

Electrochemical, morphological and theoretical evaluation of a new poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate) against corrosion of AISI 1020 steel in 0.1 N HCl solution

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Abstract

This research includes the preparation of a new poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate) (PSCOCBDL) by free radical polymerization of the preliminarily prepared *cis*-2-butene-1,4-dilinoleate with 3-sulfolene. This prepared copolymer was diagnosed using Fourier transform infrared spectroscopy and Gel permeation chromatography. The corrosion inhibition effect of poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate) on AISI 1020 steel corrosion in 0.1 N hydrochloric acid solution was studied at a temperature 298 K by means of electrochemical impedance spectroscopy and potentiodynamic polarization techniques. A set of experiments with different concentrations of the inhibitor copolymer (15, 30, 45 and 60 ppm) were conducted. The study revealed that the inhibition efficiency increases with an increase in concentration. Potentiodynamic polarization measurements detected that the PSCOCBDL copolymer was a corrosion inhibitor of anodic type. Atomic force microscopy technique was employed to determine the surface morphology of AISI 1020 steel samples after exposure both in uninhibited and inhibited medium. The morphological study indicated that adsorption of the corrosion inhibitor copolymer PSCOCBDL on AISI 1020 steel surface resulted in building a protective layer. The adsorption of the prepared copolymer on AISI 1020 steel surface obeys the Langmuir isotherm. Various quantum chemical descriptors have been calculated based on the density functional theory, such as E_{HOMO} , E_{LUMO} , ΔE , χ , η , S , and μ , which are related most closely to the anti-corrosive features of the examined copolymer. A molecule with a higher E_{HOMO} can take electrons speedily from an appropriate acceptor molecule with a lower-energy vacuous molecular orbital, while the E_{LUMO} value indicates how well the molecule can hold back electrons.

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1. Introduction

The deterioration of facilities made of steel due to corrosion is a main issue in petrochemical manufactures and in other engineering firms [1, 2], as the annual corrosion results in the closure of numerous factories and cessation of installations, as well as the loss and subsequent damage of numerous industrial products, which ultimately contribute to

environmental contamination [3–5]. In industry, acid solutions are utilized for a variety of purposes, including acid descaling, acid pickling, acid descaling in industry, and acidizing of oil wells. Corrosion assaults ensue due to the acidic solution's inherently corrosive characteristics. As a result, investment initiatives in corrosion management within the metal industry become exorbitantly costly [6, 7]. Therefore, it is fundamental to prepare some powerful corrosion inhibitors. Inhibition by organic compounds comprising heteroatoms N, S and O, especially in the presence of π -electrons in their structures. Organic polymers are among the most efficacious techniques for protection of metals against corrosion when exposed to corrosive acidic environments [8, 9]. This is due to its great liability to form complex compounds with ions of metals and be efficiently adsorbed on surfaces of metals due to the presence of diverse functional groups in the polymer molecules. Polymer molecules or their complexes with metals occupy a significant surface area, that way covering the surface and shielding the metal from corrosive compounds present in the solution [10, 11].

The adsorption mechanism is predicated on polar groups serving as efficient centers for the adsorption process; the adsorption film that is produced serves as a barrier, efficiently segregating the steel substrate from the hostile environments to which it is exposed [12]. Numerous studies have demonstrated that polymers are efficient corrosion inhibitors and coating materials. The synthesis of a collection of polymers was achieved through the reaction of hydroxyquinazoline derivatives and aminoquinazoline derivatives with *N,N*-cyclohexyl carbodiimide (DCCI) in the presence of methacrylic acid by Aly *et al.* These polymers were explored as corrosion inhibitors of AISI 1020 steel in HCl media. The protective efficiency was estimated through utilization of potentiodynamic polarization. The findings show that the inhibition efficiency increased with an increase in inhibitor concentration and was reduced with temperature. Inhibition occurred due to adsorption of polymer compounds on the mild steel surface [13]. Various factors that affect corrosion inhibition, including the structure of the molecules and concentration of 1-phenyl-2-thiourea (PTU) and 1,3-diisopropyl-2-thiourea (ITU) in 1.0 M HCl, were examined by Huong *et al.* utilizing PDP curves, EIS and quantum chemical calculations. The inhibitory efficiencies of PTU and ITU at 5×10^{-3} M and 60°C were found to be the highest at 98.96 and 92.65%, respectively. PTU and ITU are adsorbed on the metal surface according to the Langmuir adsorption isotherm. The theoretical results for the inhibitors agree well with experimental data [14]. Rahal *et al.* studied the utilization of thiobarbituric acid (TBA) and thiourea (TU) as corrosion inhibitors of mild steel in 0.5 M HNO₃ by utilizing PDP, EIS and quantum-chemical calculations. Both of these inhibitors displayed perfect inhibition efficiency in the HNO₃ solution. A number of isotherms, namely Langmuir, Flory-Huggins, Temkin and kinetic-thermodynamic models, were used fit data on adsorption of inhibitors on mild steel surface [15].

