



# Use of Seroquel as an Effective Corrosion Inhibitor for Low Carbon Steel in 1 M HCl

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## Abstract

Seroquel drug was studied for corrosion inhibition of low carbon steel in 1 M HCl solution by using experimentally with optimized concentrations at an elevated temperature range of 303–333 K. The inhibition efficiency was studied in the absence and presence of Seroquel by weight loss, electrochemical impedance spectroscopy and potentiodynamic polarization measurements. The inhibition effect of the inhibitor increases with the increasing concentration of Seroquel. Tafel polarization studies revealed that the inhibitor acts as mixed type inhibitor. The inhibition effect was attributed due to the adsorption process on low carbon steel and it obeys Temkin adsorption isotherm. The effect of temperature with the inhibition effect of inhibitor from the solution was examined by activation and thermodynamic parameters. Surface morphology of the corroded specimens were studied by SEM technique and IR spectrum of the corrosion product shows the influence of the Seroquel for corrosion inhibition.

**Keywords** Antipsychotic drug · Low carbon steel · Corrosion inhibition · FTIR

## 1 Introduction

Low carbon steel is an alloy of iron, and finds huge applications in industrial and structural field because of its superior mechanical properties. When it comes in contact with acidic media it loses its properties and undergoes dissolution. Several corrosion control approaches are used to avoid metal dissolution in acid media. But, the use of corrosion inhibitor is the most efficient and practical method to control the corrosion of metals. Corrosion inhibitors are heterocyclic molecules having heteroatoms such as nitrogen, phosphorous, sulfur, oxygen, and  $\pi$  electrons in their heterocyclic ring

system [1]. The toxicity of widely used corrosion inhibitors intends to replace them by non-toxic chemical substances (medicinal drugs or plant products) [2]. Due to non-poisonous, extensive use, and harmless effects on environment, medicinal compounds are extensively used instead of toxic organic corrosion inhibitors [3, 4]. The reduction in the rate of corrosion is due to the adsorption of organic compounds on the metal surface which blocks the active sites on the surface [5]. Presence of heteroatoms such as nitrogen, oxygen, phosphorous, sulfur, and aromatic rings makes the organic molecule to adsorb through them and blocks the active corrosion sites on the metal surface [6, 7]. The influence of inhibitors on the kinetics of electrochemical reactions modifies the dissolution of metals in acid solution [8]. Some of the medicinal drugs such as Floctafenine [9], Ziprasidone [10, 11], Clozapine [12], Cefuroxime axetil [13], Amoxicillin [14], and Modazar [15] have been investigated as good corrosion inhibitors in acid solution.

The present work is attributed to the adsorption of inhibitor molecules on low carbon steel from bulk of the solution. The adsorption phenomenon may occur due to the presence of electron-rich heteroatoms and  $\pi$  bonds which makes to study and to prove it as an effective corrosion inhibitor. The scope of this work is to investigate the influence of Seroquel drug as an effective corrosion inhibitor for low carbon

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steel in HCl solution. The molecular structure of Seroquel clearly shows the presence of hetero atoms like N, O, and S in the aromatic rings, functional groups such as  $-C=N-$ ,  $-OH$ ,  $-NH$  in its structure,  $\pi$  electron-rich aromatic rings, fair molecular size, and quite good planarity to wrap sufficient metal surface which might be supportive of its adsorption on the metal surface, giving importance to its adsorption on the metal surface.

From the literature, it has been found that, several researchers worked with drug molecule as corrosion inhibitor having properties like antifungal, antibacterial [9–12], etc., since only few literatures are available on the use of antipsychotic drug as corrosion inhibitor, like Floctafenine [9], Ziprasidone [10, 11], Clozapine [12], which set off the use of Seroquel, an antipsychotic drug to check its inhibition action for corrosion of steel.

## 2 Experimental

### 2.1 Material

The commercially available low carbon steel strips (composition: 0.35% C, 0.032% Mn, 0.028% P, 0.03% S, and remaining Fe) with a dimension of 4 cm  $\times$  1 cm  $\times$  0.1 cm were used for the present study. The surface of the steel was polished by using SiC emery papers of grade number 80 up to 2000. Weight loss method was carried out in 1 M HCl solution by these same strips and electrochemical studies were carried out by strips with 1 cm<sup>2</sup> exposed area (remaining portion was covered by epoxy resin). Aggressive corrosive media was prepared by AR grade HCl.

### 2.2 Inhibitor Solution

Seroquel is an antipsychotic medicine to treat schizophrenia and bipolar disorder. The IUPAC name of this drug is (2-[2-(4-dibenzo [b,f] [1, 4] thiazepin-11-yl-1-piperazinyloxy)-ethanol). The molecular structure of Seroquel is shown in Fig. 1. Different concentrations of the inhibitor in 1 M HCl were prepared and used for all corrosion experiments.

### 2.3 Weight Loss Measurements

Weight loss measurements were carried out by immersing steel sheets in 100 cm<sup>3</sup> of 1 M HCl solution containing different concentrations of inhibitor. The steel sheets were taken out after 4 h of immersion time and washed with tap water then with distilled water, dried in acetone, and accurately weighed. All the tests were done in triplicate and an average value was considered.

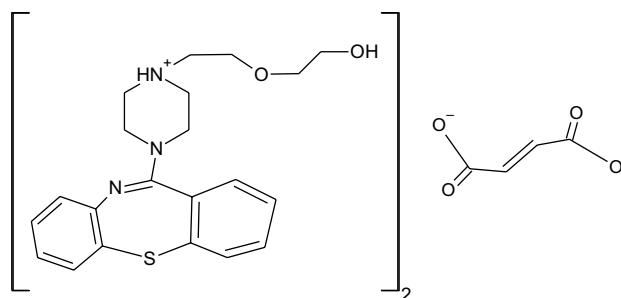


Fig. 1 Molecular structure of Seroquel

### 2.4 Electrochemical Measurements

The electrochemical measurements were carried out by using CHI-608D electrochemical work station with three electrode system. The electrode system consists of working electrode (low carbon steel), reference electrode (calomel), and an auxiliary electrode (platinum). The electrochemical parameters were recorded at different temperatures from 303 to 333 K. The working electrode was kept in contact with test solution for 30 min to attain steady-state open circuit potential. Potential–current curves were recorded by scanning at a rate of 0.01 V/s in the potential range of  $-0.2$   $\rightarrow$   $+0.2$  V to the OCP values. The impedance data were obtained using AC signal with 0.005 V amplitude in the frequency range of 1 Hz to 10 kHz.

