCS" with improving cephalexin monohydrate drug dose [28].

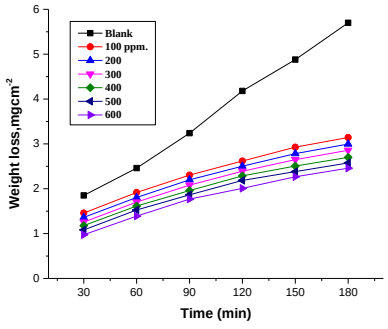


Figure 1. WL-time diagrams for the liquefaction of LCS with and without different doses of cephalexin monohydrate drug at 25^{o}C.

Table 2. % IE of LCS dissolution at 120 min. Immersion in 1 M HCl with various doses of cephalexin monohydrate drug at 25°C.

Concentration (ppm)	%Inhibition Cephalexin monohydrate drug	Θ
100	37.4	0.374
200	40.1	0.401
300	42.8	0.428
400	45.7	0.457
500	47.7	0.477
600	51.9	0.519

3.1.1. Adsorption isotherms.

The best correlation between the experimental results and the isothermal functions was obtained in the temperature studied (25ºC) utilizing the Temkin isotherm adsorption [29-30], which is given by the following balance.

$$\ln K C = a\theta \quad (5)$$

where C is cephalexin monohydrate drug dose, and K is the equilibrium of adsorption constant. It is well recognized that the ($\Delta G°_{ads}$) is related (K) and $\Delta G°_{ads}$ by the following equation [31]:

$$K = 1/55.5 \exp [-\Delta G°_{ads}/RT] \quad (6)$$

where "55.5 is the cephalexin monohydrate drug dose of water in mol l^{-1}. Fig. 2 signifies the design of (θ) versus log C for the dissolution of LCS in 1.00M HCl at 25 ºC. As can be realized from Fig. 2, the Temkin isotherm is the greatest one which elucidates the investigational results". Also, it is established that the kinetic-thermodynamic model of El-Awady *et al*. [32].

$$\log (\theta/ 1- \theta) = \log k' + y \log C \quad (7)$$

K = 'K' $^{(1/y)}$, 'K' is constant, and 1/y is the number of the surface-active sites engaged by one cephalexin monohydrate drug molecule. "Drawing log (θ/1-θ) versus log C for the cephalexin monohydrate drug for the dissolution of LCS in 1M HCl at 25ºC is specified in Fig. 3. The data of K and $\Delta G°_{ads}$ measured by Temkin and from the kinetic model are specified in Table 3. In general, the $\Delta G°_{ads}$ data obtained from El-Awady *et al*. model are similar to those Temkin isotherms. The $\Delta G°_{ads}$ sign had negative, which designate spontaneous of cephalexin monohydrate drug onto the surface of LCS [33-35]. The $\Delta G°_{ads}$ data gotten for the studied cephalexin monohydrate drug on LCS surface range from 31 kJ mol^{-1}", representative both physical and chemical adsorption [36].

Table 3. Parameters obtained from Adsorption isotherm (Kinetic model and Temkin) at 25ºC.

Kinetic model			Temkin		
1/y	**K**	**$-\Delta G°_{ads}$, kJ mol^{-1}**	**a**	**K**	**$-\Delta G°_{ads}$, kJ mol^{-1}**
2.31	**1.44**	**31.25**	**12.81**	**1.16**	**31.60**

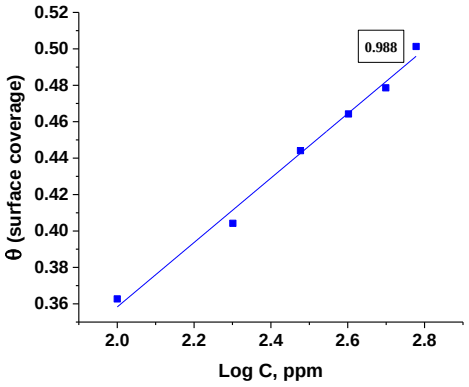


Figure 2. Diagrams fitting of dissolution data for LCS 1M HCl to Temkin adsorption isotherm at 25 ºC.