This present study aims at the synthesis and characterization of a new polymeric compound, poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate) (PSCOCBDL), and its evaluation as a corrosion inhibitor of AISI 1020 steel in 0.1 N HCl. This is due to the high

molecular weight and repeating functional groups of this prepared polymeric compound, which provide higher electron density at the inhibitor's adsorption centers and thus strengthen the interactions between the inhibitor molecules and the metal surface, resulting in protection of the metal from corrosion.

2. Experimental

2.1. Materials

The chemical composition (in wt.%) of AISI 1020 steel obtained from company metal samples (United States): 98.5% Fe, 0.2% C, and 0.6% Mn; minor amounts of P, S, Si, Sn, Cu, Ni, Cr and Mo. Sigma-Aldrich in Germany supplied the following chemicals: linoleic acid, 3-sulfolene, *cis*-2-butene-1,4-diol, zinc oxide, benzoyl peroxide, toluene, and hydrochloric acid.

2.2. Synthesis of poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate)

a. Condensation reaction

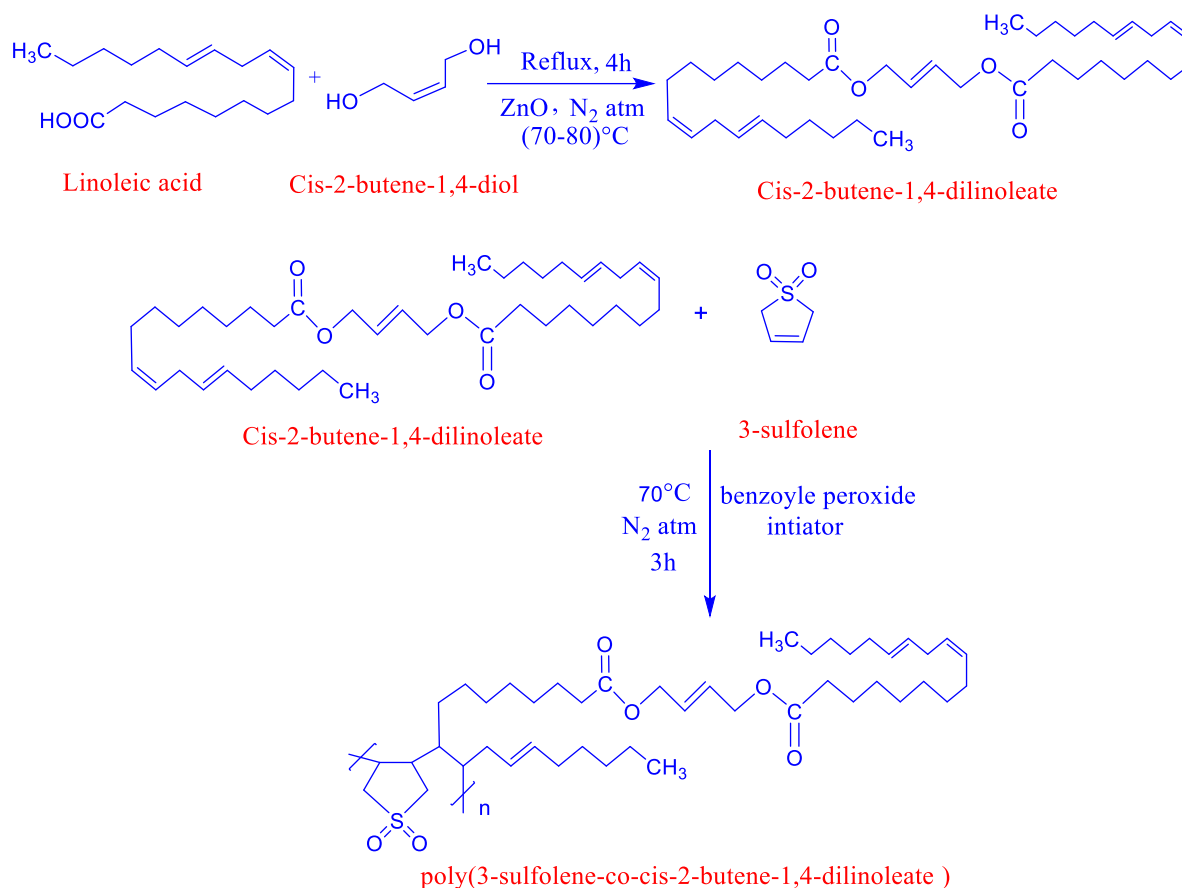
Linoleic acid (6.66 ml, 0.021 mol) and *cis*-2-butene-1,4-diol (3.45 ml, 0.042 mol) were reacted *via* condensation reaction in a 100 mL round-bottom flask equipped with a reflux condenser. The reaction was performed at a mole ratio of 1:2, with ZnO serving as the catalyst. A nitrogen atmosphere was used to heat the reaction mixture at 70–80°C for four hours while agitating continuously. Following the completion of this procedure, the product was kept in a separating funnel for 1 h in order to obtain two distinct strata. After eliminating the unreacted substances and water from the lowermost layer, the organic layer at the top was isolated. The product was kept at r.t. for 24 h [16] to give *cis*-2-butene-1,4-dilinoleate (CBDL).