### 2.5 Adsorption Isotherm

Corrosion inhibition of inhibitors on steel in acid media is due to their adsorption on the steel surface. The adsorption property of Seroquel on low carbon steel at different temperatures in 1 M HCl was studied using several adsorption isotherms and the thermodynamic data were determined using standard equations.

### 2.6 Activation Parameters

The variation in inhibition efficiency at different temperatures was studied by activation parameters [16]. Using the data obtained for corrosion rate at different temperatures, graphs were plotted and calculations were made using standard equations.

### 2.7 Scanning Electron Microscopic Studies

Low carbon steel samples were kept in contact with 1 M HCl solution in the absence and presence of optimum concentration of inhibitors over a period of 4 h of immersion time. The samples were taken out and then washed with distilled water,

dried, and analyzed by SEM technique. The SEM analysis was carried out using VEGA3 TESCAN SEM instrument at an accelerating beam of 25 kV.

## 2.8 FTIR Spectral Studies

FTIR Spectrum of the pure compound and the compound scarpred from the metal surface after corrosion was carried out by using Frontier Perkin Elmer spectrometer.

## 3 Results and Discussion

### 3.1 FTIR Spectral Studies

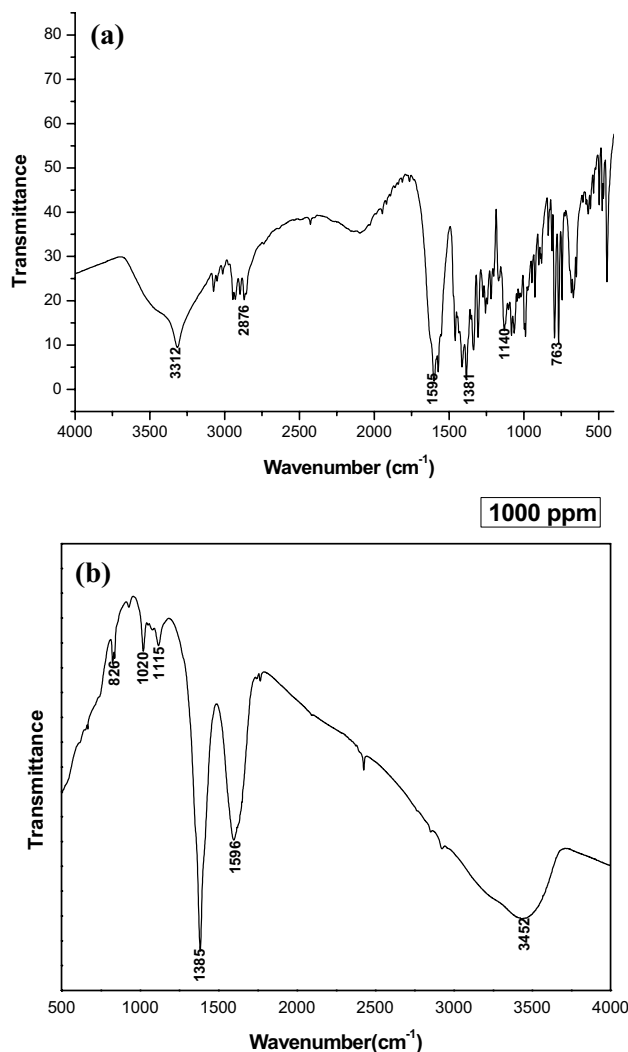
FTIR spectral studies gives the valuable information about the coordination of inhibitor molecule with the metal surface through the hetero atoms. Specific to the inhibitor used in the present study, i.e., Seroquel, adsorption may be through the heteroatoms like, N, O, and S and is confirmed by the shift of absorption peak in the IR spectrum of scarpred compound compared to IR spectrum of pure compound.

FTIR spectrum of pure Seroquel is shown in Fig. 2a. The presence of broad band at  $3312\text{ cm}^{-1}$  indicates the presence of hydroxyl group stretching vibration. The peak at  $2876\text{ cm}^{-1}$  indicates the presence of carboxylic acid O–H stretching vibration. The peak at  $1595\text{ cm}^{-1}$  shows the presence of aromatic C=C bending vibration. The narrow peak at  $1381\text{ cm}^{-1}$  is due to C–H absorption. The presence of narrow band at  $1140\text{ cm}^{-1}$  is due to the C–O group. The peak at  $763\text{ cm}^{-1}$  shows the presence of aromatic C–H bending vibration.

Figure 2b shows the FTIR spectrum of the compound scarpred from the metal surface after corrosion in 1 M HCl solution. The appearance of absorption peak at  $3452\text{ cm}^{-1}$ , compared to  $3312\text{ cm}^{-1}$  in the pure compound indicates the adsorption of molecule with the metal surface through –OH group of the Seroquel molecule. The band at  $1115\text{ cm}^{-1}$ , compared to  $1140\text{ cm}^{-1}$  for the pure compound, corresponding to C–O–C stretching vibration also indicates the coordination of molecule through O heteroatom. The peak at  $1020\text{ cm}^{-1}$  is due to the presence of aliphatic amines, which also supports the bonding of Seroquel through N atom. Slight shift in the wave number of the absorption peaks in the scarpred compound confirms the interaction of the Seroquel with steel and the presence of inhibitor molecule on the surface of the metal.