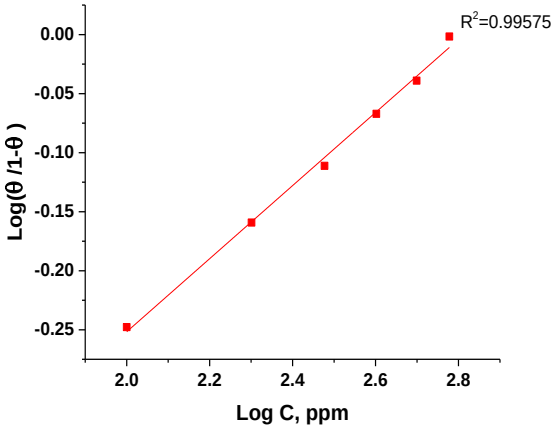


Figure 3. Diagrams fitting of dissolution data for LCS 1M HCl in the existence of cephalexin monohydrate drug to the kinetic model at 25 ºC.

3.1.2. Kinetic parameters.

The dissolution of LCS in 1 M HCl existence and nonexistence various doses of the cephalexin monohydrate drug (100-600 ppm) at temperatures range (25–45ºC) was deliberately utilizing WL test. "The %IE data at various temperatures were presented in Table 4 The outcome data exposed that the degree of the %IE improved with raising the dose of the cephalexin monohydrate drug and reduced with raising temperature [37] whereas the %IE is significantly lowered at a higher temperature. The reduction of the %IE with improving the temperature is expressive of physical adsorption of the utilized cephalexin monohydrate drug on the surface of LCS".

Table 4. IE % of LCS dissolution at 120 min. Immersion in 1 HCl attendance and lack of altered doses of cephalexin monohydrate drug at different temperatures.

Concentration (ppm)	IE %			
	30°C	35°C	40°C	45°C
100	30.4	20.9	13.1	6.5
200	33.0	23.8	15.6	8.5
300	35.2	26.9	17.7	10.4
400	38.5	29.7	20.5	12.7
500	41.0	32.0	23.0	14.8
600	43.9	34.4	25.2	17.1

The impact of temperature on both corrosion and corrosion protection of LCS in an aggressive environment in existence and lack of altered dose of cephalexin monohydrate drug at various temperatures ranging from 25ºC to 45ºC was deliberately utilizing WL. The CR improves with improving temperature both in uninhabited and inhabited acid. The parameters of activation for the liquefaction technique measured from the Arrhenius plot as next [38]:

$$k = A \exp(- E_a^*/ RT) \quad (11)$$

E^*_a can be obtained from the slope of "log (k_{corr}) against 1/T plots attendance and lack of altered doses of the cephalexin monohydrate drug as obtainable in Fig. 4. Data of E^*_a are described in Table 5 E^*_a has higher data in the existence of the cephalexin monohydrate drug than that in its nonexistence. This has attributed the physical adsorption of cephalexin monohydrate drugs on LCS surface [39]. The transition state theory was utilized to calculate the (ΔS^*) and (ΔH^*) Fig. 5. The change data of (ΔS^*) and (ΔH^*)" can be measured by utilizing the formula:

$$k_{corr} = (RT/Nh) \exp(^{\Delta S^*/R)} \exp^{(-\Delta H^*/RT)} \quad (8)$$

ΔH^* and ΔS^* were designed by applying the next balance [40-42]:

$$\Delta H^* = E^* - RT \quad (9)$$

$$\Delta S^* = (\Delta H^* - \Delta G^*)/T \quad (10)$$

The sign of ΔH^* is positive and high in the existence of the cephalexin monohydrate drug over that of the unprotected solution. "This indicates that the energy barrier of the dissolution reaction in the existence of the investigated cephalexin monohydrate drug increases. Conversely, ΔS^* data are lesser and have negative data in the existence of the cephalexin monohydrate drug; this means that the appending of this cephalexin monohydrate drug causes a lower in the disordering in going from reactants to the activated complexes" [43-44].