b. Copolymerization

cis-2-Butene-1,4-dilinoleate prepared in advance was copolymerized with 3-sulfolene in toluene at a molar ratio of 1:4 under nitrogen atmosphere with benzoyl peroxide as the initiator (1% w/w). Then, continuous stirring at 70°C for 3 h was used to complete the polymerization. The copolymer thus obtained was dried *in vacuo* for 24 h [17, 18]. Scheme 1 illustrates the PSCOCBDL synthesis.

2.3. Characterization of the synthesized copolymer

The chemical structure of the synthesized copolymer was determined using a Bruker FTIR spectrometer. The Fourier transform infrared spectra (FTIR) were recorded in the 400–4000 cm⁻¹ range and analyzed. Gel permeation chromatography (GPC) was employed to ascertain the average molecular weight (Mn) of the copolymer. A refractive index detector was utilized in conjunction with a Breeze™ 2 HPLC System. THF (Merck) was employed as the eluent fed at a rate of 1.0 mL/min.



Scheme 1. Schematic illustration of PSCOCBDL preparation.

2.4. Electrochemical measurements

Electrochemical measurements were conducted using an Ivium potentiostat/galvanostat (Vertex One, Ivium Technologies, Netherlands). The experimental setup involved three electrodes arranged in a cell assembly: AISI 1020 steel as the working electrode, a platinum counter electrode, and a saturated calomel (Hg/Hg₂Cl₂ sat. KCl) reference electrode. Samples of AISI 1020 steel were submerged at 298 K in the acid solution comprising 0.1 N HCl and various concentrations of the corrosion inhibitor PSCOCBDL (15, 30, 45, and 60 ppm). Subsequently, electrochemical impedance (EIS) measurements were conducted, yielding impedance spectra with amplitudes of 10 mV and frequencies ranging from 100 kHz to 0.1 Hz. Experiments utilizing potentiodynamic polarization (PDP) were conducted within a potential range of ± 250 mV at a scanning rate of $5 \text{ mV} \cdot \text{s}^{-1}$.

2.5. Atomic force microscope analysis (AFM)

The AFM technique was used to study the morphological properties of AISI 1020 steel surface with and without poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate). AFM analysis was carried out using NaioAFM 2022, NanoSurf AG (Switzerland).

