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Experimental and Theoretical Studies on Inhibition Effect of the *Praziquantel* on Mild Steel Corrosion in 1 M HCl

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Abstract
The corrosion inhibition behavior of *praziquantel* for mild steel in 1 M HCl was studied by theoretical and electrochemical measurements. Tafel polarization measurement indicates that the *praziquantel* inhibitor acts as a mixed type. The corrosion rate decreases with the increasing concentration of inhibitor in 1 M HCl. The effect of inhibition is attributed due to the adsorption of inhibitor molecule on it and obeys the Langmuir adsorption isotherm. Adsorption parameters reveal that the adsorption process is exothermic and spontaneous. The quantum chemical parameters support the result obtained by electrochemical techniques. The surface morphology as SEM images shows the formation of a passive layer over the metal surface is an indication of the reduction in the corrosion rate.

Keywords Praziquantel · EIS · Quantum chemical parameters

1 Introduction

Mild steel has many structural and industrial applications because of its natural availability, toughness, and most economical viability. This is used under various aggressive conditions such as alkaline, acid and salt solution in industrial applications. The aggressive corrosive environment enhances the corrosion of steel due to the presence of chlorides sulfate and nitrate ions in it. Corrosion process can be controlled by painting, cathodic protection, metal coating or by the use of corrosion inhibitors.

Therefore, the use of corrosion inhibitors is a well-known method to control the corrosion of metal in aggressive corrosive media. Usually, most of the famous inhibitors are organic/inorganic compounds containing nitrogen, sulfur and oxygen atoms [1–6]. Hence, the inhibitor molecules get adsorbed on metal surface, which retards the corrosion. This adsorption of corrosion inhibitor depends mainly on physicochemical properties of the molecule such as functional groups, steric factor, molecular size, molecular weight, molecular structure, aromaticity, the electron density of the donor atoms and *p*-orbital character of donating electrons [7–11]. Along with this, it also depends on the electronic structure of the molecules [12, 13].

The existing inhibitors are toxic. There is a need to develop the eco-friendly inhibitors. Few compounds such as ketosulfone [14], rhodanine azo sulfa drugs [15], metol [16], hydralazine [17], aspirin [18], torsemide and furosemide [19], ciprofloxacin [20], sulfa drugs [21], lamotrigine [22], rhodanine azo sulfa drugs [23] and risperidone [24] are reported to be useful inhibitors for metals.

The present study was focused on the inhibition efficiency of praziquantel for the corrosion of mild steel in 1 M HCl in a temperature range of 303–333 K. Praziquantel molecule is a heterocyclic aromatic compound, which consisting of electron-rich nitrogen, oxygen atoms and π-bonds in its structure might be favorable for its adsorption on the metal surface. Hence, its study as corrosion inhibitors was carried out for mild steel in 1 M HCl solution.

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2 Experimental

2.1 Materials and Methods

Mild steel strips with dimensions of 6 cm × 1 cm × 0.1 cm were used for weight loss method, and the same strips with an exposed area of 1 cm^2 were used for electrochemical studies. The strips are abraded with emery paper from grade no. 80 up to 2000 and washed thoroughly by using double-distilled water.AR-grade hydrochloric acid and double-distilled water were used to prepare the 1 M HCl corrosive medium for all the experiments.

2.2 Inhibitor

Praziquantel is an anthelmintic veterinary drug, which is effective against flatworms. It is white-colored and soluble in alcohol. IUPAC name of the praziquantel is [(RS)-2-(cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4H-pyrazino [2,1-a] isoquinolin-4-one]. Praziquantel is first dissolved in 1 cm^3 of ethanol and then added into HCl media. The selected molecule is a heterocyclic compound, which contains two oxygen and two nitrogen atoms. Due to the presence of these electroactive elements, it is expected to act as a good inhibitor. The range of concentrations of inhibitor used is from 50 ppm to 250 ppm. The structure of the inhibitor molecule is shown in Fig. 1.

2.3 Weight Loss Measurements

The weight loss analysis is a practical and chemical process of corrosion inhibition study. In this present work, different mild steel strips were taken and passed through a pre-treatment process. The mild steel strips were weighed accurately by digital balance with an accuracy ± 0.1 g. Different mild steel specimens were immersed in a solution with the absence and presence of various inhibitor concentrations for different periods at 303 K. After the immersion process, the mild steel strips were removed and washed using double-distilled water, dried at room temperature and weighed accurately. The weight was recorded, and weight difference before and after the immersion process was calculated. The following expression was used to calculate the corrosion rate.

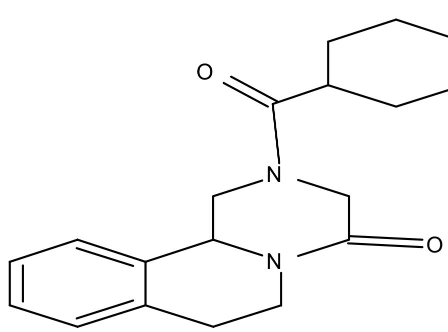

Fig. 1 Molecular structure of praziquantel

$$\nu = \frac{W^0 - W}{ST} \times 100 \tag{1}$$

where W^0 and W are the weight of mild steel strip in the absence and presence of inhibitor in 1 M hydrochloric acid, respectively. ν is the corrosion rate, S and T are the surface area of the steel strip and the time of immersion in hours, respectively. The inhibition efficiency (η_w) is calculated as follows,

$$\eta_W = \frac{\nu - \nu_i}{\nu} \times 100 \tag{2}$$

where ν and ν_i are a weight loss of the mild steel strip in the absence and presence of inhibitor solution, respectively. The corrosion parameters were computed and recorded.

