Corrosion Inhibition Effect of Anti HIV Drug Tenofovir Disproxil Fumarate on Mild Steel in Acidic Medium

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Abstract

Corrosion inhibition of mild steel by a non toxic Anti HIV drug Tenofovir Disproxil Fumarate(TDF) has been investigated by using chemical and electrochemical methods such as weight loss, polarization and electrochemical impedance techniques. The experimental results suggested that, TDF is a good corrosion inhibitor for mild steel in 1M Hydrochloric acid medium. The inhibition efficiency increased with increasing of inhibitor concentration. The adsorption of TDF obeys Langmuir adsorption isotherm by following chemisorption mechanism. The results obtained from both chemical and electrochemical techniques are in good agreement with each other. Activation parameters and The quantum chemical approaches are discussed.

Keywords: Tenofovir Disproxil Fumarate; Inhibitor; SEM; Polarisation; weight loss; quantum studies.

1.INTRODUCTION

The corrosion of steel is a fundamental academic and industrial concern that has received a considerable amount of attention 'H.Ashassi-Sorkhabi [1]. Mild steel has been extensively used under different conditions like chemical and allied industries in alkaline, acid and salt solutions. Chloride, sulphate and nitrate ions in aqueous media are particularly aggressive and accelerate corrosion.

The use of inhibitors is one of the most practical methods for controlling corrosion in acidic media [2]. HCl is generally used in the treatment of steel and ferrous alloys. Most of the well-known acid inhibitors are organic compounds containing nitrogen, sulphur and oxygen atoms. In acidic solutions, transition of metal/solution interface is attributed to the adsorption of the inhibitor molecules at the metal/solution interface, forming a protective film. The rate of adsorption is usually rapid and hence, the reactive metal surface is shielded from the acid solutions [3].

The adsorption of corrosion inhibitor depends mainly on physico-chemical properties of the molecule such as functional groups, steric factor, molecular size, molecular weight, molecular structure, aromaticity, electron density at the donor atoms, p-orbital character of donating electrons and electronic structure of the molecule. It is reported that smaller inhibitor

molecules are efficient because they facilitates electronic interactions and impede steric effects. But many of them are toxic even though they exhibit good inhibition action [4–8].

This has led to consider drugs as inhibitors [9–10],Tryptamine [11], ketoconazole [12], sulfa drugs[13],antibacterial drugs [14], tacrine [15] have been reported to be good inhibitors. The planarity of the molecule, besides other factors, decides the efficiency of an inhibitor [16]. Thus drugs with planar structure can be a promising inhibitor which encouraged us to choose a drug TDF [17].

TDF belongs to the class of antiretrovirals. It is used for the treatment of HIV-1 infections and AIDS. The IUPAC name of Tenofoir Disproxil Fumarate (TDF) is9-((R)-2-((Bis((((isopropoxycarbonyl)oxy)methoxy)phosphinyl)methoxy)propyl)adenine fumarate. The presence of electron rich N, O, P atoms and π- bonds in its structure might be in favour of its adsorption on the metal surface which gives a scope for its study as a potential corrosion inhibitor. The aim of the present investigation is to study the effect of TDF as a corrosion inhibitor for mild steel in 1M HCl.

2. Experimental

Mild Steel strips having compositions 0.04% C, 0.35% Mn, 0.022% P, 0.036% S and the rest being Fe (99.55%) were used for all experiments. Strips of dimension 4 cm x 1 cm x 0.5 cm were used for weight loss method and strips with an exposed area of 1 cm^2 were used for electrochemical methods. The strips are polished by using emery papers (Grade No. 80,120,220,320), Washed thoroughly with distilled water, degreased with acetone and dried at room temperature. The corrosive media 1M HCl solutions were prepared using AR grade HCl and distilled water.

TDF is procured from Sequent scientific Limited, Mangalore. The structure of TDF is as shown in the **Figure.1.** Different amount of TDF is dissolved in 1M HCl solution to prepare test solutions.
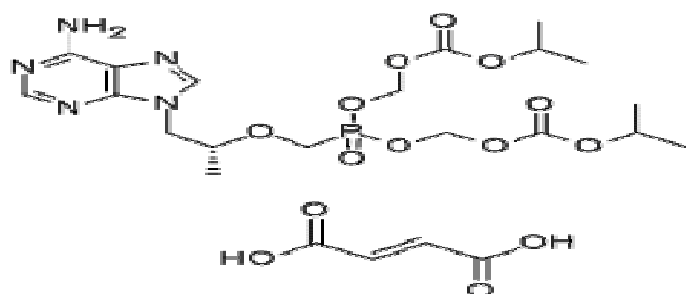

Figure.1. Structure of TDF

3. Methods

Weight loss measurements were carried out by weighing pre cleaned and dried mild steel specimens before and after immersion in acid solutions for 4 h in the absence and presence of various concentrations of inhibitors. Duplicate experiments were performed in each case and the mean value of the weight loss was noted. Corrosion rate and percentage inhibition efficiency were calculated.

The potentiodynamic polarization studies were carried out with mild steel strips having an exposed area of 1 cm^2. Conventional three electrode cell consisting of mild steel as working electrode, Platinum foil as counter electrode and Ag/AgCl electrode as reference electrode was used for measurements. The anodic and cathodic polarization values were measured under galvanostatic conditions with CH–analyzer instrument. In case of polarization measurements, the potential sweep rate was 2 mVs^{-1}. The inhibition efficiencies were calculated from corrosion currents determined using the Tafel extrapolation method.

Electrochemical impedance measurements were carried out using an electrochemical system Frequency Response Analyser (FRA). The electrochemical impedance spectra (EIS) were acquired in the frequency range of 10 KHz to 0.1Hz at the rest potential by applying 5 mV wave AC voltage. The double layer capacitance (C_{dl}) and the charge transfer resistance Rp were determined from Nyquist plots. The inhibition efficiencies were calculated from Rp value.

Generally, In order to gain more information about mode of adsorption of TDF on mild steel surface in 1 M HCl at different temperature, attempts were made to fit experimental data with several adsorption isotherms like Temkin, Langmuir, Freundlich, Frumkin, Bockris–Swinkels and Flory–Huggins isotherms.

The effect of temperature on the corrosion inhibition of TDF on mild steel is investigated by calculating activation parametersThe morphological study of mild steel in the absence of inhibitor and in the presence of inhibitor in 1M HCl was investigated by a JEOL JSM – 840A scanning electron microscope. The energy of the accelerating beam employed was 20 kV.