### 3.2 Weight Loss Method

The study was carried out by immersing mild steel strips in 1 M HCl solution containing different concentrations of the inhibitor at different temperatures for maximum of



**Fig. 2** a FTIR spectrum of Seroquel drug and b FTIR spectrum of scarpred compound

4 h. The weights of each steel strip were measured before and after immersion using an analytical balance. The percentage inhibition efficiency,  $\eta_w$  was calculated using the formula,

$$\eta_w = \frac{W^0 - W}{W^0} \times 100, \quad (1)$$

where  $W$  and  $W^0$  represent weight loss of steel in the presence and absence of corrosion inhibitor, respectively.

Rate of corrosion is determined using the following equation,

$$v_{\text{corr}} = \frac{\Delta m}{ST}, \quad (2)$$

where  $\Delta m$  is weight loss in absence of inhibitor ( $m_0$ ) – weight loss in presence of inhibitor ( $m_1$ ),  $S$  is surface area,  $T$  is time of exposure in hours.

Calculated values of corrosion rates and inhibition efficiency are listed in Table 1. It is evident from the values obtained that the corrosion rate of steel decreases with increase in the concentration of Seroquel against blank. As shown in Table 1, it is clear that inhibition efficiency of Seroquel increases with increase in concentration up to 1000 ppm. So 1000 ppm is considered as the critical concentration for maximum inhibition efficiency to be achieved. The decrease

in corrosion rate with the increase in inhibitor concentration is due to adsorption of inhibitor molecule on metal surface [17].

### 3.3 Electrochemical Measurements

#### 3.3.1 Polarization Studies

Polarization studies were carried out to obtain the knowledge of kinetics of electrode reactions (both anodic and cathodic) [18]. Electrochemical corrosion parameters, i.e., corrosion current ( $i_{\text{corr}}$ ), corrosion potential ( $E_{\text{corr}}$ ), Tafel slope ( $\beta_a$  and  $\beta_c$ ) from the extrapolation of the polarization curves, and  $\eta_p$  (inhibition efficiency according to polarization data) are given in Table 2. The polarization plots of low carbon steel in 1 M HCl in the presence and absence of different concentrations of Seroquel at different temperatures are shown in Fig. 3. The  $\eta_p$  was calculated using the following equation,

$$\eta_p = \frac{i_{\text{corr}}^0 - i_{\text{corr}}}{i_{\text{corr}}^0} \times 100, \quad (3)$$

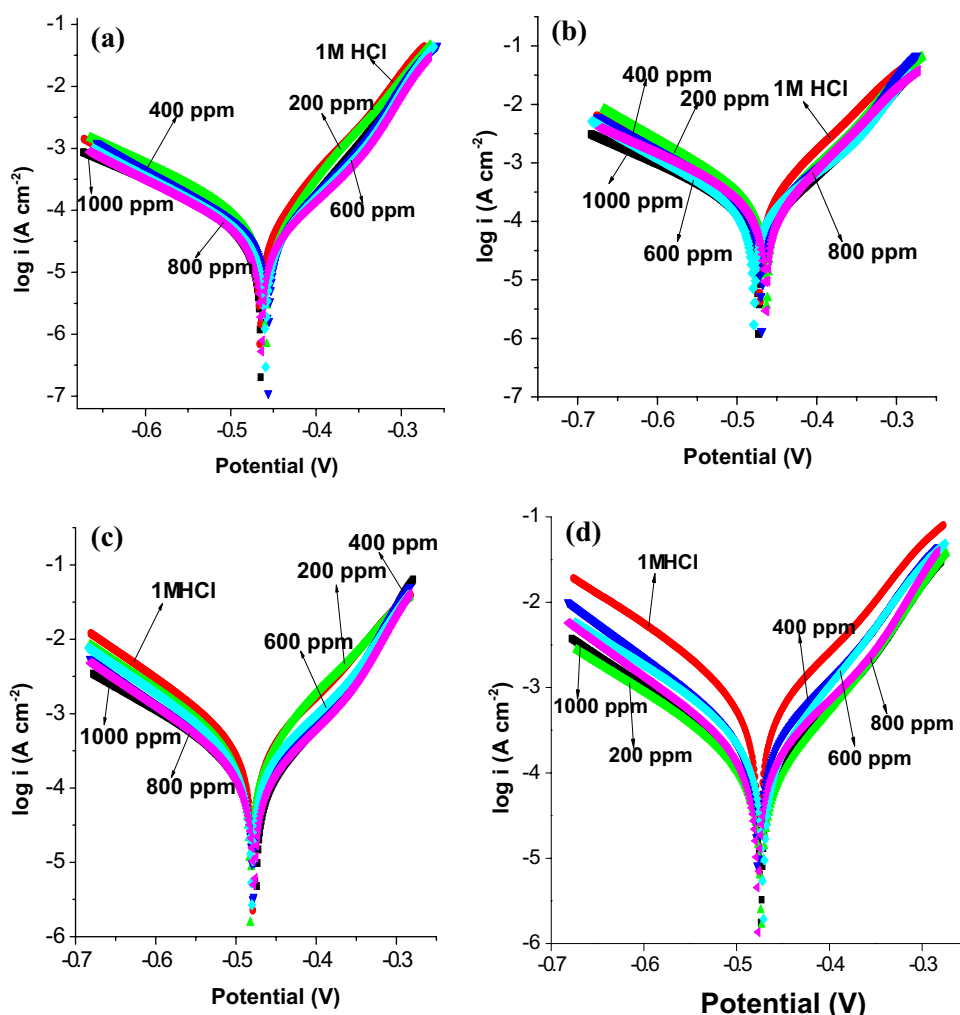
**Table 1** Corrosion parameters obtained from weight loss measurement

Concentration of Seroquel (ppm)	Corrosion rate, $\rho$ (g/cm <sup>2</sup> h)	Inhibition efficiency (% $\eta_w$ )
Blank	0.257	–
200	0.223	13.20
400	0.202	21.40
600	0.170	33.85
800	0.142	44.74
1000	0.135	47.47

**Table 2** Tafel results for the corrosion of steel in 1 M HCl in the presence of different amounts of Seroquel at different temperatures