2.4 Electrochemical Tafel Polarization Measurements

An electrochemical reaction can explain kinetics of corrosion process. In electrochemical Tafel polarization analysis, mild steel strip which is in contact with the corrosive medium assumes a potential which refers to corrosion potential (E_{corr}) [25]. This corrosion current polarizes both the anodic and cathodic current on the mild steel surface. For this polarization, current can be measured with applied potential at a specified scan rate. In this, corrosion measurement parameter, corrosion current density (i_{corr}) and corrosion rate (CR) are computed by the Tafel plot analysis. The inhibition efficiency can be calculated as follows:

$$\eta_P = \frac{i^0_{corr} - i_{corr}}{i_{corr}} \times 100 \tag{3}$$

where i_{corr} and i^0_{corr} are the corrosion current density in the presence and absence of the inhibitor concentration from the bulk of the solution, respectively.

2.5 Electrochemical Impedance Spectroscopy (EIS) Measurement

Impedance measurements were done by using AC signals with an amplitude of either scan rate 0.01 mV/s. It was at steady state corrosion potential (E_{corr}) in the frequency range of 10 k Hz to 0.1 Hz.

The obtained EIS data were fit into an equivalent circuit by using Z-simp 3.21 software. The EIS parameters such as polarization resistance (R_P) and double-layer capacitance (C_{dl}) were calculated by using the Nyquist plot. The following expression was used to calculate the inhibition efficiency (η_Z)

$$\eta_Z = \frac{R_P - R_P^0}{R_P} \times 100 \quad (4)$$

where R_P and R_P^0 are the polarization resistance in the presence and absence of inhibitor from the bulk of the solution, respectively.

2.6 Adsorption Isotherm and Thermodynamic Parameters

To learn about the mode of adsorption of *praziquantel* on mild steel surface in 1 M HCl at different temperatures, attempts were made to fit experimental data with several adsorption isotherms such as Tempkin, Freundlich and Langmuir's adsorption isotherm. By using these data, thermodynamic parameters were calculated using standard equations.

2.7 Activation Parameters

To study the activation parameters on the corrosion inhibition of mild steel, electrochemical impedance spectroscopy (EIS) measurements were taken at different temperatures from 303 to 333 K in the absence and presence of various concentrations of praziquantel.

2.8 Quantum Chemical Studies

Quantum chemical calculations were performed to analyze the adsorption and inhibition mechanism of praziquantel inhibitor on the mild steel surface in the gas phase by using Parametric Method 3 (PM3). These computations were carried out using the Hyperchem 7.5 package program.

2.9 Scanning Electron Microscopic (SEM) Studies

The mild steel strips surface morphology was recorded after immersion in 1 M HCl in the absence and presence of *praziquantel* for 4 h by using scanning electron microscope (JEOL JSM-840A model).

3 Results and Discussion

3.1 Weight Loss Measurements

The weight loss experiment for the corrosion of mild steel in 1 M HCl in the absence and presence of different concentration of the praziquantel at 303 K is conducted, and corrosion parameters are discussed. The computed ρ and η_W values from the weight loss method are reported in Table 1

Results obtained from weight loss method show that the corrosion rate decreases with praziquantel. From the observation of Table 1, we find the maximum efficiency of 85.71% at 250 ppm concentration of inhibitor. This clearly shows that weight loss decreases significantly with the addition of praziquantel inhibitor. The decrease in the rate of corrosion with an increase in concentration of praziquantel is attributed due to the surface coverage of metal increases as it adsorbs inhibitor molecules [26].

3.2 Electrochemical Tafel Polarization Measurements

The polarization measurement is carried out to analyze the nature and effect of the inhibitor on the kinetics of the anodic and cathodic reactions [27]. Figure 2 shows the Tafel polarization plots of mild steel in the absence and presence of various concentrations of praziquantel in 1 M HCl. The computed corrosion parameters from the polarization method are reported in Table 2.

From the close observation of Fig. 2, we find that the addition of praziquantel shifts both the anodic and cathodic polarization curves toward a lower E_{corr} value. This phenomenon is attributed to the adsorption of praziquantel on the mild steel surface, which inhibits anodic dissolution of mild steel and cathodic hydrogen liberation reaction. In general, if the displacement of corrosion potential (E_{corr}) value is greater than ± 85 mV concerning the corrosion potential of the blank, the inhibitor can be considered either as anodic or cathodic type. In our work, E_{corr} value is lesser than ± 85 mV (48 mV), which indicates that the inhibitor acts as a mixed type of inhibition [28]. There is no significant variation in β_a and β_c values. This confirms that the presence of praziquantel in corrosive media acts as an adsorptive inhibitor for mild steel. It retards both anodic and cathodic reactions by blocking the active corrosion sites on the surface [29, 30].

