

Inhibitive Performance of Hydroxypropyl Cellulose and Potassium Iodide on the Corrosion of Mild Steel in Sulphuric Acid Environment

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Authors' contributions

This work was carried out in collaboration between all authors. Authors SCN, OO and EEO designed the framework of the experimental study. Authors ICM and SCN performed the gravimetric experiment, electrochemical experiment and theoretical modeling. Author SCN carried out the literature research. All authors read and approved the final manuscript.

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ABSTRACT

The inhibitive performance of hydroxypropyl cellulose (HPC) and its combination with potassium iodide (KI) on mild steel corrosion in 0.5 M H₂SO₄ acid solution was studied using the potentiodynamic polarization, gravimetric measurement technique and theoretical computations. Weight loss results obtained indicate that the HPC and its combination with KI functioned as a good inhibitor in sulphuric acid environment with inhibition efficiency of 76.43% and 89.73% respectively, and inhibition efficiency increased with concentration. Changes observed in polarization parameters suggest the adsorption of HPC on the mild steel surface, leading to the formation of protective films. The adsorption characteristics of the inhibitor were approximated by Langmuir isotherm. Synergistic effect increased the inhibition efficiency in the presence of halide additives and the values of the synergistic factor with KI were higher than unity indicating that both additives act cooperatively to enhance inhibition performance. The Fukui functions revealed that HPC

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adsorbed on the corroding mild steel surface through multiple OH groups, propyl groups and aromatic structure. The experimental results corroborated with results from theoretical studies.

Keywords: Langmuir isotherm; hydroxypropyl cellulose; mild steel; corrosion; inhibitor; halide.

1. INTRODUCTION

The contribution of metals in the development of industrial sectors is seen as one of the greatest achievement attributed to man's ingenuity towards industrial revolution. However, the corrosion of metals and alloys in aggressive service environment has being a major factor undermining the impact of metals and alloys towards the modern industrial development [1]. Many practical and effective methods have been utilized in controlling the dissolution of mild steel in aggressive service environment and the use of corrosion inhibitor is one of the methods [2]. In addition, several corrosion inhibitors have been reported in literature for their effective retarding cathodic and anodic reactions of corrosion process but majority of the inhibitors are toxic, costly or not readily available [3-5]. However, concerted efforts have been made towards the development and formulation of efficient corrosion inhibitors that are eco-friendly, relatively cheap, readily available, etc, and many inhibitors of organic origin and polymeric backgrounds have been reported to give positive results [6-10].

Many polymers have proved to be effective corrosion inhibitors from the molecular point of view, because of presence of some functional and substituent's groups (hetero-atoms, conjugated double or triple bonds, aromatic or cyclic ring structure, etc) attached in their back bone or side chains which act as adsorption centres for corrosion inhibition. Also, the ability of these polymers to donate or accept electrons from surface charge on the metal via electrostatic or chemical interaction using their antibond orbitals to form feedback bonds [11] is an excellent corrosion inhibition property. The effectiveness of polymeric materials in reducing metal corrosion in aggressive solution has been reported [12-15] and mainly it is due to the ability of polymers to displace hydrated corrosion agents on the metal surface or alter the activation energy barrier of the anodic and cathodic reaction process. This is made possible as result of interaction between the polymer molecules and surface charge on the metal which leads to the formation of complex that is adsorption on the metal surface. Hence, the

adsorbed complex forms the protective film or layer that controls the sites of corrosion and reduces the corrosion damage on the metal surface. The stability or effectiveness of the protective action of polymeric inhibitors in acidic environment depends of the following factors: surface charge on the metal, nature of aggressive solution, nature and concentration of inhibitor, molecular structure of the inhibitor, temperature, etc [16-19].

Hydroxypropyl cellulose is a nontoxic, biodegradable, water-soluble organic compound whose molecular structure possesses the desirable features of a good corrosion inhibitor. It is a synthetic compound commonly used as a binder, film forming and releasing agent in many industrial, pharmaceutical and domestic products. Hydroxypropyl cellulose has been shown to be effective corrosion inhibitor of cast iron in acidic environment [20]. However, more studies are needed to understand the inhibition mechanism of hydroxypropyl cellulose in relation with other metals and alloys in varying aggressive environment. The present report focused on investigating the inhibitive performance of hydroxypropyl cellulose (HPC; Fig. 1) on corrosion of mild steel in acidic media and broadening application of synthetic polymers used for controlling mild steel corrosion. Efforts were made to enhance the inhibition efficiency by introducing iodide ions into the sulphuric acid solution containing HPC. Some quantum chemical calculations (Density Functional Theory and Molecular Dynamic Simulation) were performed to support our experimental investigations.