2.6. Theoretical evaluation

All calculations of structural parameters in this section were executed using Gaussian09 software [19]. The B3LYP 6-311 + G(d, p) method was utilized to perform comprehensive quantum chemical calculations and optimize geometric configurations. According to Koopman's theory [20], the E_{HOMO} and E_{LUMO} values are denoted by ionization potential (I) and electron affinity (A), which has reversed sign respectively.

$$I = -E_{\text{HOMO}} \quad (1)$$

$$A = -E_{\text{LUMO}} \quad (2)$$

Some chemical parameters, including electronegativity (χ), hardness (η), softness (S) and chemical potential (μ), were calculated based on density functional theory. To calculate χ , η and S , relations (3–5) were used:

$$\chi = -\mu \frac{(I + A)}{2} \quad (3)$$

$$\eta = \frac{(I + A)}{2} \quad (4)$$

$$S = \frac{1}{2\eta} \quad (5)$$

3. Results and Discussion

3.1. Characterization of the copolymer obtained

The FTIR spectrum of PSCOCBDL is illustrated in Figure 1. The peaks at 2926.81 and 2858.10 cm^{-1} correspond to aliphatic stretching vibration of C–H bonds, respectively. The peak at 1712.11 cm^{-1} corresponds to the stretching vibration of C=O in the ester group, the peak at 1120.88 cm^{-1} to the stretching vibration of C–O bonds of the ester, while the peak at 1619.17 cm^{-1} to the stretching vibration of aliphatic C=C bonds. The peaks observed at 1417.21 and 1281.02 cm^{-1} are indicative of symmetric and asymmetric stretching vibrations of S=O groups in sulfolene, respectively. The C–S bending peak corresponds to the wavenumber 648.91 cm^{-1} .

Figure 2 shows the GPC of PSCOCBDL. The molecular weights of PSCOCBDL and the polydispersity index were measured using gel permeation chromatography. The M_n (number-average molecular weight) and M_w (weight-average molecular weight) parameters of PSCOCBDL were found to be 1808 and 2219 g/mol, respectively. The peak molecular weight (M_p) of PSCOCBDL was found to be 1339 g/mol. The obtained polydispersity index (M_w/M_n) of 1.227 confirms that the polymerization is good and the number of chains is not exaggerated [21].

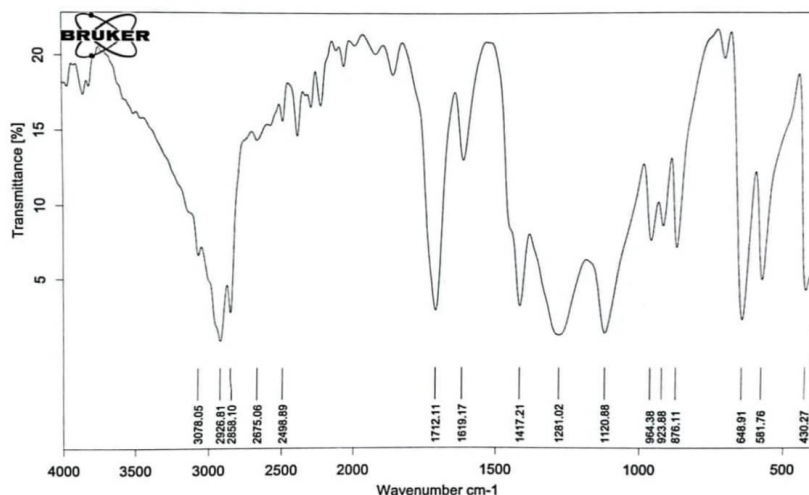


Figure 1. FTIR spectrum of PSCOCBDL copolymer.