Table 1 Corrosion parameters obtained from weight loss measurement for steel in the absence and presence of various concentrations of praziquantel hydrochloride in 1 M HCl

Corrosive medium of praziquantel (ppm)	Corrosion rate ρ (mpy)	Inhibition efficiency (η_w)
Blank	21.78	–
50	20.26	60.71
100	17.17	64.64
150	15.23	71.42
200	12.88	80.35
250	11.89	85.71

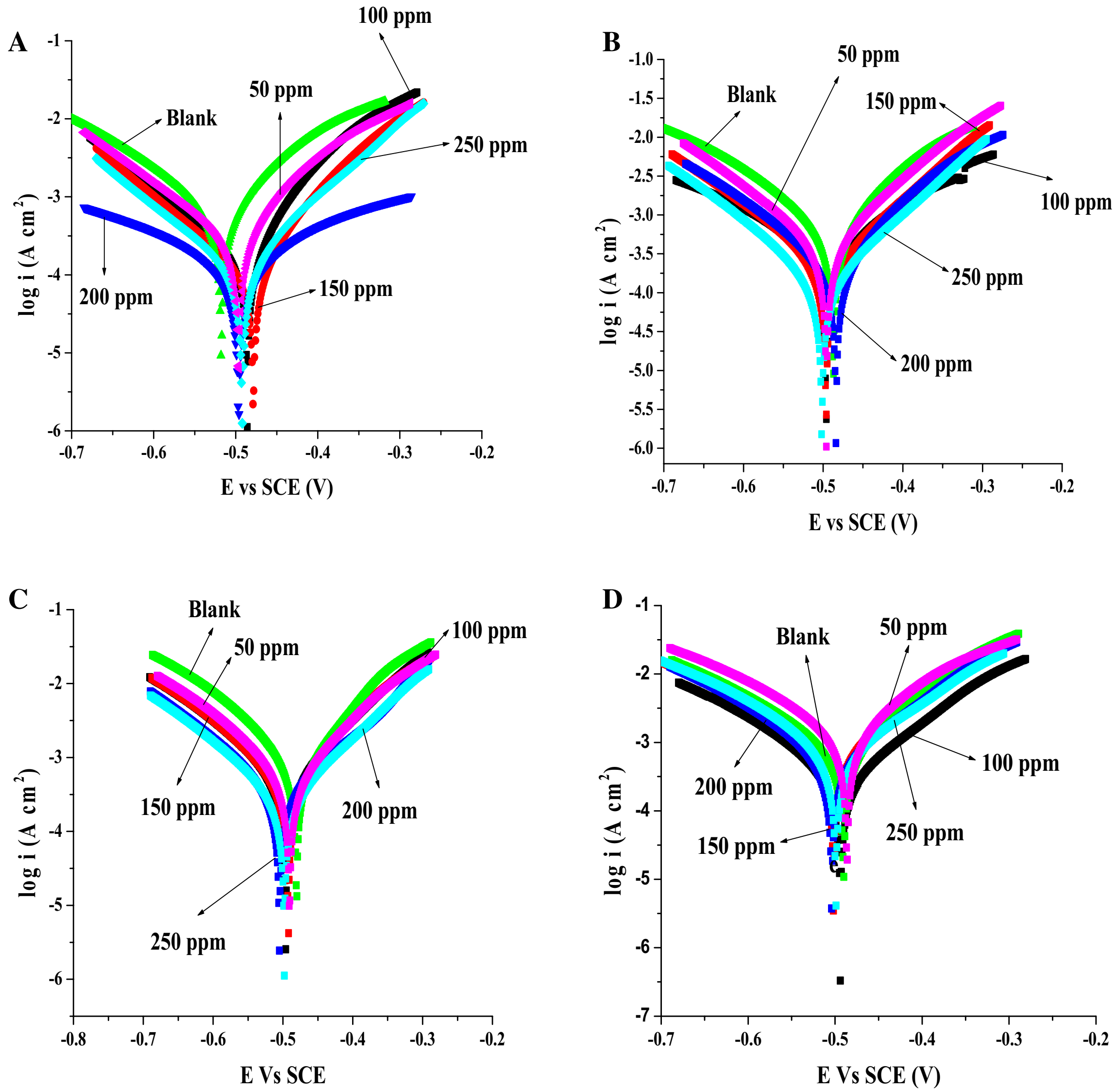

Fig. 2 Tafel plots for steel in the absence and presence of different concentrations of praziquantel in 1 M HCl at **a** 303 K, **b** 313 K, **c** 323 K, **d** 333 K

The observation of Table 2 suggests that the corrosion rate decreases and inhibition efficiency increases with the increase in inhibitor concentration. A maximum value of 80.44% at 250 ppm of praziquantel is observed [31]. The mechanism of inhibition is by the formation of a protective film on the surface of mild steel [32].

3.3 Electrochemical Impedance Spectroscopy (EIS) Measurements

EIS for mild steel in the absence and presence of various concentrations of praziquantel in 1 M HCl are presented as Nyquist plots in Fig. 3. An equivalent circuit model is used to fit the EIS results shown in Fig. 4. EIS parameters such as charge transfer resistance which is equal to polarization resistance (R_P), double-layer capacitance (C_{dl}), surface coverage (θ) and inhibition efficiency (η_Z) are calculated and reported in Table 3.