Temperature (K)	Inhibitor concentration (ppm)	Corrosion potential, $E_{\text{corr}}$ (V)	Corrosion current density, $i_{\text{corr}}$ (A/cm <sup>2</sup> )	Corrosion rate, $\nu_{\text{corr}}$ (mpy)	Cathodic slope, $\beta_c$ (mV/decade)	Anodic slope, $\beta_a$ (mV/decade)	Inhibition efficiency, $\eta_p$ (%)
303	Blank	–0.466	0.030	22.2	–7.211	14.49	–
	200	–0.458	0.028	15.7	–7.603	15.51	6.66
	400	–0.456	0.023	13.5	–7.811	15.07	23.33
	600	–0.459	0.021	12.2	7.460	14.38	30.00
	800	–0.464	0.019	3.7	–7.41	13.66	36.66
	1000	–0.465	0.017	3.3	–7.29	16.20	43.33
313	Blank	–0.471	0.041	22.3	–7.05	13.13	–
	200	0.463	0.031	19.5	–8.37	13.47	24.43
	400	–0.469	0.027	17.5	–7.99	12.07	34.14
	600	–0.479	0.024	14.1	–7.989	10.41	41.46
	800	–0.464	0.023	7.4	–7.43	13.79	43.90
	1000	–0.473	0.019	5.5	–7.19	12.68	53.65
323	Blank	–0.479	0.052	23.84	–8.35	11.06	–
	200	–0.482	0.042	19.90	–8.01	11.12	19.23
	400	–0.480	0.033	16.06	–8.22	10.77	36.53
	600	–0.479	0.027	14.39	–7.74	11.07	48.07
	800	–0.477	0.023	10.10	–8.02	11.22	55.76
	1000	–0.475	0.020	8.06	–7.47	12.90	61.53
333	Blank	–0.469	0.123	25.7	–8.20	12.76	–
	200	–0.473	0.056	23.8	–7.85	13.10	54.47
	400	–0.477	0.036	19.60	–8.51	11.76	70.73
	600	–0.471	0.027	17.10	–7.93	13.60	78.04
	800	–0.477	0.024	14.40	–8.29	11.15	80.48
	1000	–0.474	0.020	10.88	–7.83	11.60	83.73

**Fig. 3** Tafel plots for low carbon steel in the absence and presence of different concentrations of inhibitor at **a** 303 K, **b** 313 K, **c** 323 K, and **d** 333 K temperature



where  $i_{\text{corr}}^0$  and  $i_{\text{corr}}$  are the current densities in the absence and presence of corrosion inhibitor, respectively. As shown in Fig. 3, it can be observed that the addition of Seroquel shifts both the anodic and cathodic curves toward lower values of current densities. This is due to the adsorption of Seroquel on steel surface which inhibits metal dissolution at anode and hydrogen liberation at cathode causing a remarkable decrease in the corrosion rate. As reported in many literatures, the inhibitor can be classified as anodic or cathodic type, if the displacement of corrosion potential is greater than  $\pm 85$  mV compared to the corrosion potential of the blank [19]. In our present work, since corrosion potential value is lesser than  $\pm 85$  mV, the inhibitor acts as mixed type inhibitor [20–23].

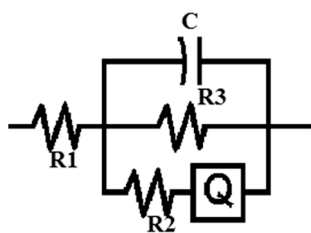
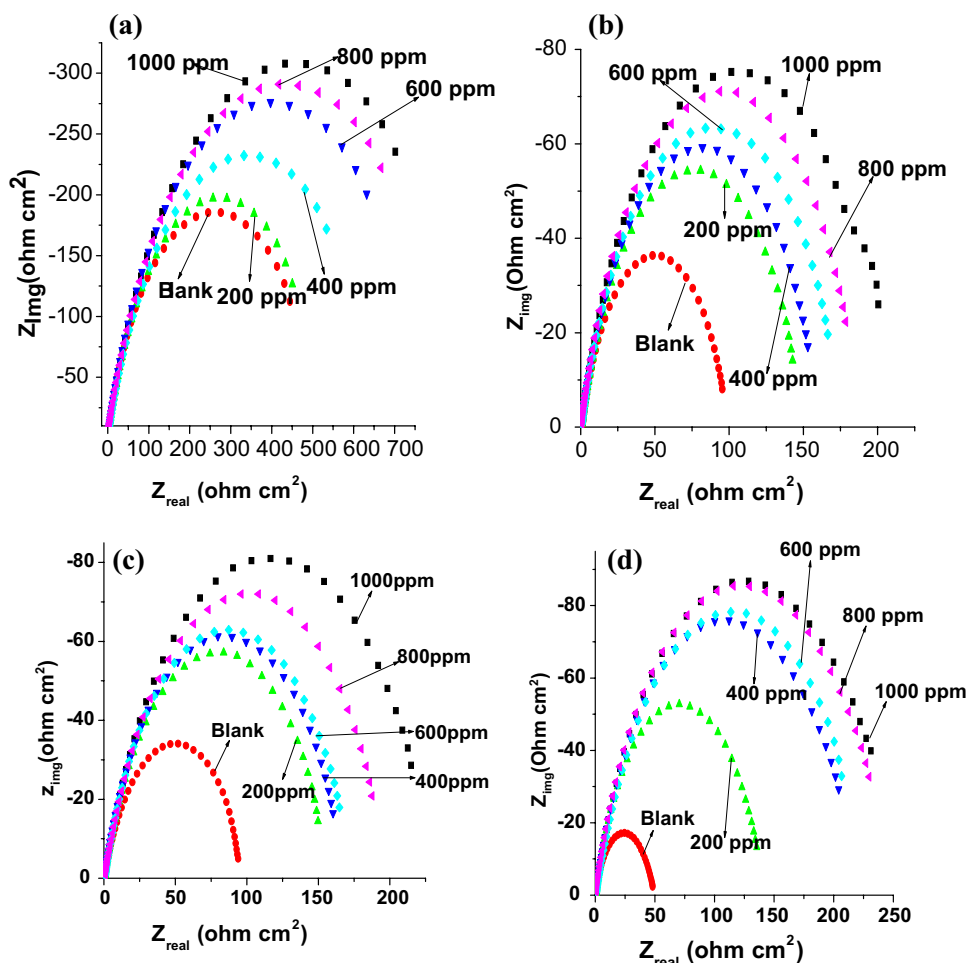
The effect of temperature on corrosion of steel in the absence and presence of Seroquel was studied in the temperature ranging from 303 to 333 K and the results are tabulated in Table 2. From the values obtained it is clear that the corrosion rate of low carbon steel increased as the temperature increases in the absence of the inhibitor. But in the presence of the inhibitor, the corrosion rate diminished with the rise