The interaction of metal and the inhibitor is discussed by quntum chemical approaches. Quantum chemical calculations for TDF were carried out in the gas phase by using Parametric Method 3 (PM3). The Polak–Rieberre algorithm which is fast accurate and has been used for computation. The energy parameters in the form of the root mean square gradient were kept at 0.05 kcal/A mol and convergence limit at 0.05. These calculations were performed by using Hyperchem 7.5 package program (Hypercube Inc., Florida, 2003).

3. Result and Discussions

3.1 Weight loss method

The percentage inhibition efficiency obtained from weight loss experiment η_w for the corrosion of mild steel in 1M HCl with different concentration of TDF at room temperature for an immersion time of 4 hours is given in **Table 1**. The % I.E was calculated from the following relationship.

$$\eta_w\,(\%) \;=\; \frac{W^o - W}{W^o} \times 100 \quad\text{-------------------------------------(1)}$$

Where, W^o and W are weight loss of steel in absence and presence of inhibitor.

The rate of corrosion ρ (g cm^{-2} h^{-1}) was calculated from equation

$$\rho = \frac{W^o - W}{ST} \times 100 \quad\text{------------------------------------ (2)}$$

Here, S is the surface area of the steel specimen and T is the immersion time in hours. Corrosion parameters for mild steel in 1M HCl in the absence and presence of different concentrations of the TDF is provided in **Table 1**.

The variation of η_w with the concentration of TDF for 4 hour of immersion time at 303 K is given in the **figure.2.** η_w is increased with increasing TDF concentration upto 1000 ppm and above this concentration almost same trend was observed. The increase in η_w with increase in concentration of TDF is due to the strong adsorption of the TDF on the steel surface. So 1000 ppm is considered as an optimum concentration for achieving the maximum efficiency.

Table 1.Corrosion parameters obtained from weight loss measurements for steel in 1M HCl in presence of different concentrations of TDF.

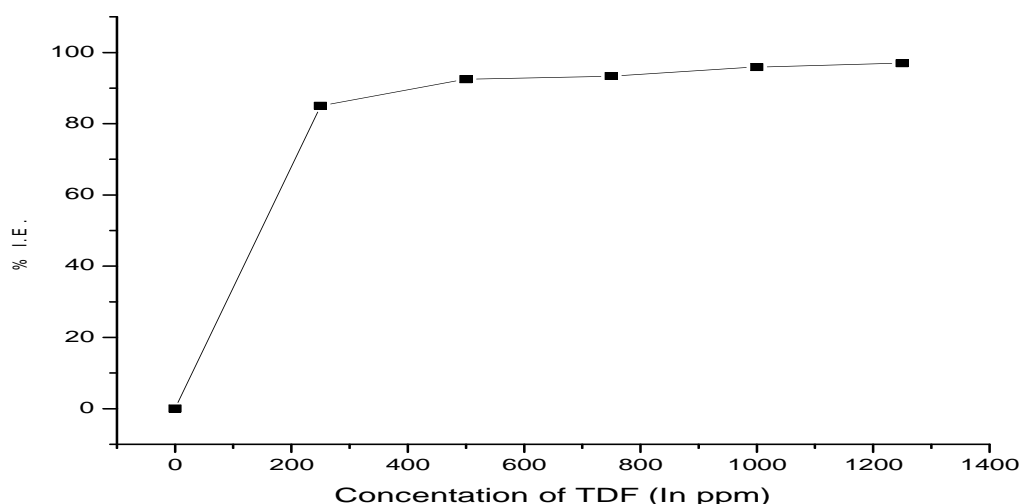| Inhibitor Concentration (in ppm)	Corrosion rate (mg cm^{-2} h^{-1})	η_w
1M HCl (Blank)	0.00347	–
250	0.00295	85
500	0.00321	92.5
750	0.00324	93.37
1000	0.00333	95.96
1250	0.00322	92

Figure.2. Variation of %E with concentration of TDF (In ppm) at 303 K .

3.2. Polarization studies

The polarization behavior of steel immersed in 1 M HCl at room temperature in absence and presence of different concentration of TDF is shown **Figure. 3.** Electrochemical parameters like corrosion potential (E_{corr}), corrosion current density (i_{corr}), cathodic Tafel slope (β_c), anodic Tafel slope (β_a) and percentage inhibition efficiency according to polarisation studies (η_p) are listed in Table 2. The η_p was calculated from following relation.

$$\eta_P = \frac{i^o_{corr} - i_{corr}}{i^o_{corr}} \times 100 \quad\text{-- (3)}$$