The Nyquist plots (Fig. 3) consist of semicircles with their centers on the real axis. These are described as polarization resistance (R_P). The R_P value increases with the increase in the inhibitor concentrations. These semicircles are not perfect, and there is frequency dispersion effect due to the roughness and inhomogeneity nature of the working electrode (mild steel). The increase in R_P value is an indication of the corrosion inhibition of mild steel due to the formation of protective layer by the adsorption of praziquantel molecule onto the surface of the mild steel. The decreasing in the C_{dl} values (Table 3) with the addition of inhibitor is attributed due to the decrease in dielectric constant or

Table 2 Electrochemical Tafel polarization parameters for steel in the absence and presence of various concentrations of praziquantel in 1 M HCl at a temperature range of 303–333 K

Temperature (K)	Inhibitor Conc^n (ppm)	Corrosion potential E_{corr} (V)	Corrosion current density i_{corr} (μA cm^{-2})	Corrosion rate ν_{corr} (mpy)	Cathodic Tafel slope β_c (mV/decade)	Anodic Tafel slope β_a (mV/decade)	Inhibition efficiency η_P
303	Blank	− 0.518	0.170	22.65	− 220	160	–
	50	− 0.496	0.067	20.10	− 170	130	60.58
	100	− 0.486	0.061	17.30	− 150	110	64.11
	150	− 0.479	0.046	15.00	− 120	120	72.94
	200	− 0.474	0.045	13.95	− 220	250	73.52
	250	− 0.470	0.042	12.56	− 110	140	75.29
313	Blank	− 0.510	0.465	25.80	− 170	200	–
	50	− 0.494	0.141	21.00	− 130	140	69.67
	100	− 0.485	0.113	19.20	− 250	220	75.69
	150	− 0.476	0.110	16.80	− 140	130	76.34
	200	− 0.469	0.094	15.00	− 150	150	79.78
	250	− 0.466	0.076	12.30	− 110	150	83.65
323	Blank	− 0.491	0.486	28.60	− 180	170	–
	50	− 0.488	0.264	25.30	− 160	170	45.67
	100	− 0.483	0.208	23.35	− 110	160	57.20
	150	− 0.472	0.189	19.30	− 150	150	61.11
	200	− 0.466	0.159	18.60	− 280	300	67.28
	250	− 0.458	0.158	16.80	− 100	120	67.48
333	Blank	− 0.488	0.506	34.90	− 160	170	–
	50	− 0.486	0.307	32.80	− 180	200	39.32
	100	− 0.480	0.261	28.30	− 140	130	48.41
	150	− 0.465	0.258	26.90	− 170	180	49.01
	200	− 0.462	0.195	25.80	− 130	140	61.46
	250	− 0.450	0.181	23.40	− 140	150	64.22

increase in the electric double layer on metal surface [33]. Inhibition efficiency obtained from EIS method is in good agreement with weight loss and Tafel polarization method and is shown in Fig. 5.

3.4 Adsorption Isotherm and Thermodynamic Parameters

Adhesion of dissolved inhibitor molecules on a metal surface from the inhibited solution is referred to as adsorption. The inhibition effect is attributed to the adsorption of inhibitor molecule on the surface of mild steel as a protective film, which reduces the corrosion rate [34]. The adsorption on the corroding surfaces never reaches the real equilibrium and tends to enter a steady adsorption state. When corrosion rate is sufficiently decreased in the presence of an inhibitor, the steady adsorption state manages to attain quasi-equilibrium state. Hence, it is reasonable to consider quasi-equilibrium adsorption in a thermodynamic way using the appropriate adsorption isotherm. The degree of surface coverage (θ) for inhibitor is obtained from EIS measurement data.

The linear regression coefficient (R^2) of Langmuir adsorption isotherm is found more close to unity. Hence, it can be said that the adsorption of praziquantel molecule on mild steel surface in 1 M HCl solution obeys the Langmuir's adsorption isotherm (Fig. 6). This isotherm assumes that the adsorbed molecule occupies only one site, and it does not interact with other adsorbed species. Table 4 shows the calculated values of K_{ads} and ΔG^0_{ads}.

A plot of $\Delta G^0_{ads}/T$ v/s $1000/T$ is provided in Fig. 7, and the computed ΔH^0_{ads} and ΔS^0_{ads} values are reported in Table 4.

The adsorption of the inhibitor takes place on the steel surface by replacement of water molecules with praziquantel molecules, and it can be explained by the following expression [35],

$$\text{Praziquantel}_{sol} + x\text{H}_2\text{O}_{ads} \Leftrightarrow \text{Praziquantel}_{ads} + x\text{H}_2\text{O}_{sol}.$$

The value of K_{ads} indicates a strong adsorption ability of praziquantel on the surface of the mild steel. The higher is its value, the higher is the ability of adsorption. This adsorption process can take place in two ways such as physisorption and chemisorption. Physisorption involves an electrostatic