in temperature; this also says that the increased adsorption of the inhibitor on the surface of metal thereby blocks metal sites which are prone for corrosion at high temperature. The inhibitor attained maximum inhibition efficiency in the range of 70–84% at an optimum concentration of 1000 ppm of Seroquel.

### 3.3.2 Electrochemical Impedance Spectroscopy Measurements

Figure 4 represents EIS spectra for low carbon steel in 1 M HCl at different temperatures in the presence and absence of different concentrations of Seroquel inhibitor which are presented as Nyquist plots. The equivalent circuit model is shown in Fig. 5 which was used to analyze the current response as a function of frequency. Calculated EIS experimental parameters such as charge transfer resistance which is equivalent to polarization resistance ( $R_p$ ), double layer capacitance ( $C_{dl}$ ), inhibition efficiency ( $\eta_2$ ), and surface coverage ( $\theta$ ) are listed in Table 3. It is clear from Table 3 that  $R_p$  value increases and  $C_{dl}$  value decreases with increase in inhibitor concentration. This

**Fig. 4** Nyquist plots for low carbon steel in 1 M HCl in the absence and presence of different Inhibitor concentrations at **a** 303 K, **b** 313 K, **c** 323 K, and **d** 333 K temperatures



R1, R2, R3- Resistance, C-Capacitance  
Q-Constant phase element

**Fig. 5** Electrical equivalent circuit model to fit impedance data

is due to the adsorption of inhibitor molecules on the metal surface thereby decreasing the extent of metal dissolution [24]. The decrease in  $C_{dl}$  values with increase in inhibitor concentration is probably due to the decrease in dielectric constant and/or due to the increase in the thickness of the double layer on the metal surface [25]. The deviations from perfect semicircles are involved with the frequency dispersion of interfacial impedance which is due to many physical factors like active sites, surface roughness, and non-homogeneity of the mild

steel. The increase in diameter of the semicircle with increase in the inhibitor concentration indicates that the charge transfer process is the main factor in controlling the corrosion of mild steel, which is mainly due to increase in charge transfer resistance and formation of more compact monolayer on metal surface [26].

Impedance study was also carried out in the temperature range of 303–333 K, and the results are shown in Table 3. It has been found that the value of  $R_p$  decreases as the temperature increases in the absence of the inhibitor, which indicates the increase of corrosion at high temperature. But, value of  $R_p$  increased significantly by the addition of Seroquel at high temperature which indicates that the increase of adsorption thereby decreases the corrosion rate.

The  $\eta_z$  values were calculated using the following relation,

$$\eta_z = \frac{R_p - R_p^0}{R_p} \times 100, \tag{4}$$

where  $R_p$  and  $R_p^0$  are polarization resistance values in the presence and absence of inhibitor.



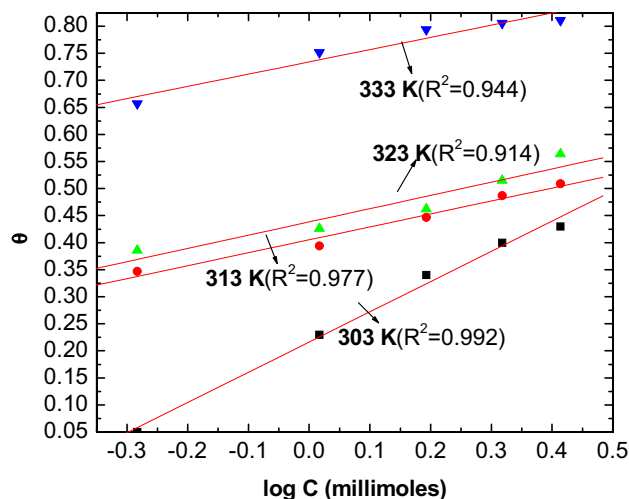
**Table 3** EIS results for the corrosion of steel in 1 M HCl in the presence of different amounts of Seroquel at different temperatures

Temperature (K)	Inhibitor concentration (ppm)	$R_p$ ( $\Omega$ cm <sup>2</sup> )	$C_{dl}$ ( $\mu$ F/cm <sup>2</sup> )	$\eta_z$ (%)	Surface coverage, $\theta$
303	Blank	537.2	0.014	–	
	200	562.8	0.013	4.80	0.048
	400	705.4	0.010	23.80	0.230
	600	824.6	0.009	34.85	0.348
	800	898.5	0.008	40.20	0.402
	1000	951.7	0.005	43.57	0.435
313	Blank	98.79	0.020	–	
	200	151.3	0.013	34.70	0.347
	400	163.1	0.014	39.40	0.394
	600	178.5	0.014	44.70	0.447
	800	192.4	0.013	48.70	0.487
	1000	201.5	0.011	50.90	0.509
323	Blank	97.25	0.014	–	
	200	158.4	0.014	38.60	0.386
	400	169.4	0.013	42.60	0.426
	600	180.7	0.013	46.20	0.462
	800	200.6	0.012	51.50	0.515
	1000	223.0	0.016	56.40	0.564
333	Blank	48.27	0.022	–	
	200	140.8	0.017	65.70	0.657
	400	194.5	0.011	75.20	0.752
	600	233.8	0.021	79.40	0.794
	800	249.1	0.010	80.60	0.806
	1000	255.2	0.011	81.10	0.811

### 3.4 Adsorption Isotherm

Adsorption isotherm is the most important topic in the field of corrosion because it provides some fundamental information about interactions between adsorbate (inhibitor) and adsorbent (metallic surface). Depending on the electronic structure of inhibitor molecule, nature of metal and electrolyte, solution temperature, etc., adsorption may be chemisorption, physisorption, or both. Physical adsorption is associated with weak van der Waals or electrostatic interactions between the adsorbent and the adsorbate in the neutral or ionic form, respectively.