2. MATERIALS AND METHODS

2.1 Materials Preparation

2.1.1 Metal coupons

Mild steel plate (with % compositions listed as follow: C = 0.16%, Si = 0.04%, Mn = 0.05%, Cu = 0.05%, Cr = 0.07%, and remainder was Fe) was mechanically press cut to 3 x 3 x 0.1 cm coupons. The mild steel coupons were wet-polished with grade silicon carbide paper (from # 400- #1200)

to ensure smooth surface, degreased with acetone rinsed with distilled water and dried with warm air. The test coupons were kept in a desiccator prior to use.

2.1.2 Corrodent

Sulphuric acid (H₂SO₄) was the corrodent used for the study. It was BDH grade AR and 98%. Blank acid solution was prepared using H₂SO₄ and double distilled water.

2.1.3 Inhibitor

The inhibitor used was powdered hydroxypropyl cellulose (HPC). It was a product of sigma Aldrich from USA. Inhibited solutions were prepared by adding hydroxypropyl cellulose (HPC) to the blank solution to obtain desired concentrations (0.2 g/L, 0.4 g/L, 0.6 g/L and 0.8 g/L). For all synergistic studies 0.4 gKI was used.

2.2 Electrochemical Measurements

PARC-2273 Advanced Electrochemical Equipment was used for the potentiodynamic polarization measurements. A glass electrolytic cell that consists of a test solution, platinum plate (counter electrode), saturated calomel electrode (reference electrode), and the metal (working electrode) was used. The metal electrode was embedded in epoxy resin leaving a surface area of 1 cm² uncovered and connected with a Cu-wire the electrochemical equipment for electrical contact. Polarization studies were carried out in a potential range -250 to +250 mV and at a scan rate of 0.333mV/s. Each test was run in triplicate to verify the reproducibility of the result.

2.3 Gravimetric Measurement

The prepared mild steel coupons were suspended in 200 ml of test solutions in 250 ml capacity glass beakers with the aid of glass rod, nylon rope, and hook. All measurements were kept at 30±1°C. To determine the weight loss, the coupons were retrieved at 24 h interval progressively for 5 days, cleaned, dried and reweighed. The difference between the initial weight of coupons before suspending in the test solution and the final weight of coupons after suspending in the test solution was calculated as weight loss. The values recorded were mean values of triplicate determinations. The corrosion rate (CR) values were determined according to Equation 1 stated below.

$$CR \text{ (mm/yr)} = \left(\frac{87600\Delta W}{\rho A t} \right) \quad (1)$$

where, ΔW = weight loss in gram (g), ρ = density of the metal coupons (g/cm³), A = exposed surface area of the metal coupon (cm²) and t = time of exposure (in hrs).

The percentage inhibition efficiency, % IE was calculated respectively using the Equation 2 stated below:

$$IE \% = 1 - \left(\frac{CR_0}{CR_i} \right) \times 100 \quad (2)$$

where CR_i and CR_0 are corrosion rates in the presence and absence of inhibitor respective.

2.4 Theoretical Computation Studies

The theoretical calculations were performed using DFT electronic structure programs DMol³ and Molecular dynamic simulations (MD) as contained in Materials Studio 7.0 software (Accelrys, Inc.).

3. RESULTS AND DISCUSSION

3.1 Potentiodynamic Polarization Result

Polarization measurements were undertaken to distinguish the effect of HPC on the cathodic and anodic corrosion reactions of mild steel immersed in 0.5 M H₂SO₄. The resulting polarization curves of mild steel are illustrated in Fig. 1. Polarization parameters including corrosion potential (E_{corr}), corrosion current density (i_{corr}), cathodic (b_c) and anodic (b_a) Tafel slopes were estimated from the polarization curves and presented in Table 1. The presence of HPC reduced the values of cathodic and anodic current compared to the blank acid solution. This is an indication that HPC altered the anodic dissolution of mild steel and cathodic hydrogen evolution reaction processes, but cathodic process was predominantly controlled. In addition, the E_{corr} values were shifted towards negative direction but the change was not significant to any extent. This implies that corrosion inhibition process is under mixed control since the displacement in E_{corr} is less than 85mV [21]. Hence, the changes in polarization parameters were attributed to difference in the inhibitor concentration, surface modification due to adsorption interaction between the functional groups and charge on the metal surface and corrosive agent present in solution. The inhibition efficiency, IE% was

obtained from the values of corrosion current density in the absence (i_{corr}^0) and presence of HPC (i_{corr}) according to Equation 3 stated as follow:

$$IE \% = (1 - i_{corr}^0 / i_{corr}) \times 100 \quad (3)$$

The results of IE% obtained are shown in Table 1 and the maximum value of IE% for HPC is at the highest inhibitor concentration.