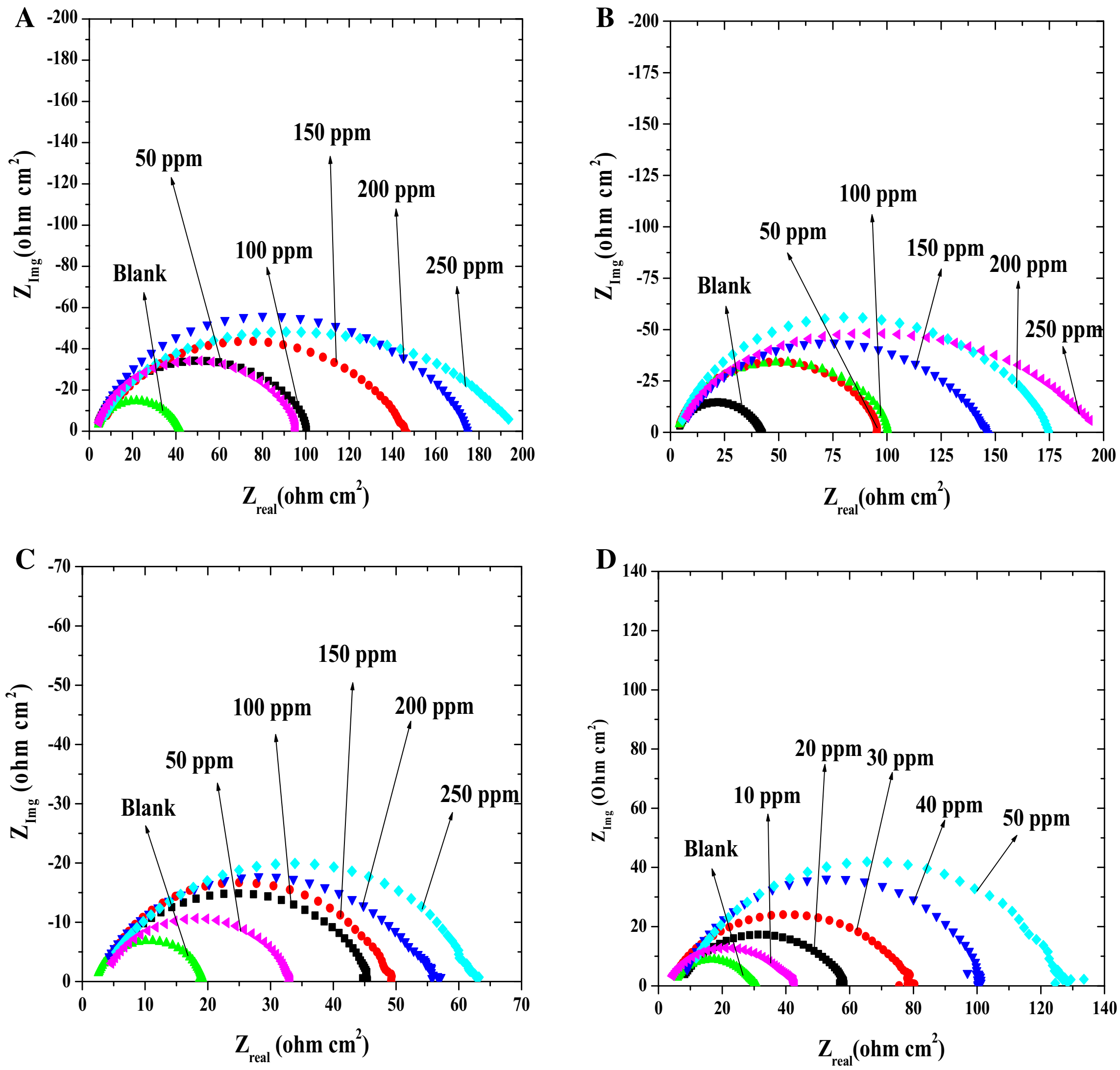

Fig. 3 Nyquist plots for steel in 1 M HCl in the absence and presence of different concentrations of praziquantel at **a** 303 K, **b** 313 K, **c** 323 K, **d** 333 K

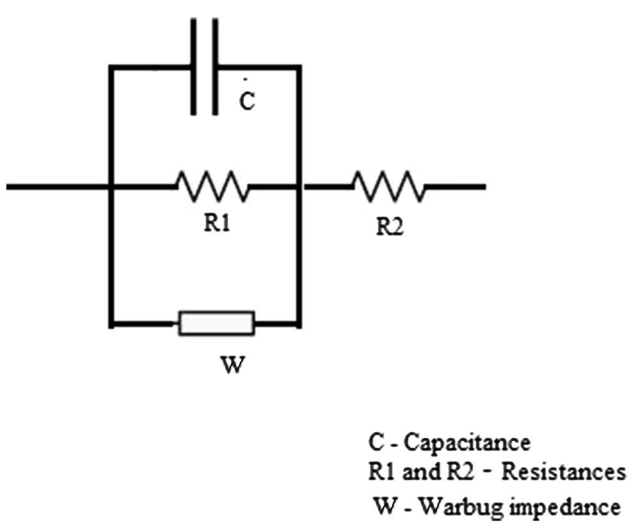

Fig. 4 Equivalent circuit used to fit the EIS results

interaction of inhibitor molecules with the metal surface. Chemisorption involves a chemical interaction (i.e., the interaction of nonbonding electrons with vacant *d*-orbital of metal) between the inhibitor molecule and the metal surface [36].

In general, if the value of ΔG^0_{ads} is less than − 20 kJ/mol, the adsorption process occurs through physisorption. If the ΔG^0_{ads} value is greater than − 40 kJ/mol, it is chemisorption [37]. The negative sign of ΔG^0_{ads} indicates the spontaneity of the adsorption (Table 4). In this study, ΔG^0_{ads} values are found in a range of − 32.71 to − 34.52 kJ/mol. This shows that the adsorption of praziquantel on mild steel surface at different temperatures (303–333 K) involves both physisorption and chemisorption [38].