where, i^o_{corr} and i_{corr} are corrosion current densities in absence and presence of inhibitor, respectively. i_{corr} values ~~are~~ decreased and Inhibition efficiency increased with increasing concentration of TDF. This is because the formation of TDF protective layer in between the corrosive media and the Steel surface.
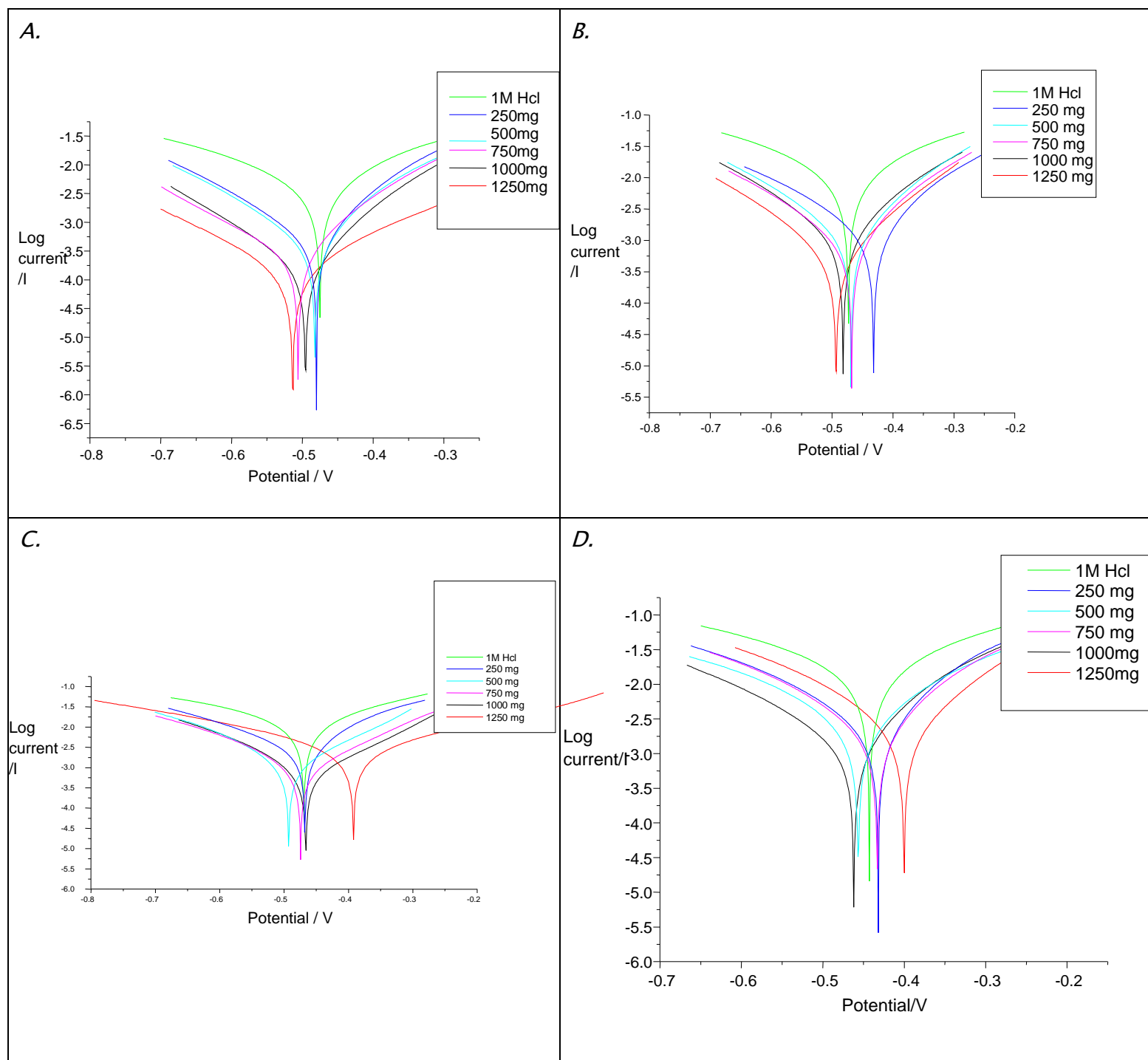
Figure.3. Polarization curves for the corrosion of mild steel in 1M HCl at (A)303 K (B) 313 K (C) 323K (D)333K in the absence and presence of different concentrations of TDF.

Generally, in corrosion, there are two types of reactions; they are anodic and cathodic reactions. The liberation of hydrogen gas in an acidic media is concerned with the cathodic reaction, whereas the oxidation of metal is concerned with the anodic reaction. If the inhibitor is able to inhibit the anodic reaction, then such inhibitor is categorized as an anodic inhibitor and if the inhibitor is able to inhibit the cathodic reaction, then such inhibitor is categorized as a cathodic inhibitor. The Tafel plot explains the type of inhibitor as follows.

The displacement of E_{corr} is not always in the regular trend and can observe the change in E_{corr} either to the anodic side or cathodic side with reference to the blank solution [18–20]. The magnitude of E_{corr} displacement plays very important role to explain the type of inhibitors. If the value of E_{corr} displacement is more than 85mV to the anodic side or cathodic side, then the inhibitors are called as anodic type inhibitors or cathodic type inhibitor respectively. Otherwise the inhibitor is called as mixed type inhibitor [21, 22]. In the present study, the maximum E_{corr} displacement is less than 85mV and hence TDF is a mixed type inhibitor, Meanwhile the decrease in current density and corrosion rate reveals that the inhibitor forms a protective layer in between aggressive media and the metal.

3.3. EIS studies

Electrochemical impedance spectra for steel in 1 M HCl without and with different concentration of inhibitor at different temperature are presented as Nyquist plot in **Figure.4.** The size of semicircle increased with inhibitor concentration reflects the effectiveness of inhibitor. An equivalent circuit model (**Figure.5**) was proposed to fit and analyze EIS data. EIS parameters calculated in accordance with equivalent circuit are listed in **Table 2**. According to Popova et al. [23], the sum of charge transfer resistance (R_{ct}) and adsorption resistance (R_{ad}) is equivalent to polarisation resistance (R_p). Inhibition efficiency (η_z) was calculated using following equation.

$$\eta_Z = \frac{R_p - R_p^o}{R_p} \times 100 \qquad -------------------------------(4)$$