Table 5. Kinetic Parameters for the utilized cephalexin monohydrate drug on the dissolution of LCS in 1.00 M HCl solution.

Concentration, (ppm)	E_a^*, kJ mol^{-1}	ΔH^*, kJ mol^{-1}	$-\Delta S^*$, k^{-1}J mol^{-1}
100	61.5	62.0	20.9
200	64.5	62.2	23.8
300	64.9	63.2	26.9
400	65.4	63.3	29.7
500	65.9	64.8	32.0
600	66.2	65.1	34.4

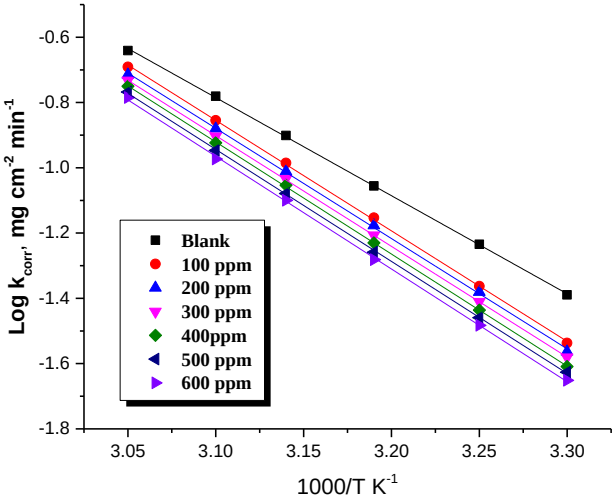


Figure 4. log k- 1000/T bends for LCS dissolution existence and nonexistence of altered doses of cephalexin monohydrate drug.

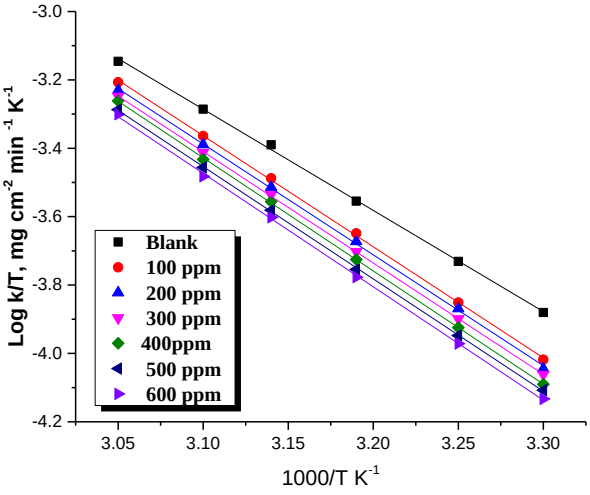


Figure 5. log (k/T) vs. (1000/T) bends for LCS dissolution existence and nonexistence of altered doses of cephalexin monohydrate drug.

3.2. Polarization tests (PP).

Fig. 6 demonstration PP bends registered for LCS in 1.00 M HCl solutions attendance and nonattendance of an altered dose of cephalexin monohydrate drug at 25ºC. "With the increment of the dose of cephalexin monohydrate drug diagrams shifts both anodic and cathodic sections to the lesser data of i_{corr}, which leads to dropping in the CR. The PP bends recognized in Table 6 as the alternation of the data of (log i_{corr}) with the (E_{corr}), (βa, βc), (C.R.), (θ) and (%IE). This means that cephalexin monohydrate drug hinders both cathodic and anodic reactions of LCS in HCl medium. The slopes of anodic and cathodic Tafel lines (βa and βc), were lightly varied with the rasing the dose of cephalexin monohydrate drug". This designates that a cephalexin monohydrate drug inhibitor signifies as mixed-type inhibitors [45].