Further, the negative sign of ΔH^0_{ads} indicates that the adsorption of praziquantel on mild steel surface is exothermic. This exothermic adsorption may involve

Table 3 Electrochemical impedance spectroscopy (EIS) results for the corrosion of mild steel in the absence and presence of praziquantel in 1 M HCl at a temperature region of 303–333 K

Temperature (K)	Inhibitor concentration (ppm)	R_P (Ω cm^2)	C_{dl} (μF cm^{-2})	η_Z	Surface coverage θ
303	Blank	39.21	0.037	–	–
	50	96.23	0.031	59.25	0.592
	100	101.2	0.029	61.25	0.612
	150	147.8	0.020	73.47	0.0734
	200	180.5	0.015	78.27	0.782
	250	200.5	0.012	80.44	0.804
313	Blank	25.85	0.038	–	–
	50	40.88	0.031	36.76	0.367
	100	53.17	0.028	51.38	0.513
	150	79.42	0.025	67.45	0.674
	200	96.42	0.024	73.19	0.731
	250	124.1	0.012	79.17	0.791
323	Blank	17.62	0.042	–	–
	50	30.13	0.039	41.52	0.415
	100	44.37	0.034	60.28	0.602
	150	47.28	0.031	62.73	0.627
	200	55.64	0.025	68.33	0.683
	250	62.21	0.022	71.67	0.716
333	Blank	15.40	0.051	–	
	50	24.98	0.047	38.35	0.385
	100	31.72	0.044	51.45	0.514
	150	32.74	0.028	52.96	0.529
	200	38.16	0.026	59.64	0.596
	250	42.07	0.025	63.39	0.633

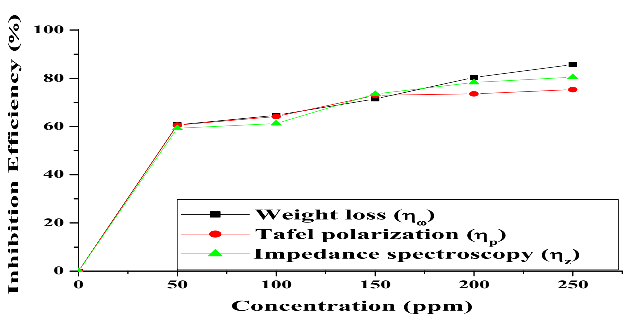

Fig. 5 Variation of inhibition efficiency versus praziquantel concentration (ppm) at 303 K

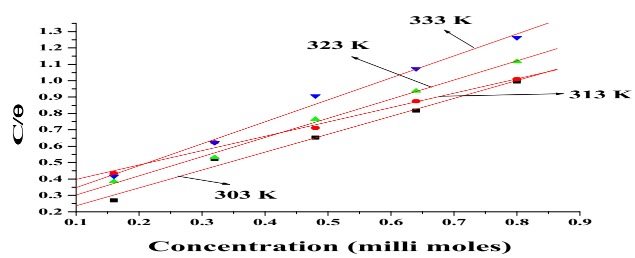

Fig. 6 Langmuir adsorption plot of steel solution containing different concentrations of praziquantel in 1 M HCl at a temperature range of 303–333 K

physisorption, chemisorption or both. In an exothermic process, physisorption can be distinguished from chemisorption by considering the absolute ΔH^0_{ads} value. The ΔH^0_{ads} value which is lesser than − 40 kJ/mol involves physisorption processes. For chemisorption, this value approaches − 100 kJ/mol. In the present work, ΔH^0_{ads} is − 63 kJ/mol, and it suggests that praziquantel gets adsorbed on the mild steel surface, predominately by chemisorption [39, 40].

The negative value of entropy (ΔS^0_{ads}) indicates that the reaction suffers a loss in the degree of freedom during the complexation process [41]. Also, as the adsorption process is exothermic, it should be accompanied by a decrease in entropy [42].

3.5 Activation Parameters

The temperature plays a vital role in the mechanism of corrosion and its inhibition. The effect of temperature is investigated using Arrhenius and transition state theory.

Table 4 Thermodynamic parameters for steel in the absence and presence of various concentrations of praziquantel in 1 M HCl at a temperature range of 303–333 K

Temperature (K)	R^2	K_{ads} (M^{-1})	ΔG^0_{ads} (kJ mol^{-1})	ΔH^0_{ads} (kJ mol^{-1})	ΔS^0_{ads} (kJ mol^{-1})
303	0.994	7874	– 32.71	– 63.00	– 99.96
313	0.995	6100	– 33.10	– 63.00	– 95.52
323	0.998	5376	– 33.85	– 63.00	– 90.24
333	0.996	4694	– 34.52	– 63.00	– 85.52