3.2 Weight Loss Measurement Results

3.2.1 Corrosion rate

This is used to measure extent at which a metal exposed to aggressive environment degrades or deteriorates with time. The dissolution of mild steel in aggressive environment is usually

electrochemical in nature [22] involves two reaction processes (anodic and cathodic reactions) which is facilitated by some factors such as corrosive agent, nature of metal, temperature, etc surrounding the metal surface. The resultant effect of exposing metal to corrosion process leads to material (metal) loss, hydrogen gas evolution, pollution, economic loss, etc. Clearly, it is seen in Table 2 that mild steel suffered material loss due to corrosion damage with respect to time, though the presence of HPC within the system reduced the effect. This can be attributed to the weakness of the corroded mild steel product in depressing the diffusion of corrosive agent in the medium. Hence, visual observation and experimental data confirmed that mild steel did not show any sign of passivation within the period of study.

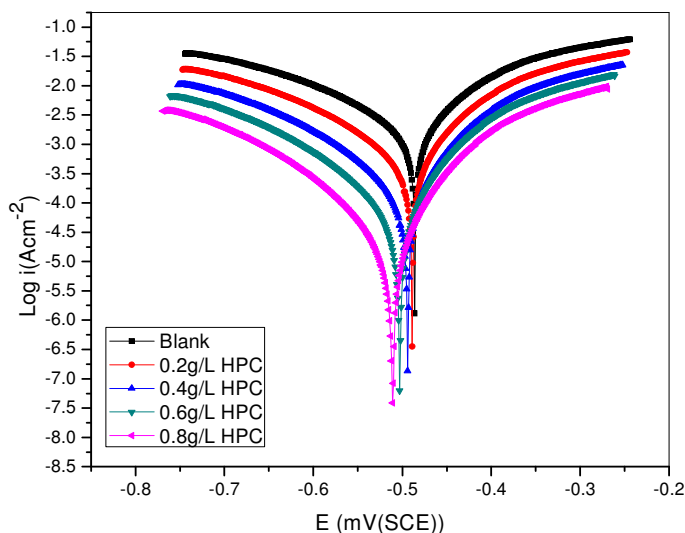


Fig. 1. Polarization curves for mild steel corrosion in 0.5 M H₂SO₄ in the absence and presence of HPC

Table 1. Polarization parameters for mild steel corrosion in 0.5 M H₂SO₄ in the absence and presence of HPC and HPC +KI

System	E _{corr} (mV(SCE))	i _{corr} (μAcm ⁻²)	b _c (mVde ⁻¹)	b _a (mVde ⁻¹)	IE (%)	θ
Blank	-480.76	782.39	173.15	116.07	–	–
0.2 g/LHPC	-510.76	265.56	131.62	99.31	66.48	0.66
0.4 g/LHPC	-503.45	215.23	123.12	91.56	72.83	0.73
0.6 g/LHPC	-495.87	188.49	112.08	90.56	76.21	0.76
0.8 g/LHPC	-489.36	163.05	95.32	88.78	79.42	0.79
0.2 g/LHPC+ 0.4 gKI	-482.47	235.03	121.45	83.61	70.34	0.70
0.4 g/LHPC+ 0.4 gKI	-478.86	181.72	98.05	79.09	77.07	0.77
0.6 g/LHPC+ 0.4 gKI	-473.78	143.46	86.78	77.11	81.90	0.82
0.8 g/LHPC+ 0.4 gKI	-470.03	110.51	71.63	76.07	86.05	0.86

3.2.2 Inhibition efficiency

The ability of an inhibitive material to resist or cover more corrosion sites or regions on the metal surface subjected to corrosion. The corrosion reaction process of metal cannot be prevented or stopped completely, since it is a means of returning a metal to their natural state or ores from which they were originally obtained [23] but the process can be controlled or reduced using various means. Hence, it was observed that introduction of HPC in acidic solution reduced the dissolution of mild steel and the trend was concentration dependent (Table 2 and Fig. 2). This protective effect of HPC on mild steel is as a result of inhibitive action of some functional groups such as hydroxyl group, propyl group, cyclic ring structure, etc which form the basis of structure of the polymer. Although, it is difficult to ascertain which functional group or groups played more active role in inhibition adsorption, but it is suggested that the interaction between the functional groups and charge on the metal surface leads to the formation of complex which accelerates the corrosion control by either blocking more corrosion sites [24] or altering the energy barrier of the corrosion process.