where, R_p and R_p^o are polarisation resistance values in presence and absence of inhibitor.
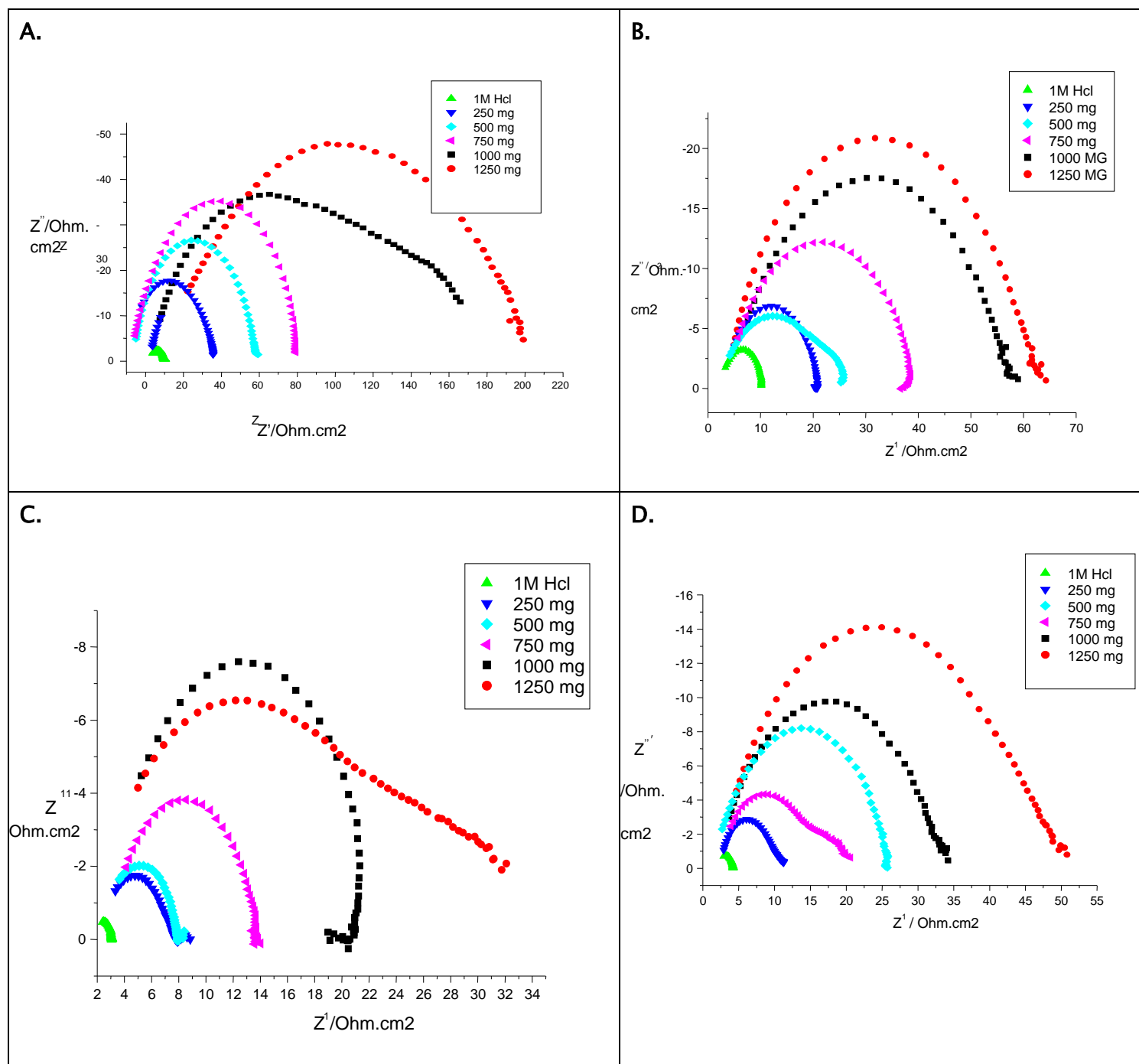
Figure. 4. Nyquist plots for the corrosion of mild steel in 1M HCl at (A)303 K (B) 313 K (C) 323 K (D) 333 K in the presence of different concentrations of TDF(Inhibitor).
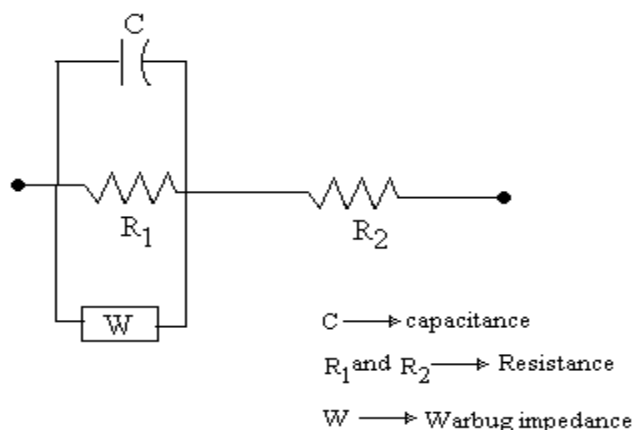
Figure.5. Equivalent circuit used to interpret the results of EIS.

Table. 2. revealed that R_p values increased and capacitance values decreased with inhibitor concentration . Decrease in capacitance may be resulted from a decrease in local dielectric constant and/or an increase in the thickness of electrical double layer, suggests that the inhibitor molecules act by adsorption at metal/solution interface. This indicated the formation of a surface film on steel. The general overview of the electrochemical impedance results meets the expectations from the theory of the technique, but it must be noted that the capacitive loops are depressed ones with centers under the real axis even though they have a semicircle appearance. Deviations of this kind are mostly referred to as frequency dispersion and they are attributed to irregularities and heterogeneities of the solid surfaces [24–26].

Table. 2: Tafel and AC impedence results for the corrosion of mild steel in 1 M HCl in the presence different weights of TDF at different temperatures.

Temperature (in K)	Inhibitor con^n (ppm)	$-E_{corr}$ (V)	i_{corr} A cm^{-2}	Corrosion rate(mpy)	$-\beta c$ V/decade	βa V/decade	% η_p	R_p Ωcm^2	C_{dl} (μF cm^{-2})	% η_z
	Blank	0.496	0.177	34.70	5.663	6.274	-	6.536	246	-
	250	0.489	0.09	17.91	7.757	9.630	49	23.57	230	72
	500	0.483	0.077	15.91	7.903	9.096	56	52.24	200	87
	750	0.499	0.050	10.09	6.667	9.951	71	59.7	123	89
303	1000	0.521	0.0192	14.04	7.743	8.532	89	89.37	50	92
	1250	0.500	0.013	11.32	6.835	6.795	92	90.75	40	92
	Blank	0.482	0.43	85.34	5.313	5.515	-	1.593	6340	-
	250	0.444	0.059	43.12	6.247	8.159	86	19.27	6000	91
	500	0.472	0.054	38.85	7.090	8.569	87.5	34.64	4500	95
	750	0.470	0.053	30.09	7.029	8.413	87.6	48.66	3600	96.7
313	1000	0.485	0.052	27.56	7.293	8.031	88	66.71	2200	97.6
	1250	0.491	0.046	16.92	7.543	8.651	89.3	28.51	170	98.4
	Blank	0.476	7.91	104.26	4.996	5.396	-	0.6429	1990	-
	250	0.480	0.144	28.24	6.070	7.49	98	22.67	640	87.1
	500	0.501	0.0575	21.36	7.420	7.678	99.2	24.0	580	97.3
323	750	0.500	0.090	15.29	6.761	8.058	98.8	44.17	470	98.5
	1000	0.464	0.129	12.18	7.347	7.952	98.3	44.2	390	98.5
	1250	0.528	0.102	11.21	7.077	7.374	98.7	62.9	30	99
	Blank	0.450	0.194	139.7	4.887	5.374	-	3.239	320	-
	250	0.400	0.141	27.56	8.001	10.853	27.3	14.16	116	77.12
	500	0.464	0.136	26.65	6.408	7.921	29.8	15.12	104	78.57
333	750	0.490	0.110	21.51	6.550	8.090	43.2	11.51	100	71.85
	1000	0.467	0.064	16.59	6.936	8.778	67	11.37	78	71.5
	1250	0.408	0.105	10.60	6.920	8.814	46	11.0	44	70.0