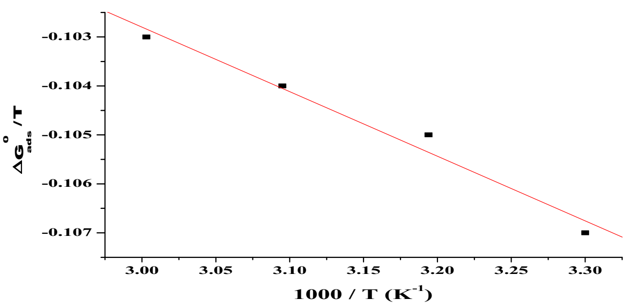

Fig. 7 The relationship between $\Delta G^0_{ads}/T$ and $1000/T$

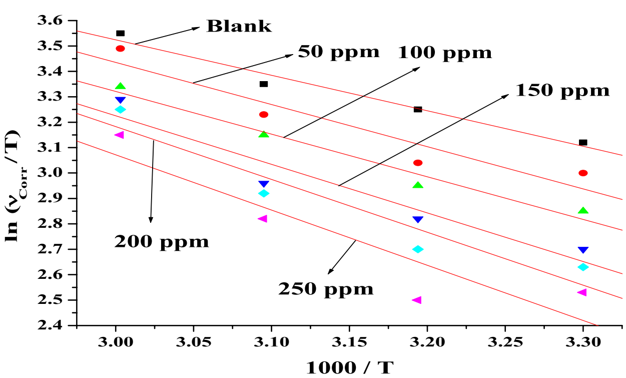

Fig. 8 Arrhenius plot for steel in the presence of different concentrations of praziquantel in 1 M HCl

Electrochemical Tafel data are fitted to study the activation parameters.

Figure 8 represents the Arrhenius plot of ln ν_{corr} against $1/T$ for the mild steel corrosion in 1 M HCl solution in the absence and presence of praziquantel. The computed E_a^* and A values are reported in Table 5.

The values of apparent activation energy (E_a^*) are higher in inhibited solution than those of the uninhibited solution. Thus, activation parameters mainly control the corrosion rate of mild steel. The increase in apparent activation energy for the mild steel dissolution in inhibited solution may be interpreted as physical adsorption [43]. Szauer and Brand have explained that as the temperature increases, the increase in activation energy can be attributed to an appreciable decrease in the adsorption of the inhibitor on the mild steel surface in 1 M HCl solution [44].

According to the Arrhenius equation, the corrosion rate (υ_{corr}) is affected by both apparent activations energy (E_a^*) value and Arrhenius pre-exponential factor (A). The Arrhenius pre-exponential factor (A) in the Arrhenius equation for corrosion process and different reactions are related to the number of active centers. In the present work, E_a^* value of the inhibited solution is higher than that of the uninhibited solution. This is an indication that the inhibitor is adsorbed on the active adsorption sites, and corrosion process occurs predominantly on the other active sites of higher energy. Values of E_a^* and A obtained in the presence of praziquantel are higher than in the blank acid solution. This means that the presence of praziquantel results in a high number of active centers remaining uncovered with the inhibitor (Fig. 9).

The calculated ΔH^* and ΔS^* values are listed in Table 5. The positive values of ΔH^* indicate that the dissolution reaction is an endothermic process and difficult. The negative value of ΔS^* suggests that the formation of the activated complex in the rate-determining step represents an association rather than a dissociation step. Therefore, this shows that the decrease in disorder takes place during the transition from reactants to activated complex [45].

Table 5 Activation parameters for steel in 1 M HCl in the absence and presence of various concentrations of praziquantel at a temperature range of 303–333 K

Concentration of inhibitor (ppm)	E_a^* (kJ/mol)	A (g cm^{-2} h^{-1})	ΔH^* (kJ mol^{-1})	ΔS^* (J mol^{-1} K^{-1})
Blank	11.61	22.46×10^2	9.09	– 22.80
50	13.79	45.05×10^2	11.27	– 22.10
100	13.95	42.59×10^2	11.44	– 22.16
150	15.89	78.00×10^2	13.11	– 21.65
200	17.29	123.82×10^2	14.44	– 21.21
250	18.07	146.76×10^2	15.48	– 20.95

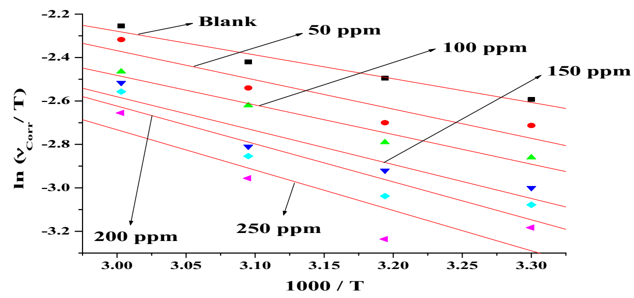

Fig. 9 Transition state plots for steel in the absence and presence of different concentrations of praziquantel in 1 M HCl

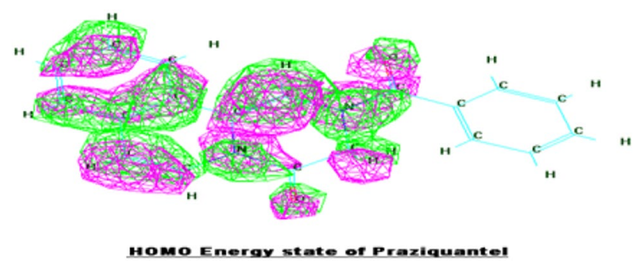

Fig. 10 Structure of HOMO energy state of praziquantel

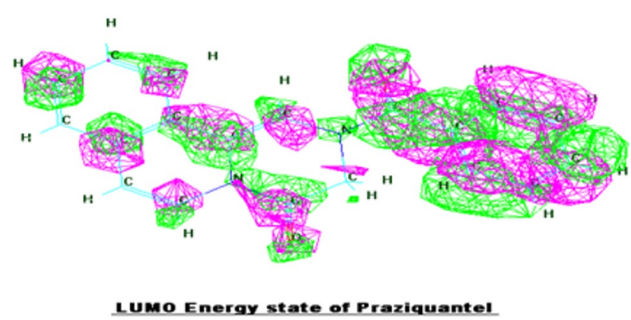

Fig. 11 Structure of LUMO energy state of praziquantel

3.6 Quantum Chemical Studies

Quantum chemical calculation deals with molecular orbital energy calculation based on Parametric Method 3(PM3) in Hyperchem 7.5 package program. This review is performed on praziquantel to get its structural and electronic properties and co-relate these features with its inhibition efficiency [46]. According to the Frontier molecular orbital theory, the formation of a transition state is due to an interaction between the frontiers orbitals [HOMO and LUMO].