3.3 Adsorption and Thermodynamic Studies

The adsorbed water molecule covers the metal surface in solution whereas in a competitive substitution reaction process inhibitor molecule displaces the water molecule and adsorb on the metal surface [25]. To understand the nature of adsorbing characteristics of HPC and HPC+KI on mild steel surface, the corrosion inhibition was investigated using potentiodynamic polarization and gravimetric measurement technique respectively. Resulting experimental data (degree of surface coverage) obtained were fitted to a number adsorption isotherms to determine the mode of adsorption process of HPC and HPC+KI complex on the mild steel surface undergoing dissolution. The correlation coefficient, R^2 (closeness to unity) was used to determine the isotherm that best fit experimental result and Langmuir adsorption isotherm gave the best fit. Langmuir isotherm is represented by a correlation between surface coverage ($\theta = \text{IE}\%/100$) and inhibitor concentration (C_{inh}) according to Equation 4 as shown below:

$$\frac{C_{\text{inh}}}{\theta} = \frac{1}{b} + C_{\text{inh}} \quad (4)$$

where b is the adsorption equilibrium constant. The calculated data from polarization and weight

loss results were used for the plots of C_{inh}/θ against C_{inh} and presented in Figs. 3a and 3b.

Straight lines were obtained with slopes of 1.0729 ($R^2 = 0.9980$), 1.185 ($R^2 = 0.9993$), 1.0184 ($R^2 = 0.9897$) and 1.2679 ($R^2 = 0.9987$). This suggests that the adsorption of HPC and HPC+KI respectively on the mild steel surface obeyed the Langmuir adsorption isotherm. From the intercepts of the linear plots of weight loss measurement results, the values of b in the presence of HPC and HPC+KI were calculated as 10.7434 and 22.1043. The high value of b for HPC+KI suggests strong adsorption because of the presence of potassium iodide. The relationship between the adsorption equilibrium constant, b and standard free of adsorption, ΔG_{ads} in an adsorption-desorption process according to Equation 5 is given as:

$$b = \frac{1}{55.5} \exp\left(-\frac{\Delta G_{\text{ads}}}{RT}\right) \quad (5)$$

where R , T and 55.5 represents universal gas constant (8.3142KJ/mol), absolute temperature (K) and water concentration of solution in ml/l [25] respectively. The computed values of ΔG_{ads} at $30 \pm 1^\circ\text{C}$ are -16.099 KJ/mol and -17.917 KJ/mol for HPC and HPC+KI respectively. The negative value of ΔG_{ads} suggests the stability of HPC and HPC+KI adsorbed on the mild steel surface and spontaneous adsorption process. Since the value of ΔG_{ads} accepted as a threshold value for chemisorptions and physisorption is -40 KJ/mol [26], the obtained values of ΔG_{ads} indicates that physisorption adsorption mechanism.

3.4 Potassium Iodide Additive Effect

The effect of combination of HPC and KI on the corrosion inhibition of mild steel was investigated using weight loss technique. The results obtained were shown in Table 2. Careful inspection of the data revealed that corrosion rate of mild steel in 0.5 M H_2SO_4 in the presence of HPC+KI was significantly reduced in the presence of HPC+KI in comparison to blank solution and HPC alone. This is could be attributed to the modification of the metal surface as a result of large ionic radius, high hydrophobic character, low electronegativity of the iodide ion [27] and combining effect between HPC and KI. Furthermore, the polarization curve (Fig. 4) showed that presence of KI reduced the values of corrosion current leading to increase in inhibition efficiency (Table 1). Also, the cathodic and anodic reaction

rates were decreased and corrosion potential shifts towards anodic potential, thus indicating that anodic reaction is predominantly controlled.

3.5 Synergism Considerations

The synergism parameter, S_1 was determined using the relationship between inhibition efficiency of inhibitors and inhibition efficiency of mixed inhibitors [28] according to Equation 6 shown below:

$$S_1 = \frac{1 - I_{1+2}}{1 - I_1 - I_2} \quad (6)$$

where $I_{1+2} = (I_1 + I_2)$, I_1 is the inhibition efficiency of KI, I_2 is the inhibition efficiency of HPC, and I_{1+2} is the inhibition efficiency of HPC+KI. The synergism parameter was estimated using the inhibition efficiency obtained from weight loss measurement technique. The results obtained are presented in Table 3. The synergistic effect of HPC+KI may be as a result of co-adsorption involving the two molecules which could be either competitive adsorption ($SI < 1$) or co-operative adsorption ($SI > 1$). The calculated values of synergism parameters were greater than unity, thus suggesting a co-operative synergistic adsorption caused the enhancement in the inhibition.