3.4.Adsorption isotherm

Organic inhibitors are found to protect mild steel corrosion in acid medium by adsorbing themselves on metal surface. In order to gain more information about mode of adsorption of

TDF on mild steel surface in 1M HCl at different temperature, attempts were made to fit experimental data with several adsorption isotherms like Temkin, Langmuir, Freundlich, Frumkin, Bockris–Swinkels and Flory–Huggins isotherms. The best fit was obtained with Langmuir's isotherm which is in good agreement with Eq. (4).

$$C/\theta = 1/K + C \quad \text{--} \quad (4)$$

where C is the inhibitor concentration, θ is the degree of surface coverage defined as $\eta_z/100$ at different concentration of inhibitor evaluated from AC impedence measurement and K_{ads} is the equilibrium constant of adsorption process which is related to $\triangle G_{ads}$ by the following relation

$$K_{ads} = 1/55.5 \ \exp(-\triangle G_{ads}/RT) \quad \text{--} \quad (5)$$

The plots of C/θ against C were straight lines with almost unit slopes and are shown in **Figure.6.**

It is found that all the regression coefficients are very close to 1 which indicates that the adsorption of TDF on the mild steel surface obeys Langmuir adsorption isotherm. The thermodynamic parameters for the adsorption process obtained from the **Figure.6.** The values

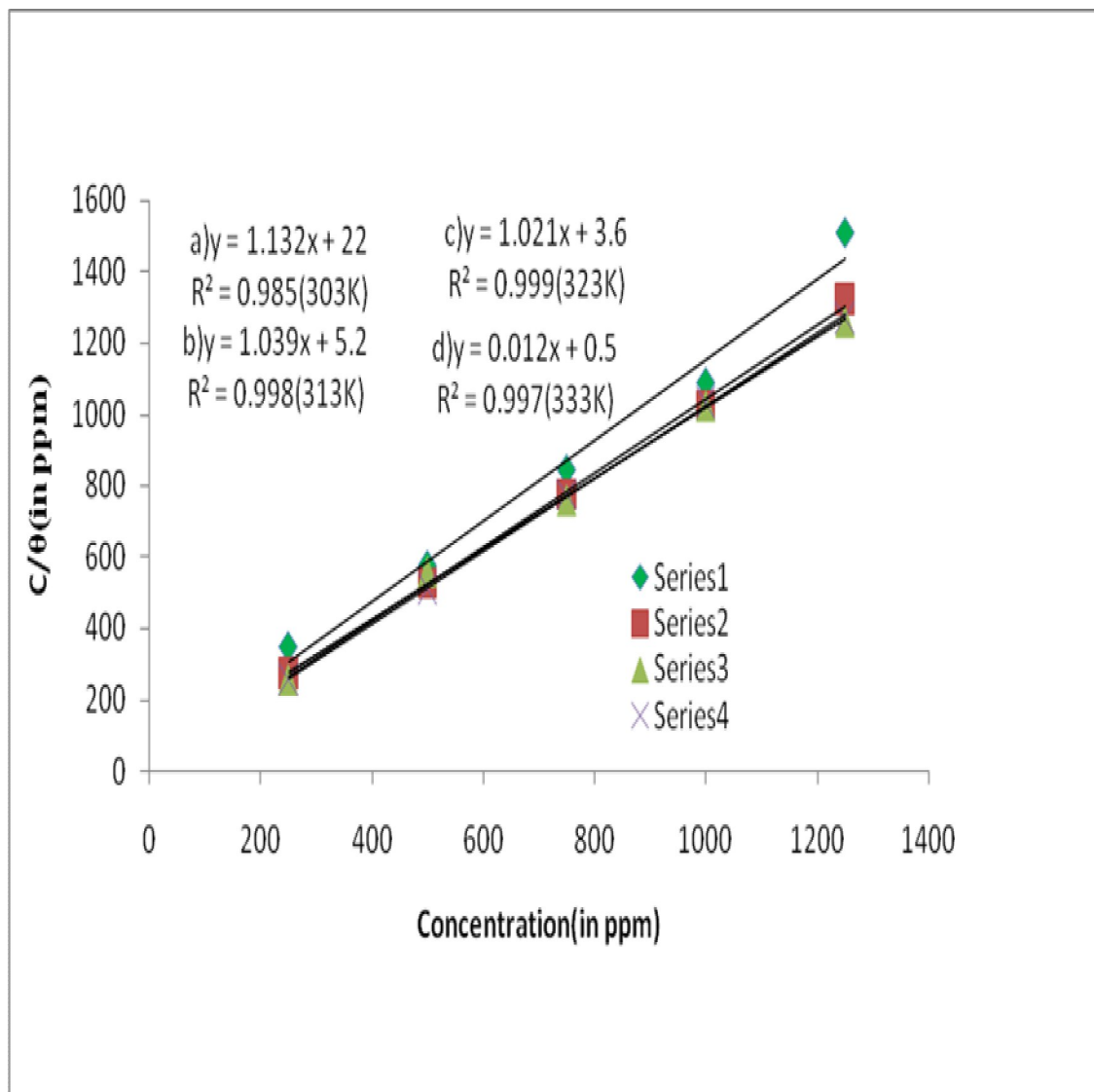are depicted in **Table 3.**

Figure.6. Langmuir adsorption plots of mild steel in 1M HCl solution containing different concentrations of TDF at different temperatures.

Table 3: Thermodynamic parameters for the adsorption of TDF on mild steel surface in 1 M HCl solution

Temperature (K)	K_{ads} (M^{-1})	ΔG^0_{ads} (kJ mol^{-1})	ΔH^0_{ads} (kJ mol^{-1})	$-\Delta S^0_{ads}$ (Jmol^{-1}K^{-1})
303	2.8×10^{10}	-38.45	-93.5	181.6
313	12×10^{10}	-39.37	-93.5	175.8
323	17.6×10^{10}	-39.96	-93.5	165.7
333	17.0×10^{10}	-37.5	-93.5	168.1

The value of K_{ads} is calculated from the intercept of isotherm line. The large values of K_{ads} indicate that the TDF molecules are strongly adsorbed on the mild steel surface. Generally, values of ΔG^0ads around -20 kJ mol^{-1} or lower are consistent with physisorption and that around -40 kJ mol^{-1} or higher involves chemisorptions [27]. O Ghasemi et al [28] obtained the values of ΔG^0_{ads} in the range of -32 kJ mol^{-1} to -35 kJ mol^{-1} and they reported the mode of adsorption occurs through the mixture of physiorption and chemisorption. R.T.Loto et al [29] obtained the values of ΔG^0_{ads} are varied from 28 to 34 kJ mol^{-1} and the investigator reported the mode of adsorption is mixture of physiorption and chemisorption. In the present study the value of ΔG^0_{ads} are found to be much closed to -40 kJ mol^{-1}. It means that the adsorption of TDF on mild steel surface involves chemisorptions [30].The negative values of ΔG_{ads} indicate the spontaneous adsorption of inhibitor on mild steel surface. The enthalpy of adsorption was deduced from the Gibbs Helmholtz equation.

$$\left[\left(\partial(G)/T\right)\big|\partial T\right]_p = -\frac{H}{T^2} \quad \text{---(6)}$$

where R is the universal gas constant, T is the absolute temperature and 55.5 is the molar concentration of water in the solution.