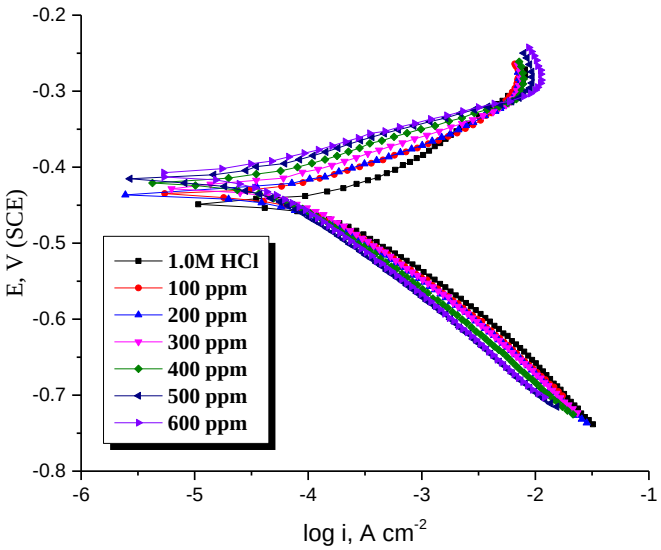


Figure 6. PP bends for LCS existence and nonexistence of altered dose of cephalexin monohydrate drug at 25ºC.

Table 6. PP values of LCS in 1.0 M HCl in existence and nonexistence of altered dose of cephalexin monohydrate drug at 25ºC.

[Inh.] ppm	-E_{OC} mV vs.SCE	-E_{corr} mV vs.SCE	j_{corr} µA cm^{-2}	β_c mV dec^{-1}	β_a mV dec^{-1}	R_p Ω cm^2	C.R. (mmyr^{-1})	IE%, j_{corr}	IE%, R_p
blank	438	449	199.1	126	94	117.6	2.311	--	--
100	429	442	126.5	116	64	141.8	1.468	36.5	17.4
200	436	436	120	114	63	147.1	0.974	39.7	20.1
300	423	427	116	115	61	149.4	0.874	41.7	21.3
400	424	422	107	112	62	162.2	0.648	46.3	27.5
500	443	434	97.2	115	60	176.4	0.436	51.2	33.3
600	399	436	94.1	113	63	186.9	0.402	52.8	37.1

3.2.1. Synergistic effect.

The rise in %IE of cephalexin monohydrate drug in the existence of some anions has been experiential by numerous detectives [46] and was recognized as a synergistic effect. "Test to improve the effectiveness of the investigated cephalexin monohydrate drug by appending of KI were carried out utilizing PP tests. Fig. 7 shows PP bends for LCS in 1.00 M HCl in existence and lack of 600 ppm of cephalexin monohydrate drug without and with different doses ($1x10^{-4}$, $1x10^{-3}$, $1x10^{-2}$ M) of KI at 25 ºC as an example. The obtained electrochemical values (E_{OC}, E_{corr}, i_{corr}, β_c, β_a, R_p, and %IE) are shown in Table 7. Results revealed in Tables 7 exposed that the existence of various doses of KI improves the lowering of i_{corr} values for LCS

in 1.0M HCl and the lessening in the CR with improving the dose of KI representative that appending of KI increases the protecting action of the cephalexin monohydrate drug. The detected synergistic influence results from rising surface coverage arising from ion-pair interaction between I^- anion and Cephalexin monohydrate drugs. There are altered schools of thought [47] on the actual role of the anions as respects increase the adsorption of the cephalexin monohydrate drug. The increment in the %IE of cephalexin monohydrate drug on the appending of iodide ions during LCS was qualified for the mechanism by Wu *et al*. [48] while the results of Oguzie *et al*. [49] and other authors [47]. Stabilization of the iodide ions adsorbed with cephalexin monohydrate drug cations indications higher surface coverage and thus increase inhibition productivity". The better %IE caused by the appending of iodide ions to cephalexin monohydrate drugs is only due to the synergistic effect.

Table 7. Synergistic effect of various doses of KI with 600 ppm of cephalexin monohydrate drug on the PP method and IE % of LCS at 25 °C.