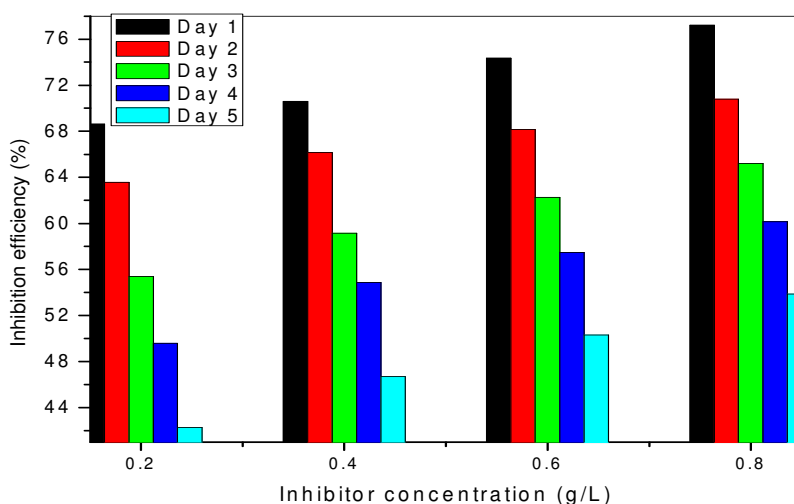


Fig. 2. Variation of inhibition efficiency (%) against Inhibitor concentration (g/L) for mild steel corrosion in 0.5 M H₂SO₄ in the presence of HPC

Table 2. Calculated values of corrosion rate (mm/yr) and inhibition efficiency for mild steel corrosion in 0.5 M H₂SO₄ in the absence and presence of HPC from weight loss measurement at different days

System	Corrosion rate (mm/yr)					Inhibition efficiency (IE%)				
	1	2	3	4	5	1	2	3	4	5
Blank	42.35	30.32	20.71	15.71	12.70	—	—	—	—	—
0.4 g/LKI	28.23	22.35	15.88	12.65	10.43	33.34	26.29	23.32	19.48	17.87
0.2 g/LHPC	13.29	11.05	9.03	7.92	6.93	68.62	63.56	56.40	49.59	45.43
0.4 g/LHPC	12.45	10.26	8.27	7.09	6.16	70.60	66.16	60.08	54.87	51.65
0.6 g/LHPC	10.86	9.36	7.82	6.68	5.93	74.36	69.13	62.24	57.48	53.31
0.8 g/LHPC	9.98	8.76	6.69	5.73	4.98	76.43	71.11	67.70	63.52	60.79
0.2 g/LHPC + 0.4 gKI	12.03	9.56	7.23	5.98	5.36	71.59	68.47	65.09	61.94	57.80
0.4 g/LHPC + 0.4 gKI	9.95	7.89	6.05	5.08	4.58	76.51	73.98	70.79	67.66	63.94
0.6 g/LHPC + 0.4 gKI	6.21	6.10	4.90	4.12	4.02	82.98	79.88	76.34	73.77	68.35
0.8 g/LHPC + 0.4 gKI	4.35	3.66	3.40	3.13	3.02	89.73	87.93	83.58	80.08	76.22