This equation can be rearranged to give the following equation

$$\Delta S^0_{ads} = (\Delta H^0_{ads} - \Delta G^0_{ads})/T \ \text{---} \ (7)$$

A plot of $\Delta G^0_{ads}/T$ versus $1000/T$ gives straight lines as shown in **Figure. 7** with the slope equal

to $-\Delta S^0_{ads}$, and the value of ΔH^0_{ads} can be calculated from the intercept.
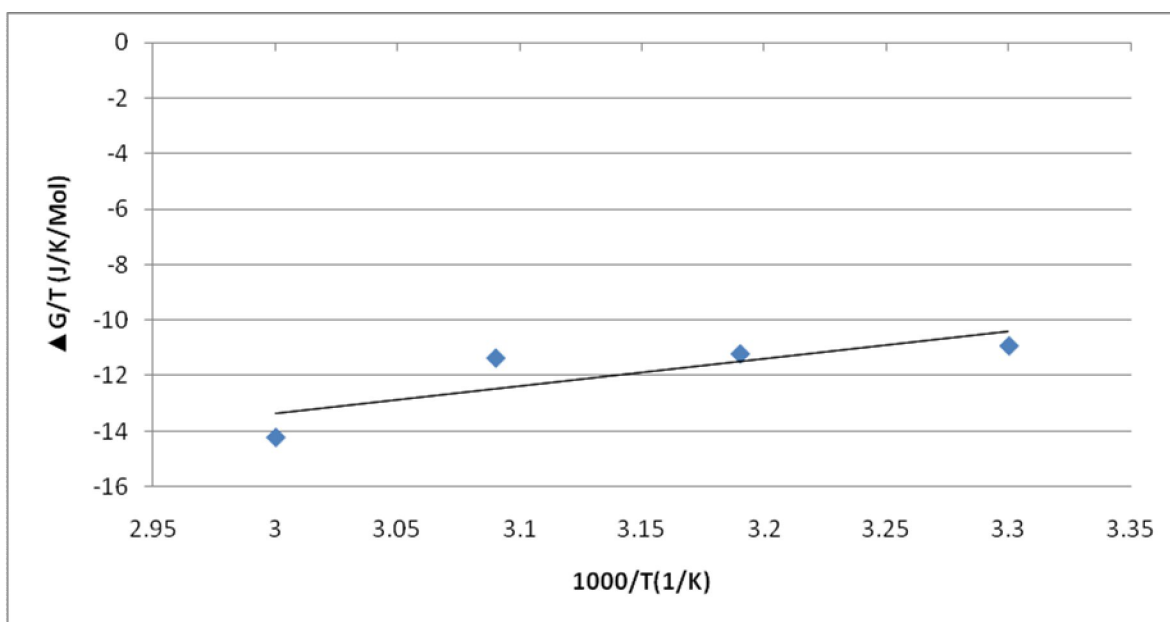

Figure.7.Adsorption isotherm plot for $\Delta G^0_{ads}/T$ Vs $1000/T$.

The change in enthalpy (ΔH^0_{ads}) also explains the mode of adsorption and sign explains whether adsorption is exothermic or endothermic in nature. According to reported literature [31], if the sign of ΔH^0_{ads} is positive, the adsorption process is endothermic in nature and if the sign is negative, then the adsorption is exothermic in nature. In the present study, the investigator got the negative sign of ($-\Delta H^0_{ads}$) change in enthalpy. Therefore investigator concludes that the adsorption process is exothermic in nature. The numeric value of ΔH^0_{ads} shows the mode of adsorption (physiorption or chemisorption).

If the value of ΔH^0_{ads} is less than 40 kJ/mol, the adsorption occurs through the physiorption and if the value of ΔH^0_{ads} approaches to 100 kJ mol^{-1}, then the adsorption occurs

through the chemisorption. This aspect is discussed in many literatures [32, 33]. In the present study, the calculated value of ΔH^0_{ads} is 93.5 kJ mol^{-1} which shows the mode of adsorption of inhibitor on metal surface is chemisorption. The ΔS^0_{ads} values in the presence of TDF are large and negative meaning a decrease in entropy is due to decrease in disordering on going from reactants to the metal adsorbed species [34].

3.5. Activation parameters

The corrosion rate is directly proportional to the temperature and hydrogen over potential decreases with increasing the temperature in acidic media [35]. The corrosion process can be explained by Arrhenius equation. The Arrhenius equation can be written as,

$$\ln \vartheta_{corr} = \ln A - \frac{E_a}{RT} \quad\text{------------------------------------- (8)}$$

where, ϑ_{corr} is the corrosion rate, E_a is the apparent activation energy of the corrosion process, R is the universal gas constant, T is the absolute temperature and A is Arrhenius pre-exponential

Factor. The graph of $\ln \vartheta_{corr}$ Vs 1000/T is plotted in the **figure.8.** in the absence and presence of inhibitor in 1M HCl solution at different temperatures (303K–333K). The parameters A, and E_a are depicted in the **Table 4.** The increase in E_a values in the presence of inhibitor indicates the decrease in adsorption process of the inhibitor on the mild steel surface with the raise in the temperature [36]. The values of E_a and A increased with the TDF concentration which shows the

formation of protective barrier between the aggressive media and the metal surface [37]. Therefore there is decrease in the corrosion rate.

Apparent change in enthalpy (ΔH^*) and Apparent change in entropy (ΔS^*) are calculated by the transition-state equation as follows,

$$\ln \frac{\vartheta_{Corr}}{T} = \left[\ln \frac{R}{Nh} + \frac{\Delta S^*}{R}\right] - \frac{\Delta H^*}{RT} \quad\text{------------------------------- (9)}$$

where N is the Avogadro number and h is the plank's constant.