Corrosion inhibition tendency of Seroquel on steel surface is due to the adsorption phenomenon which decreases the corrosion rate and this is due to formation of protective film by adsorbed inhibitor molecule [27]. The adsorption process on the surface of corroding metal always tends to attain an adsorption steady state rather than equilibrium state. But when the rate of corrosion decreases in the presence of an inhibitor, the steady adsorption state tends to attain quasi-equilibrium state. Hence, it is required to consider quasi-equilibrium state in a thermodynamic way by proper adsorption isotherm. The



**Fig. 6** Temkin adsorption plots of low carbon steel in 1 M HCl solution at different concentrations of Seroquel at different temperatures

adsorption isotherm study explains the interaction between mild steel surface and the inhibitor molecules [28]. For this, surface coverage ( $\theta$ ) values were calculated at different concentrations of the inhibitor in 1 M HCl solution. Adsorption process can be explained by two types of interaction [29]: physisorption which involves electrostatic attraction between ionic charges, low heat of adsorption, and hence less stability at relatively low temperatures, and chemisorptions which involves charge transfer to the metal surface from the inhibitor molecules, stronger adsorption energy, and hence more stability at high temperatures.

The mode of adsorption of Seroquel on steel in 1 M HCl at different temperatures was studied by fitting the experimental data into different adsorption isotherms. In this study, several commonly used isotherms, namely, Langmuir, Temkin (Fig. 6), and Freundlich were tested. In each case, a function of the fractional surface coverage ( $\theta$ ) is plotted against a function of the concentration of inhibitor ( $C$ ) and the associated adsorption parameters are deduced from slope or intercept or both. The routine involves fitting the surface coverage data into different adsorption models and the isotherm that best fits the data is used to describe the adsorption behavior. The best fit is usually the one that gives the highest regression coefficient ( $R^2$ ) value from the linear plots. Among the various isotherms, Temkin adsorption isotherm gave the best line of fit, with the values of regression coefficient ( $R^2$ ) very close to unity and is shown in Fig. 6. This suggests that the adsorption of inhibitor molecule on the metal surface obeys Temkin adsorption isotherm [30] and it is given by the following equation:

$$\exp(f\theta) = K_{ads} \cdot C, \tag{5}$$

where  $\theta$  is the degree of surface coverage,  $C$  is the inhibitor concentration,  $f$  is the molecular interaction parameter,  $K_{ads}$

is the adsorption equilibrium constant which indicates the interaction between adsorbent and adsorbate [31].  $K_{ads}$  is related to  $\Delta G_{ads}^{\circ}$  by the following equation:

$$K_{ads} = \frac{1}{55.5} e^{\left(\frac{-\Delta G_{ads}^{\circ}}{RT}\right)}, \tag{6}$$

where  $R$  is the gas constant,  $T$  is the absolute temperature in K, and 55.5 is the molar concentration of water in the solution. Thermodynamic parameters for the adsorption of inhibitor at different temperatures derived from Temkin adsorption isotherms are given in Table 4. As reported in literature the higher values of  $K_{ads}$  attribute to strong and stable adsorption of inhibitor layer on the metal surface [31, 32]. It is clear from Table 4 that the higher value of  $K_{ads}$  contributes to strong interaction between the inhibitor molecule and the steel surface.

Literature also reveals that the negative value of  $\Delta G_{ads}^{\circ}$  indicates the spontaneous adsorption of inhibitor molecule on the metal surface. It is evident from Table 4 that the reported  $\Delta G_{ads}^{\circ}$  values at different temperatures are negative which indicates that the adsorption of Seroquel inhibitor molecule on the low carbon steel surface in 1 M HCl solution is a spontaneous process. Generally, the values of  $\Delta G_{ads}^{\circ}$  lesser than or equal to  $-20$  kJ/mol represent the electrostatic interaction between the metal surface and the inhibitor molecules, i.e., physisorption, and the values greater than or equal to  $-40$  kJ/mol represent the charge transfer between the metal surface and inhibitor molecules, i.e., chemisorptions [33]. In this work,  $\Delta G_{ads}^{\circ}$  values were found to be ranging from  $-30.77$  to  $-31.55$  kJ/mol, which indicates that the adsorption process of the inhibitor on the steel was due to both physisorption and chemisorption (comprehensive adsorption) [34, 35].

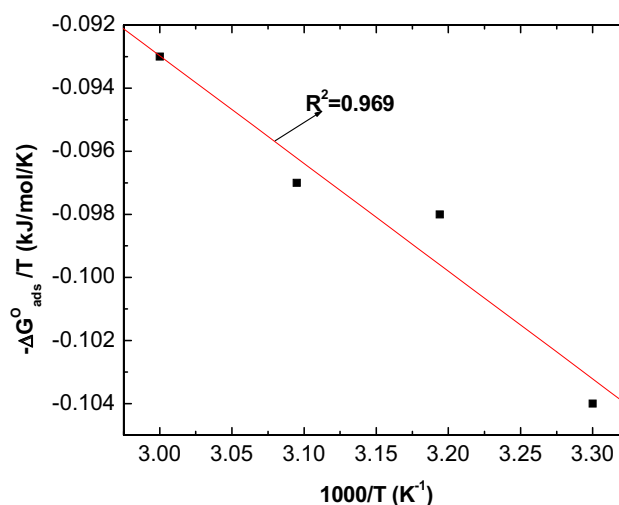
A linear graph of  $\Delta G_{ads}^{\circ}/T$  against  $1000/T$  is shown in Fig. 7, and the calculated values of  $\Delta H_{ads}^{\circ}$  and  $\Delta S_{ads}^{\circ}$  are listed in Table 4. Slope of the straight line gives  $\Delta H_{ads}^{\circ}$ , and  $\Delta S_{ads}^{\circ}$  values were calculated using the standard equation,

$$\Delta G_{ads}^{\circ} = \Delta H_{ads}^{\circ} - T\Delta S_{ads}^{\circ}. \tag{7}$$