[KI] M	$-E_{OC}$ mV	$-E_{corr}$ mV	j_{corr} μA cm^{-2}	$-\beta_c$ mV dec^{-1}	β_a mV dec^{-1}	R_p ohm cm^2	CR mm yr^{-1}	IE%, j_{corr}	IE%, R_p
——	399	436	94.1	187	63	186.9	1.092	52.8	37.1
1x10^{-4}	350	379	31.2	103	64	549.6	0.363	84.3	78.6
1x10^{-3}	307	344	18.4	110	72	1026.0	0.213	90.8	88.5
1x10^{-2}	238	307	18.0	139	87	1292.0	0.209	91.0	90.9

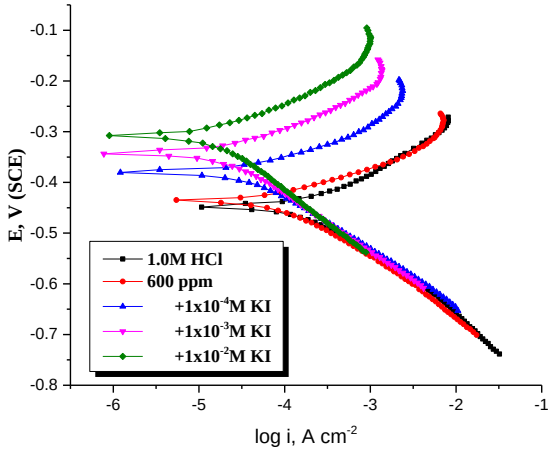


Figure 7. PP diagrams of LCD in 1.0 M HCl existence and nonexistence of 600 ppm of cephalexin monohydrate drug and an altered dose of KI at 25°C.

3.3. EIS tests.

The dissolution of LCS in 1 M HCl in the existence of cephalexin monohydrate drug was examined by EIS test at 25°C after 20 min dipping. "Nyquist and Bode bend in the attendance, and lack of altered doses of cephalexin monohydrate drug exist in Figs. 8 and 9, correspondingly. It seems that all Nyquist bends show a single capacitive loop, both in unprotected and protected solutions. The EIS data of LCS in 1 M HCl are investigated in terms of an equivalent circuit model (Fig. 10) [50].

The circuit has the solution resistance R_s and the double layer capacitance C_{dl} that put parallel to R_{ct} [51]. C_{dl}, for a circuit including a CPE calculated from the following balance [52-53]:

$$C_{dl} = (1 / 2\pi f_{max} R_{ct}) \quad (11)$$

where f_{max} is maximum frequency. Table 8 includes the obtained impedance data. As shown, R_{ct} rises, and hence %IE increases, with the increase in cephalexin monohydrate drug concentration, while C_{dl} lowered. That is because the adsorption of the cephalexin monohydrate

drug on the LCS surface, forming a film on it". The (% IE) and θ were founded from the next balance:

$$IE\ \% = \theta \times 100 = [(R_{ct(inh)} - R_{ct}) / R_{ct(inh)}] \times 100 \quad (12)$$

Table 8. EIS parameters technique for the dissolution of LCS at different doses of cephalexin monohydrate drugs at 25 °C.

[Inh.] ppm	C_{dl} μF cm^{-2}	-Phase degree	R_{ct} ohm cm^2	θ	IE%
1.0 M HCl	71.4	71.2	234.6	----	----
300	66.9	71.7	496.8	0.528	52.8
400	64.5	71.6	527.3	0.555	55.5
500	53.8	73.0	647.2	0.638	63.8
600	53.9	73.1	710.4	0.670	67.0

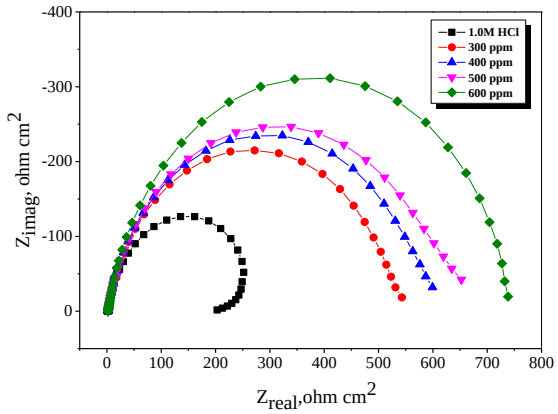


Figure 8. The Nyquist bends for dissolution of LCD in 1.0 M HCl in existence and nonexistence of altered of cephalexin monohydrate drug at 25 °C.