A graph of $\ln \frac{\vartheta_{corr}}{T}$ Vs $\frac{1000}{T}$ is as shown in the **figure.9.** The values of ΔH^* and ΔS^* are depicted in the **table 4.**

The positive value of ΔH* shows the endothermic nature of mild steel dissolution process .The negative values of ΔS* pointed to a greater order produced during the process of activation. This can be achieved by the formation of activated complex represented association or fixation with consequent loss in the degrees of freedom of the system during the process [38].
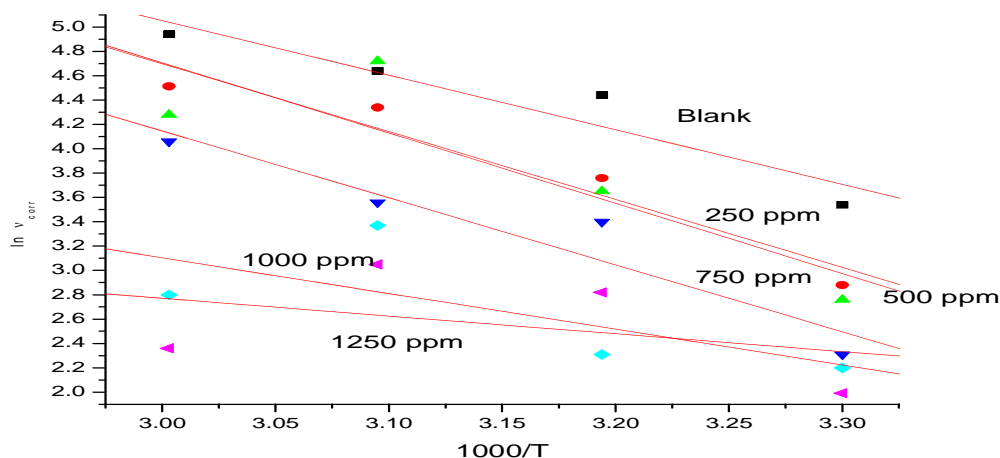

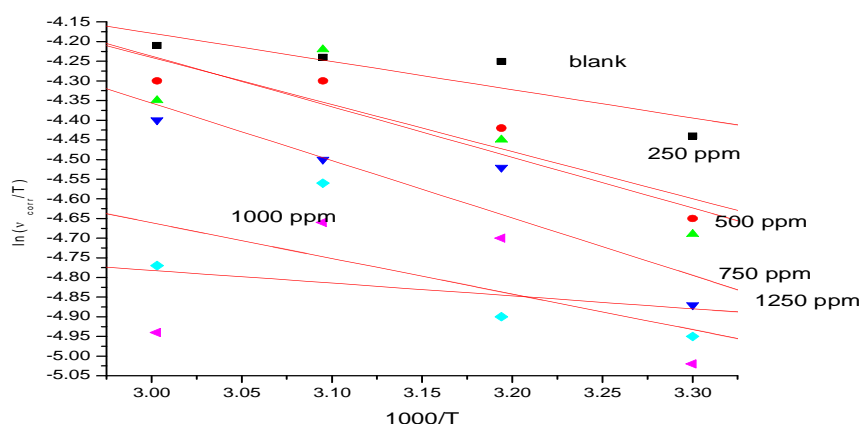Figure.8 . Arrhenius plot for mild steel in 1M HCl in the absence and presence of different Concentrations of TDF.

Figure.9. Transition State plot for mild steel in 1M HCl in the absence and presence of different concentrations of TDF.

Table 4.Activation parameters for mild steel in 1M HCl in the absence and presence of different concentrations of TDF

Concentration Of Inhibitor (ppm)	E_a^* (kJ mol^{-1})	A (g cm^{-2} h^{-1})	ΔH^* (kJ mol^{-1})	ΔS^* (J mol^{-1}K^{-1})
Blank	41.0	666.31	201.50	187.0
250	52.5	772.24	222.5	256.63
500	55.6	1174.21	224.0	261.5
750	59.23	1225.78	239.8	273.33
1000	66.4	1244.21	240.2	273.63
1250	67.47	1354.05	242.72	277.66

3.6.SEM analysis:

The surface morphology of steel surface was studied by scanning electron microscopy (SEM). Figure.10. shows the SEM photograph of the steel surface with and without inhibitor after weight loss measurements in hydrochloric acid media. The SEM photographs showed that the surfaces of metal have pits and corrosion product, but in presence of inhibitor they are minimized on the metal surface. It indicates the formation of passive layer on the metal surface. So the corrosion rate is decreased in the presence of inhibitor and reduces the electrochemical reaction.
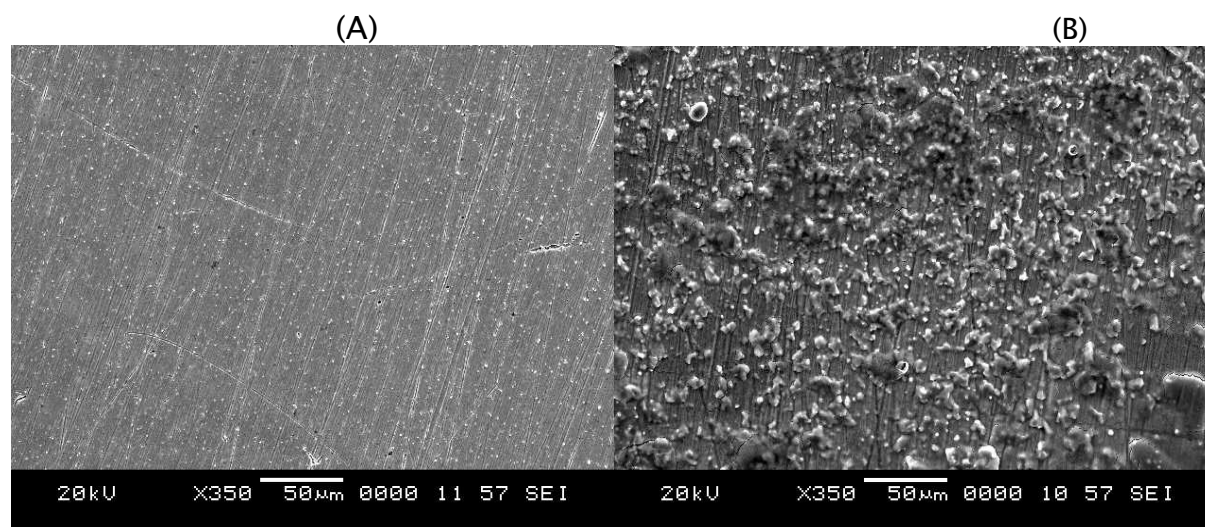
(A)   (B)