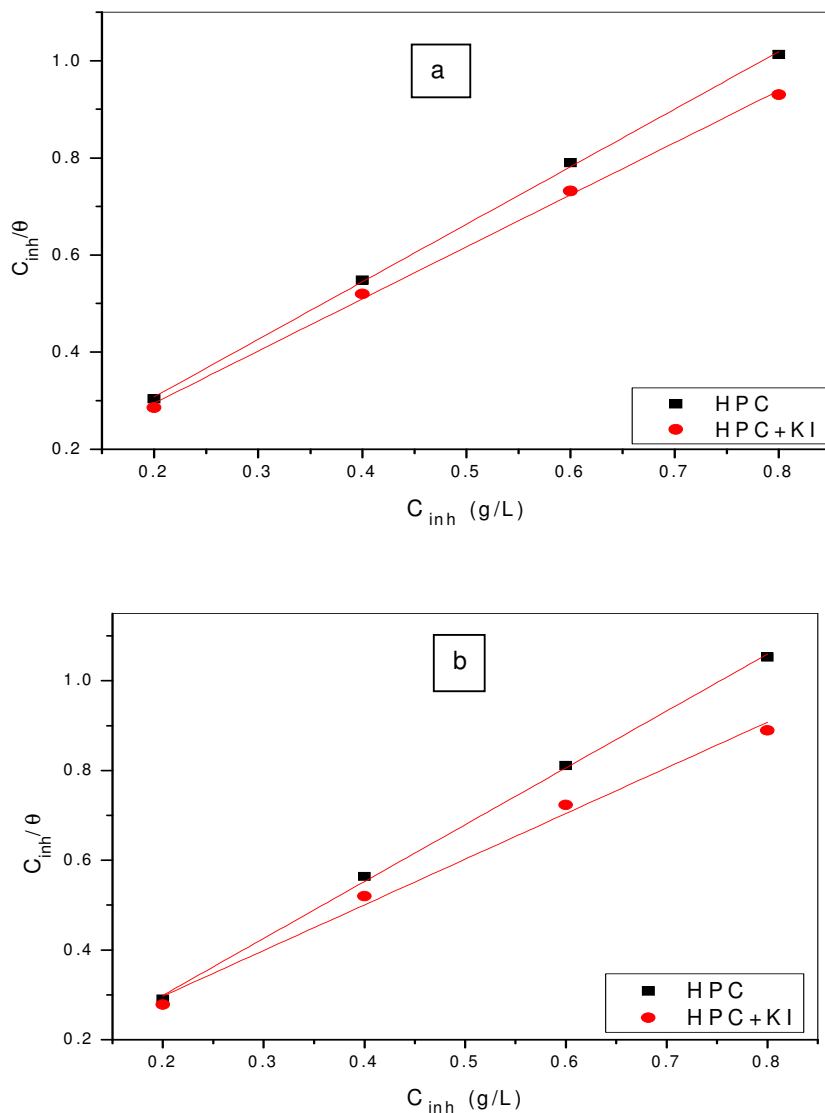


Fig. 3. Langmuir adsorption isotherm plots of HPC and HPC+KI on mild steel in 0.5 M H₂SO₄
 (a) Polarization data (b) Weight loss data

3.6 Theoretical Computational Studies

3.6.1 Molecular reactivity

Theoretical quantum chemical calculations were carried out using the density functional theory (DFT) procedure as contained in the Material Studio 7.0 to study the effect of molecular electronic structure on the inhibition effectiveness of HPC. All the calculations were performed with complete geometry optimization using the following parameters: Electronic structure program DMol³, COMPASS force field and Smart

minimization method, Mulliken population analysis, Electronic parameters involving Perdew-wang (PW) local correlation density functional and restricted spin polarization (DND basis set), Self-consistent field (SCF) procedure with a convergence of 10^{-3} , Fermi smearing parameter of 0.005 hartree, etc. The optimized structure, electron density, highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), Fukui function for electrophilic and nucleophilic attack of HPC obtained from the simulation are shown in Fig. 5.

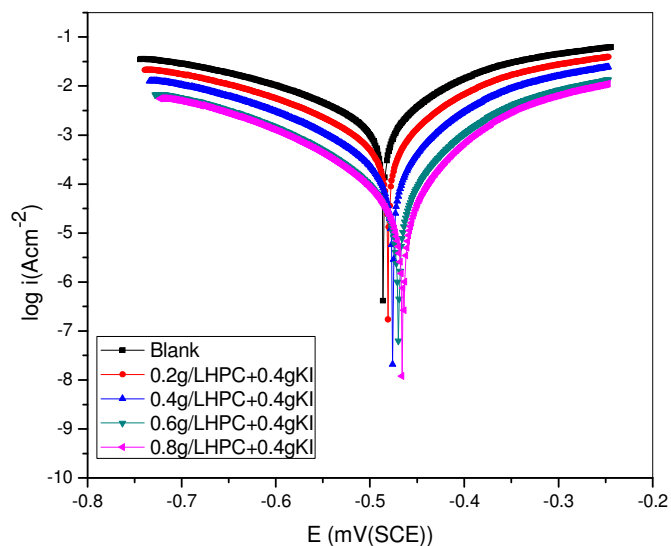


Fig. 4. Polarization curves for mild steel corrosion in 0.5 M H₂SO₄ in the absence and presence of HPC+KI

E_{HOMO} , E_{LUMO} and ΔE_{gap} are the energies of the frontier molecular orbital (FMO) and they are very important quantum parameter used for the prediction of the reactivity of chemical species. E_{HOMO} represents the electron donating ability of a molecule whereas E_{LUMO} is often associated with the electron accepting ability of a molecule. A molecule has the tendency to donate electron to a metal surface with unoccupied molecular when E_{HOMO} value is high while the low value of E_{LUMO} indicates more propensity to acceptance electron from a metal surface. ΔE_{gap} is the gap between the LUMO and HOMO energy levels at a molecule. Low value of energy gap ($\Delta E_{\text{gap}} = E_{\text{LUMO}} - E_{\text{HOMO}}$) is an indication of good inhibitive effectiveness or performance [29-31]. The calculated values of E_{HOMO} , E_{LUMO} and ΔE_{gap} are shown in Table 4 and they are in good agreement with the inhibition efficiency (IE %) of the experimental results.

The local reactivity of HPC molecule was analyzed using the Fukui function as a measurement of the chemical reactivity, thereby indicating the reactive regions in terms of nucleophilic (F^+) and electrophilic (F^-) behaviour of the molecule (Fig. 5e). Highest electron density (HOMO) regions are the sites at which electrophiles attack and represent the active centres with the highest ability to bond to the metal surface, whereas the LUMO orbital regions are sites at nucleophile attack and represent areas through which electrons are accepted from

the metal (Fe) using anti-bonding orbitals to form feedback bonds. For HPC, both HOMO orbital and LUMO orbital are dominated around the phenyl ring and along the side chains (hydroxypropyl group). In assessing reactive regions in terms of nucleophilic and electrophilic attack, the F^- corresponds with the HOMO locations, indicating the sites through which the molecule may be adsorbed on the Fe surface, whereas F^+ correspond with the LUMO locations, showing sites through which the molecules could interact with the non-bonding electrons in the metal (Fig. 5). In addition, high value of E_{HOMO} indicates the disposition of the molecule to donate electrons to an appropriate acceptor with vacant molecular orbitals.