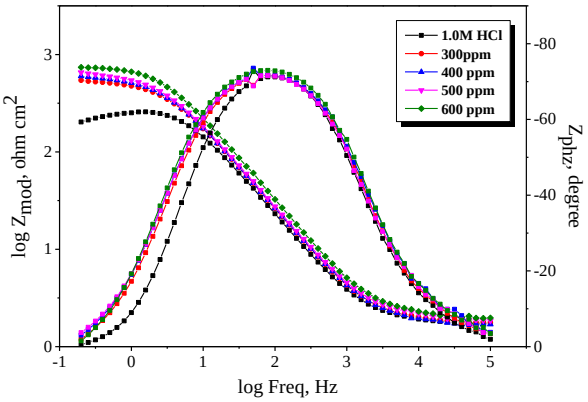


Figure 9. The Bode bends for dissolution of LCD in 1.0 M HCl in existence and nonexistence of altered of cephalexin monohydrate drug at 25 °C.

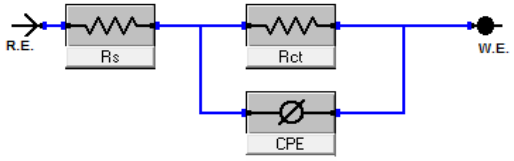


Figure 10. The equivalent circuit model used to fit the experimental results.

3.4. Quantum chemical calculation.

The capability of quantum calculations practical to the cephalexin monohydrate drug to predict their productivities as corrosion drug was studied. "Fig. 11 and Table 9 demonstrations the quantum parameters (E_{HUMO}, E_{LUMO}) and the energy band gap

($\Delta E = E_{LUMO} - E_{HOMO}$) is also listed. E_{HOMO} is related to the electron-donating ability of the molecule. The high value of E_{HOMO} is pointed to the affinity of the cephalexin monohydrate drug to give electrons to be suitable for the molecules acceptor, which devising small energy and empty molecular orbitals [54]. The protection efficiencies improve with the upper or less negative E_{HOMO} energies, with raising data of the dipole moment with diminishing the data of ΔE (energy gap) [55,56] and the stronger interaction among cephalexin monohydrate and LCD surface. The IE values increase with the lower ionization potential of the cephalexin monohydrate drug molecule, which means that the cephalexin monohydrate drug acts as an electron donor when blocking the dissolution reaction sites" [57].

Table 9. Quantum chemical parameters for 600 ppm of cephalexin monohydrate drug for the liquefaction of LCS.

cephalexin monohydrate drug	**$-E_{HOMO}$ eV**	**$-E_{LUMO}$ eV**	**ΔE eV**	**μ Debye**
	7.857	1.025	6.832	28.164