Figure.10.   SEM Images   (A) In the Presence of inhibitor
and
(B) In the Absence of inhibitor

3.7. Quantum chemical study

Quantum methods are used to emphasize experimental data obtained from chemical and electrochemical methods. The optimized minimum energy geometrical configurations of test compounds are given in **Figure.11**. The computed quantum chemical parameters like energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), HOMO –LUMO energy gap ($\Delta E_{H–L}$) dipole moment (μ) and inhibition efficiency η_q are summarized in **Table 5.** From **Figure.11.** it can be observed that HOMO and LUMO energy orbitals are extensively distributed on either sides of the TDF compound, indicating that TDF has a good adsorption centres. It has been well documented in literature that [39] higher the value of E_{HOMO} of the inhibitor, greater is the ease of inhibitor to offer electrons to unoccupied d orbital of metal atom and higher is the inhibition efficiency of the inhibitor. Further lower the E_{LUMO}, easier is the acceptance of electrons from metal atom to form feedback bonds. The gap between HOMO–LUMO energy levels of molecules was another important parameter and smaller the value of $\Delta E_{H–L}$ of an inhibitor, higher is the inhibition efficiency of the inhibitor [40]. Further higher values of dipole moment will favour the enhancement of corrosion inhibition [41]. The μ value of our compound is 6.94 and it strengthens the results.

The bonding tendencies between inhibitor molecule and metal surface atom can be discussed on the basis of HSAB theory and the frontier-controlled interaction concepts [42]. Steel metal atom being an electron pair acceptor is an acid while inhibitor molecule an electron pair donor is a base. According to HSAB theory, hard acids prefer to react with hard bases and soft acids prefer to react with soft bases. Here metal atoms are known to be soft acids, inhibitor molecules with a large HOMO–LUMO energy gap are hard bases and molecules with small HOMO–LUMO energy gap are soft bases. In the present study HOMO–LUMO energy gap is 7.1715 and it indicated the tendency of interaction of inhibitor molecules with steel. Molecular orbital (MO) theory can also be considered to highlight the findings. Since iron atom (acid) is the electron pair acceptor and inhibitor (base) is the electron pair donor, the energy difference of the LUMO of the acid and the HOMO of the base must be considered. MO theory suggests that the overlap between LUMO (acid) and HOMO (base) is the governing factor in bonding [43]. Lower the HOMO–LUMO energy gap, higher the HOMO–LUMO overlap and consequently higher inhibition efficiency. In our case Inhibition efficiency of 99% is obtained from theoretical calculation and it is more than the experimental results.

Tang. et al. [44] is of the opinion that the presence of more adsorption centers can cause flat orientation of inhibitor molecule on the surface of steel, thus high degree of surface coverage and inhibition efficiency can be achieved. Keeping all facts in mind it can be suggested that tested molecule is excellent inhibitor.

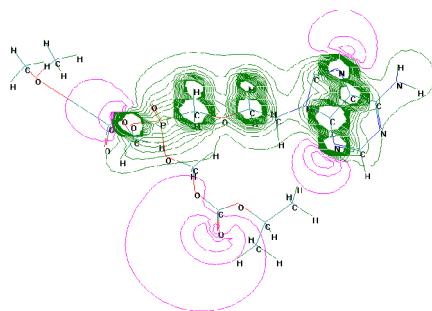### Table.5.Quantum chemical parameters of TDF.

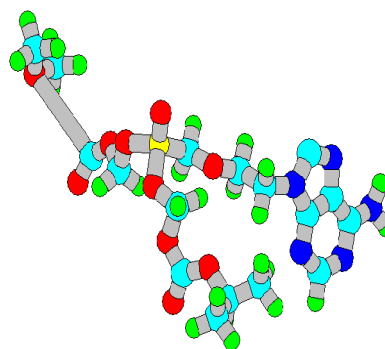| E_{HOMO}	E_{LUMO}	$\Delta E(eV)$	$\mu(Debye)$	$\eta_q(\%)$
−9.302542	−0.865166	−8.437	6.940	99.0
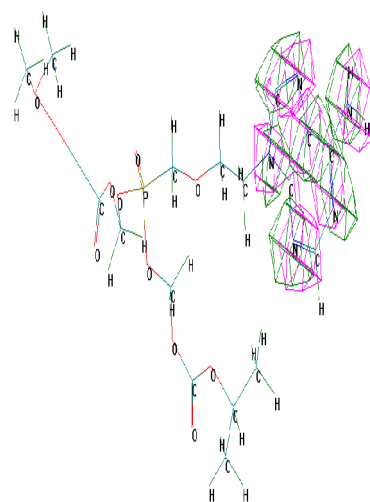
HOMO Energy state of Tenofovir
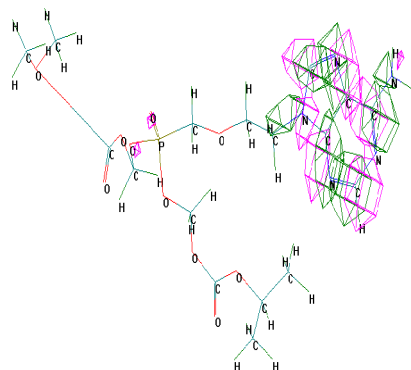
LUMO Energy state of Tenofovir

Electrostatic potential map of Tenofovir

Optimized geometry of Tenofovir

Figure.11. Structure of HOMO Energy State, LUMO Energy state and optimized geometry of TDF.

4. conclusions:

1) TDF is an excellent corrosion inhibitor for Mild steel in 1M HCl and inhibition efficiency was more pronounced with increase in the inhibitor concentration upto certain level.

2) Quantum studies are confirmed by experimental studies

3) Inhibition efficiency was increased with increase in temperature upto 323 K.

4) Adsorption of the inhibitor on steel surface is mainly due to the chemisorption

5) Adsorption of the TDF on the mild steel surface from the HCl solution obeyed Langmuir adsorption isotherm..

6) The inhibition action of the TDF against corrosion is due to the adsorption process revealed by SEM.

Acknowledgements

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