Figures 10 and 11 show the HOMO and LUMO Frontier energy distribution of the molecule, respectively. The calculated quantum chemical parameters such as the energy of highest occupied molecular orbital (E_{HOMO}), the strength of lowest unoccupied molecular orbital (E_{LUMO}), energy gap in between HOMO and LUMO ($\Delta E_{HOMO–LUMO}$), total energy, binding energy and dipole moment (μ) are reported in Table 6.

Table 6 Quantum chemical parameters of praziquantel

E_{HOMO}	E_{LUMO} (eV)	ΔE (eV)	Total energy (kcal/mol)	μ (Debye)
− 8.282	− 0.467	− 7.815	− 77,882	1.074

According to the Frontier molecular orbital theory, transition states are formed due to the interactions between HOMO and LUMO of the inhibitor molecule. HOMO is directly related to the ionization potential and gives the electron-donating ability of the inhibitor molecule. Higher energy values of HOMO indicate that it provides the π-electrons to the vacant *d*-orbital of the metal atom. This high value also facilitates the adsorption of the inhibitor on the metal surface. The energy of LUMO is related to electron affinity, and lower E_{LUMO} value indicates the acceptance of electrons by the metal from the inhibitor. Due to these donor–acceptor, electronic interaction takes place to give rise to better adsorption of the inhibitor on the surface of the metal. Large HOMO–LUMO gap implies high stability for the molecule. A decrease in energy gap usually leads to easier polarization of the molecule. The lower ΔE ($E_{LUMO} - E_{HOMO}$) values give the higher inhibition because the excitation energy gap is more polarizable and is associated with chemical reactivity [47]. The energy required for removing an electron from the last occupied orbital will be low as well. For the praziquantel molecule system, ΔE value is found as − 7.815 eV. This small energy gap of an inhibitor is expected to be a useful corrosion inhibitor.

The binding energy of the praziquantel is found to be a negative value of − 4311 k cal/mol, which suggests that the inhibitor is very stable and less prone to split apart. Hence, the inhibitor gets spontaneously adsorbed on the mild steel surface with higher stability to reduce the corrosion rate.

Dipole moment (μ) is the measure of the polarity of a polar covalent bond. Higher dipole moments increase the adsorption of inhibitors on the mild steel surface, thus improving the inhibition efficiency [48, 49]. The calculated dipole moment (μ) of praziquantel is 1.074.

3.7 Scanning Electron Microscopy (SEM) Analysis

The surface investigation of the mild steel in 1 M HCl solution in the absence and presence of praziquantel by using scanning electron microscopy (SEM) is as shown in Fig. 12. From close observation of Fig. 12, a damaged surface is obtained whenever mild steel is immersed in an uninhibited 1 M HCl solution because of the attack by corrosion. However, in the presence of an inhibitor, the surface is improved

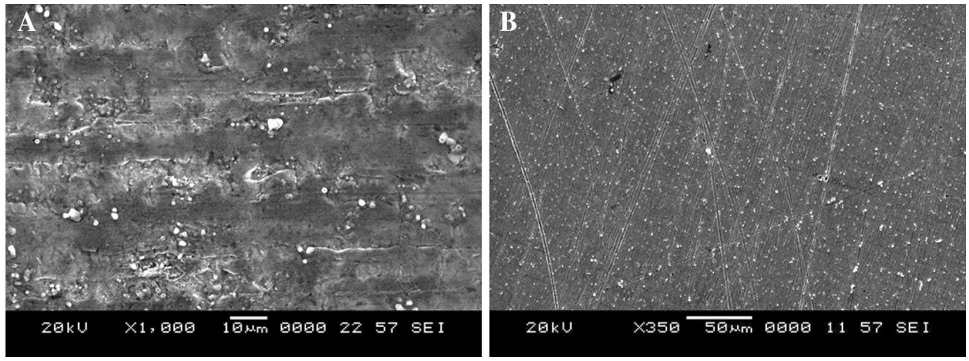

Fig. 12 SEM micrographs of steel surface (**a**) in the absence of inhibitor and (**b**) in the presence of praziquantel in 1 M HCl solution

markedly regarding smoothness. Usually, a protective film gets coated on the mild steel surface, which reduces the corrosion process considerably.

4 Conclusions

- Praziquantel acts as an active corrosion inhibitor for the corrosion of mild steel in 1 M HCl solution. Inhibition efficiency values increase with an increase in the inhibitor concentration.
- Praziquantel acts as a mixed-type inhibitor.
- Corrosion inhibition mechanism is achieved by adsorption of praziquantel molecule on the mild steel surfaces. Adsorption isotherm obeys the Langmuir model.
- The decrease in enthalpy and entropy is the driving force for the adsorption of praziquantel on the surface of the mild steel.
- Quantum chemical parameters strengthen the experimental result of this study.

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