Generally, negative values of enthalpy of adsorption indicate physical adsorption, i.e., endothermic adsorption,

**Table 4** Thermodynamic parameters for the corrosion of steel in 1 M HCl in the presence of different amounts of Seroquel at different temperatures

Temperature (K)	$K_{ads}$	$-\Delta G_{ads}^{\circ}$ (kJ/mol)	$-\Delta H_{ads}^{\circ}$ (kJ/mol)	$-\Delta S_{ads}^{\circ}$ (J/mol/K)
303	4065	31.38	34.15	91
313	2469	30.77	34.15	107
323	2283	31.55	34.15	80
333	1362	31.09	34.15	92



**Fig. 7** Relationship between  $\Delta G_{ads}^{\circ}/T$  and  $1000/T$

whereas positive values indicate chemical adsorption, i.e., exothermic adsorption [36]. The values of enthalpy of adsorption lesser than  $-40$  kJ/mol involve physical adsorption, whereas enthalpy of adsorption equal to  $-100$  kJ/mol involves chemical adsorption [37]. In this work, the value of enthalpy of adsorption is  $-34.15$  kJ/mol which represents that the adsorption of the Seroquel inhibitor on the steel surface is endothermic and it suggests physical adsorption. The entropy is maximum when there is a free mobility of inhibitor molecule in the solution [37]. The negative value of the entropy of adsorption indicates that the adsorption is accompanied by a decrease in entropy and is due to orderly adsorption of the inhibitor molecules on the steel surface [38].

### 3.5 Activation Parameters

The corrosion rate of metal is largely influenced by the temperature as it modifies the inhibition property due to decomposition and/or rearrangements of inhibitor [39]. To evaluate thermodynamic parameters in order to explain inhibition and the adsorption process, electrochemical experiments were carried out in the absence and presence of different concentrations of the inhibitor in the temperature range of 303–333 K. The temperature dependence of corrosion rate can be explained by Arrhenius equation and transition state theory [40]. The Arrhenius equation and transition state equation can be written as,

$$\log(\gamma_{corr}) = \frac{-E_a}{2.303RT} + \log A, \tag{8}$$

$$\gamma_{corr} = \frac{RT}{Nh} e^{\frac{\Delta S^{\ddagger}}{R}} e^{\frac{\Delta H^{\ddagger}}{RT}}, \tag{9}$$



where  $\gamma_{\text{corr}}$  is the corrosion rate,  $E_a$  is the apparent activation energy,  $A$  is the Arrhenius pre-exponential factor,  $R$  is the gas constant,  $T$  is the temperature in Kelvin,  $h$  is Planck's constant,  $N$  is the Avogadro number,  $\Delta S^*$  is the apparent entropy of activation, and  $\Delta H^*$  is the apparent enthalpy of activation. Arrhenius plot, obtained by plotting a graph of  $\ln(\gamma_{\text{corr}})$  versus  $1000/T$ , is shown in Fig. 8. The calculated values of  $E_a$ ,  $A$ ,  $\Delta H^*$ , and  $\Delta S^*$  are reported in Table 5. From the slope of each straight line shown in Fig. 8,  $E_a$  values were calculated using the relation  $E_a = (\text{slope} \times R)$ . Figure 9 represents a plot of  $\ln(\gamma_{\text{corr}}/T)$  versus  $1000/T$ . From the straight line of the graph,  $\Delta H^*$  values were calculated by the slope of the straight line using the equation  $\Delta H^* = -\text{slope} \times R$  and  $\Delta S^*$  values were calculated by the intercept using the equation,

$$\Delta S^* = \text{intercept} - \ln\left(\frac{R}{Nh}\right). \tag{10}$$

From the  $E_a$  values reported in Table 5, it is clear that the higher value of  $E_a$  than that of the blank suggests that the metal dissolution is suppressed by the addition of inhibitor

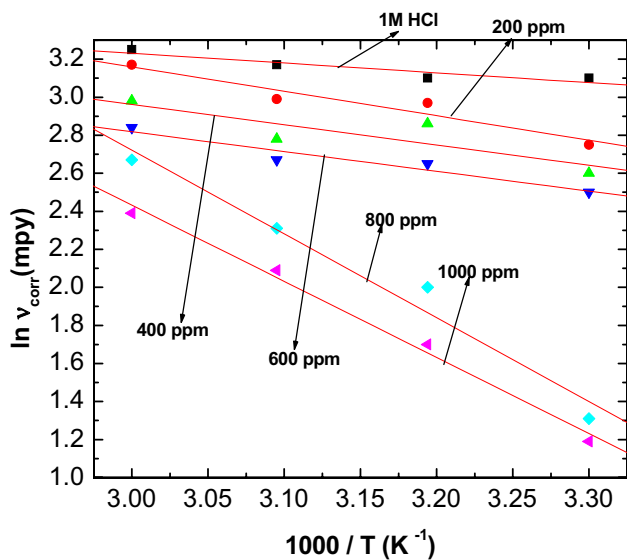


Fig. 8 Arrhenius plot for low carbon steel in 1 M HCl in the absence and presence of different concentrations of Seroquel

**Table 5** Activation parameters for the corrosion of steel in 1 M HCl in the presence of different amounts of Seroquel at different temperatures

Concentration, $C$ (ppm)	$E_a$ (kJ/mol)	$A$ (g/cm <sup>2</sup> /h)	$\Delta H^*$ (kJ/mol)	$\Delta S^*$ (J/mol/K)
Blank	4.28	$5.98 \times 10^2$	1.42	-25.83
200	10.66	$1.023 \times 10^7$	7.90	-23.56
400	8.85	$1.43 \times 10^6$	6.02	-24.43
600	8.65	$8.66 \times 10^5$	5.86	-24.63
800	36.66	$8.91 \times 10^{15}$	34.12	-14.53
1000	33.28	$2.75 \times 10^{14}$	30.45	-16.16