Some other quantum chemical parameters such as ionization potential (IP), electron affinity (EA), chemical potential (μ), absolute electronegativity (χ), hardness (η), softness (σ) and number of electrons transferred (ΔN) were calculated using the following Equations 7, 8, 9, 10, 11,12 and 13 stated below:

$$\text{IP} = -E_{\text{HOMO}} \quad (7)$$

$$\text{EA} = -E_{\text{LUMO}} \quad (8)$$

$$\chi = \frac{\text{IP} + \text{EA}}{2} \quad (9)$$

$$\mu = -\chi \quad (10)$$

$$\eta = \frac{IP-AE}{2} \quad (11)$$

$$\sigma = \frac{1}{\eta} \quad (12)$$

$$\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} - \eta_{inh})} \quad (13)$$

Table 4 provides the results of calculated quantum chemical parameters. The ability of a molecule to donate or accept electron can be obtained from the chemical potential, hardness and electronegativity. However, the lower the values of these chemical parameters, the higher the electron donating and accepting power of a molecule [32] and thus higher the inhibitive performance of a molecule. The values of the chemical parameters obtained for a HPC repeat unit (Table 4) is an indication that HPC repeat unit has a good inhibition effectiveness which is also in agreement with the analysis of frontier molecular orbital. To determine ΔN , a theoretical value for the electronegativity of bulk iron ($\chi_{Fe} \approx 7\text{ev}$) and chemical hardness ($\eta_{Fe} \approx 0$) were used

by assuming that for metallic bulk $IP = AE$, since they are softer than the neutral metallic atoms [33]. The value of ΔN obtained is less than 3.6, thus an indication that inhibition efficiency increased with increasing electron donating ability at the mild steel surface [34]. Hence, it can be inferred from the calculated result that HPC repeat unit investigated in this study was electron donors whereas mild steel surface was the electron acceptors.

3.6.2 Molecular simulation dynamics

To evaluate quantitatively the most suitable adsorption between the HPC single molecule and Fe surface, the adsorption energy (E_{Bind}) was calculated using Equation 14 stated below:

$$E_{\text{Bind}} = E_{\text{Fe-HPC}} - (E_{\text{Fe}} + E_{\text{HPC}}) \quad (14)$$

where $E_{\text{Fe-HPC}}$ is the total energy of the Fe crystal together with the adsorbed HPC molecule. (E_{Fe} and E_{HPC}) is the total energy of Fe crystal and