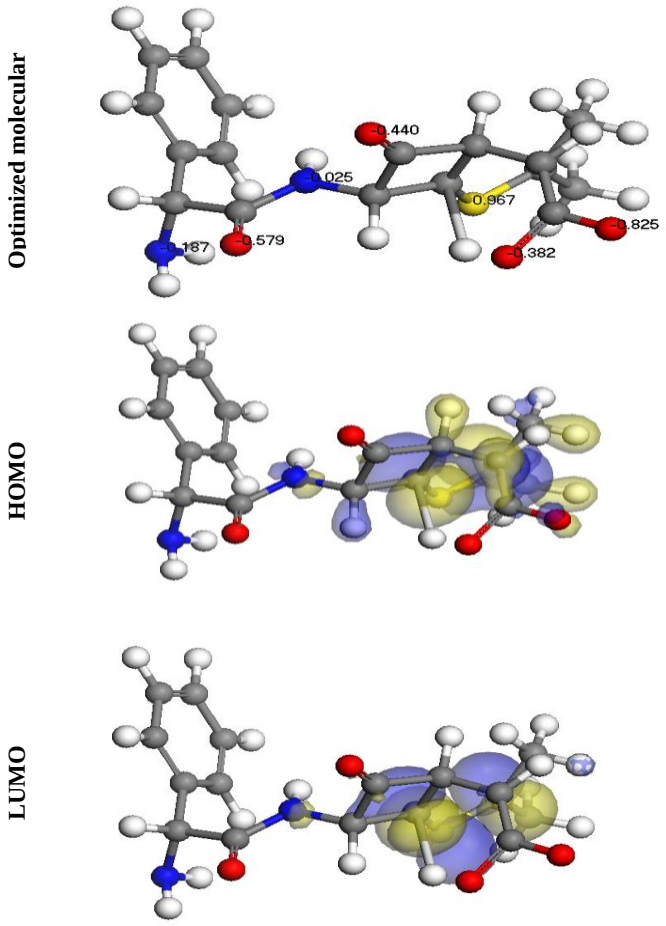


Figure 11. Optimized molecular structure and (HOMO and LUMO) of cephalexin monohydrate drug.

3.5. Mechanism of corrosion inhibition.

The cephalexin monohydrate drug-containing S, N, and O are recognized to be an effective drug. "Its efficiency relies on the electron density at the functional groups. The corrosion protection of the cephalexin monohydrate drug can be qualified for the existence of heteroatom and π electrons on the benzene ring. In the aqueous acidic environment, cephalexin monohydrate drug occurs either as neutral molecules or in the form of cations (protonated form). Fig. 12 show the protonated cephalexin monohydrate drug may adsorb through

electrostatic interactions among positively charged molecules and the negatively charged LCS surface. In other words, there may be a synergism between Cl^- and cephalexin monohydrate drugs, which improves the inhibitive ability of the cephalexin monohydrate drug. When the protonated form is adsorbed on the LCS surface, a coordinate bond may be formed by the partial transference of electrons from N, O, and S atoms to the metal surface [58-59]. In addition, owing to lone-pair electrons of N, O, and S atoms in the cephalexin monohydrate drug or the protonated form may combine with freshly generated Fe^{2+} ions on LCS" surface forming metal drug complexes

$$Fe \rightarrow Fe^{2+} + 2e \quad (13)$$

$$Inh + Fe^{2+} \leftrightarrow [Inh\text{-}Fe]^{2+} \quad (14)$$

$$[Inh]^{n+} + Fe^{2+} \leftrightarrow [Inh_n\text{-}Fe]^{(2+n)+} \quad (15)$$

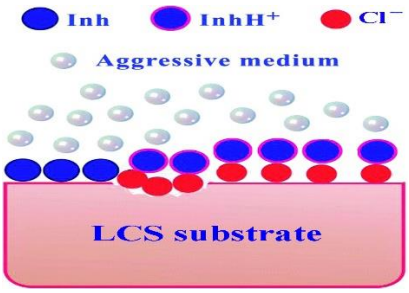


Figure 12. Proposed mechanism for the adsorption of cephalexin monohydrate drug on the LCS surface in HCl medium.

4. Conclusions

Cephalexin monohydrate drug has verified to be an environmentally friendly inhibitor for the dissolution of LCS in 1 M HCl solution. This cephalexin monohydrate drug acts as a mixed kind inhibitor, and IE% was established to rise by improving the cephalexin monohydrate dose and reduction with temperature increasing. The inhibition action of Cephalexin monohydrate drug inhibitor due to the creation of adsorbed insoluble complex on LCS. The adsorption technique obeys Temkin and Kinetic model isotherm. The outcome data from EIS test runs parallel with PP tests, prove the creation of a protective film on the surface of LCS surface in 1.0 M HCl. The KI added to raise the protecting action of the cephalexin monohydrate drug. The IE improves with raising the energy of the highest occupied molecular orbital (E_{HOMO}), which means that the Cephalexin monohydrate drug acts as an electron donor when blocking the dissolution reaction sites.

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Conflicts of Interest

The authors declare no conflict of interest.

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