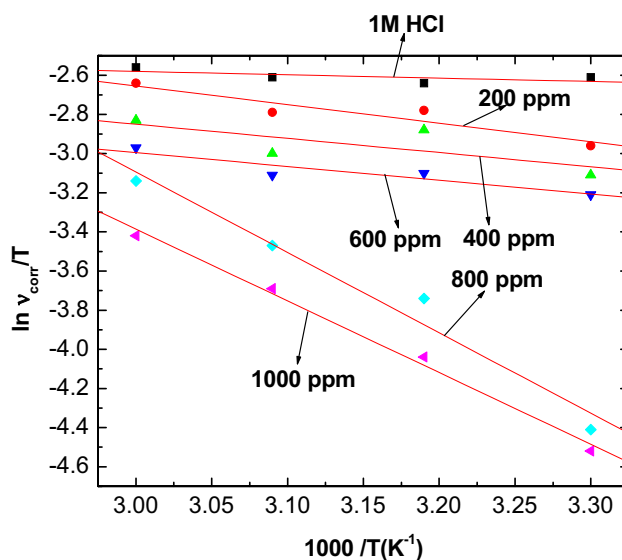
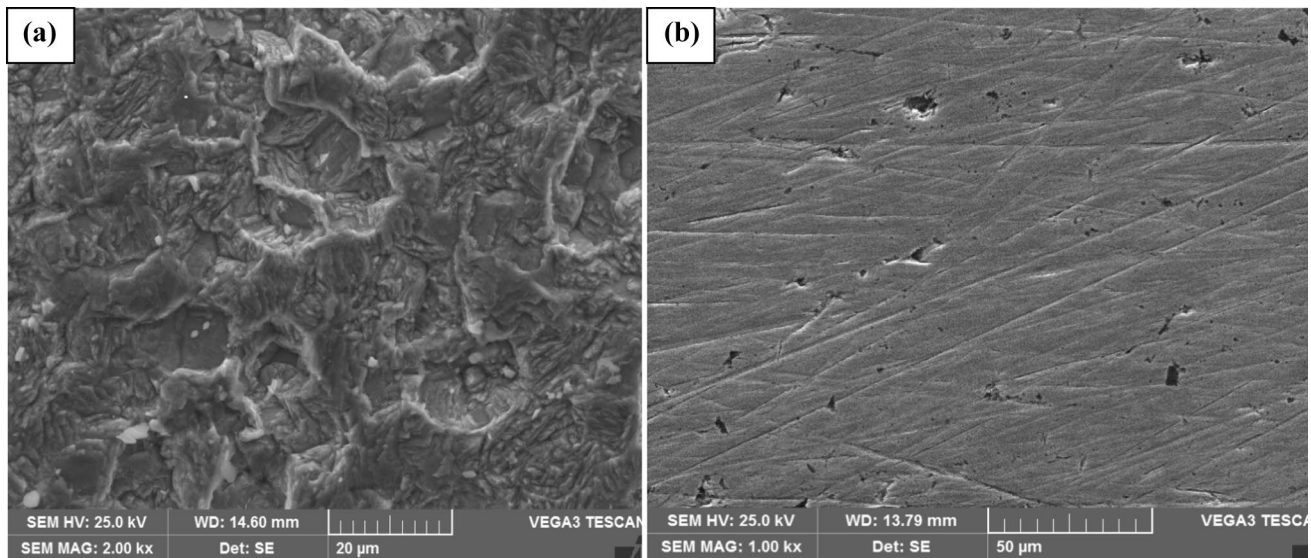


Fig. 9 Transition plot for low carbon steel in 1 M HCl in the absence and presence of different concentrations of Seroquel

[41]. The increase in  $\Delta H^*$  value is an indication of the formation of protective layer on the steel surface in contact with the inhibited solution. The less negative value of  $\Delta S^*$  in the presence of inhibitor than compared to blank is due to adsorption of inhibitor on the steel surface (quasi substitution) [42, 43].

### 3.6 SEM Studies

SEM micrographs of the mild steel surface in 1 M HCl in the absence and presence of Seroquel inhibitor are shown in Fig. 10a, b. Surface morphology of the corroded steel surface in 1 M HCl solution in the absence of inhibitor for 4 h immersion time is shown in Fig. 10a, b, which shows the corroded steel surface in 1 M HCl solution in the presence of 1000 ppm of Seroquel inhibitor for the same immersion time. The SEM image of corroded metal sample clearly shows that the surface is rough and damaged in the absence of inhibitor compared to the surface in the presence of 1000 ppm of inhibitor due to decrease in the corrosion rate. This indicates that the surface



**Fig. 10** **a** SEM image of corroded low carbon steel surface in the absence of Seroquel inhibitor and **b** SEM image of corroded low carbon steel surface in the presence of Seroquel inhibitor

damage was decreased considerably compared to the blank solution, indicating the formation of protective layer by the inhibitor on the mild steel surface.

## 4 Conclusions

Seroquel drug was found to be a good corrosion inhibitor for low carbon steel in 1 M HCl solution in the temperature range of 303–333 K. From the experimental evidence, it can be concluded that, Seroquel acts as better inhibitor even at high temperature and is confirmed by the values of surface coverage ( $\theta$ ),  $i_{\text{corr}}$  and  $R_p$  values. Inhibition efficiency was found to increase with increase in inhibitor concentration in the range of 200–1000 ppm. Maximum inhibition efficiency was found to be around 83% at 333 K. Polarization studies revealed that the inhibitor behaves as mixed type. EIS parameters and activation parameters showed that the inhibition action is due to adsorption process and the corrosion process is due to endothermic effect. FTIR spectrum reveals the adsorption of Seroquel molecule on the metal surface through heteroatoms and SEM analysis showed that the corrosion rate is retarded due to the formation of the protective layer on the steel surface.

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