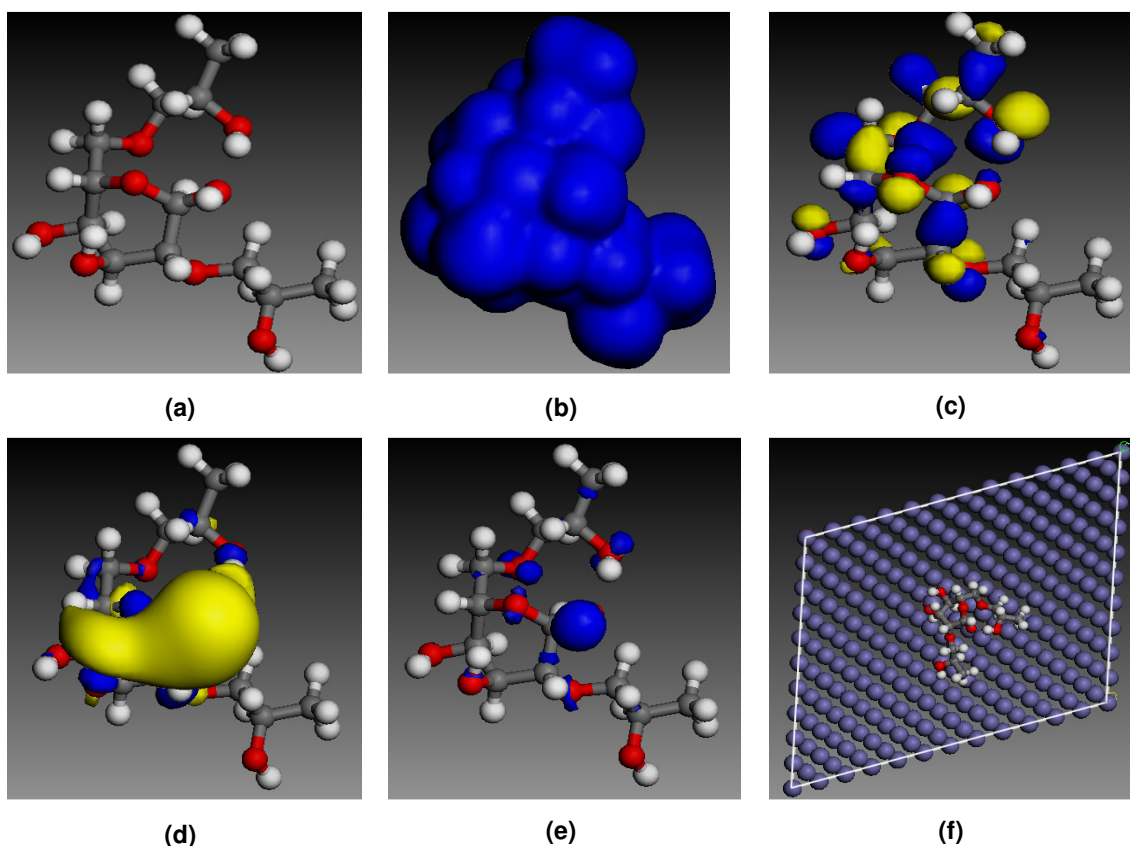


Fig. 5. Electronic properties of Hydroxypropyl Cellulose repeat unit [C = grey; H = white; O = Oxygen] (a) Optimized Structure, (b) Total electron density, (c) HOMO Orbital, (d) LUMO Orbital (e) Reactive regions (both F^+ & F^-) (f) Top view of the lowest energy adsorption orientation for a single HPC molecule on the Fe (110) surface

Table 3. Calculated synergism parameter for mild steel corrosion in 0.5 M H₂SO₄ in the presence of HPC+KI from weight loss measurement at different days

System	Synergism parameter (SI)				
	1	2	3	4	5
0.2 g/LHPC+KI	1.43	1.36	1.22	1.11	1.09
0.4 g/LHPC+KI	1.36	1.25	1.18	1.10	1.08
0.6 g/LHPC+KI	1.30	1.19	1.12	1.04	1.04
0.8 g/LHPC+KI	1.22	1.10	1.09	1.03	1.03

free HPC molecule respectively. The parameters used include: Forcite quench molecular dynamics, Cleaved Fe crystal along the (110) plane with 12×10 supercell, COMPASS force field, Smart algorithm with NVE (microcanonical) ensemble, a time step of 1 fs and simulation time 5 ps with 250 steps quenched, Fixed temperature (273 K) and geometrical optimized structures of HPC and Fe. The large negative value of E_{Bind} obtained points toward strong adsorption of HPC on the Fe surface, in agreement with the experimental findings. During the simulation, the potential energies were calculated by averaging the energies of the five structures of the lowest energy. The obtained adsorption energy value is -168.5121 kcal/mol and adsorption orientation for a single HPC molecule on the Fe (110) surface is shown in Fig. 5f.

Table 4. Quantum chemical parameters of hydroxypropyl cellulose (HPC)

Parameters	Values
E_{HOMO} (eV)	-5.4414
E_{LUMO} (eV)	1.9203
ΔE_{gap} (eV)	7.3617
χ (eV)	-1.7606
η (eV)	-3.6809
σ (eV)	-0.2717
μ (eV)	1.7606
ΔN (eV)	1.1900
Binding energy (Kcal/mol)	-171.7494

4. CONCLUSION

Hydroxypropyl cellulose (HPC) exhibited good inhibitive effectiveness in controlling the dissolution of mild steel in 0.5 M H₂SO₄ and the performance was improved further using potassium iodide (KI). The gravimetric measurement data obtained followed Langmuir adsorption isotherm. Potentiodynamic polarization results showed that HPC inhibited both the cathodic and anodic reaction processes and thus classified it as a mixed-type inhibitor. The inhibitive performance of HPC is probably

due to electrostatic interaction between the functional groups and charge on the mild steel surface and as well as adsorption of the complex formed which covered a large surface area of the metal. The combination effect of HPC and KI on corrosion inhibition behaviour was proposed to be synergistic in action. The uncertainty associated with the experimental data shown in Table 2 is a revelation that inhibitive performance or stability of HPC decreases with time, indicating that time variation should of optimum consideration in the choice of application of HPC as inhibitor. Also, the polarization curves revealed that HPC alone predominantly controlled cathodic reaction process whereas HPC+KI controlled the anodic dissolution of mild steel in sulphuric acid induced corrosion process. The Fukui functions revealed that HPC adsorbed on the corroding mild steel surface through multiple OH groups, propyl groups and aromatic structure. Finally, theoretical computation studies revealed the relationship between the electronic molecular structure and the inhibition efficacy of HPC.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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