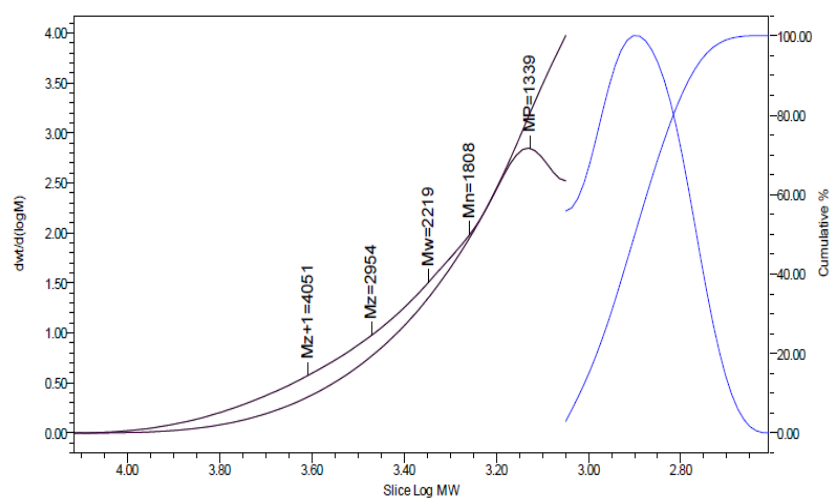


Figure 2. GPC chromatograms of PSCOCBDL copolymer.

3.2. Electrochemical measurements

3.2.1. Open circuit potential measurements (OCP)

Open circuit potential (OCP) plots were recorded for uninhibited and inhibited solutions for 30 min (until a constant potential was obtained). Figure 3 shows that the OCP of AISI 1020 steel at 298 K was attained after 30 min of exposure. It is obvious that the potential of AISI 1020 steel electrode immersed in 0.1 N HCl solution (blank curve) initially tends to more negative potentials, which represents the breakdown of the pre-immersion air-formed surface oxide film [22]. This is followed by the growth of a new oxide film in the solution, so that the potential shifts again in the noble direction until a steady state potential is established. The addition of PSCOCBDL inhibitor at a concentration of 15 ppm to the acid medium caused no difference in OCP, whereas the corrosion potential of AISI 1020 steel at concentrations of 30, 45 and 60 ppm moved in the positive direction.

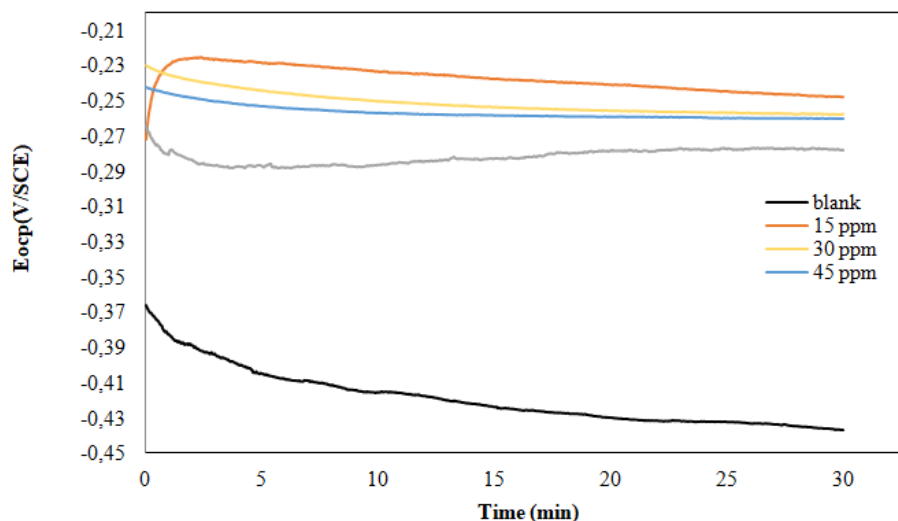


Figure 3. Open circuit potential of AISI 1020 steel in 0.1 N HCl without inhibitor and with different concentrations of PSCOCBDL.

3.2.2. Electrochemical impedance spectroscopy (EIS)

Electrochemical impedance measurements were conducted to give insights into the acid-interface kinetics of AISI 1020 steel and the manner in which the inhibitor copolymer PSCOCBDL modifies this kinetics. The Nyquist plots depicting corrosion of AISI 1020 steel in 0.1 N HCl solution at 298 K are shown in Figure 4. The plots were obtained with and without different concentrations of PSCOCBDL inhibitor. As shown by semicircles in Figure 4 of Nyquist plots, charge transfer is the primary mechanism governing the corrosion of AISI 1020 steel [23, 24]. This indicates that the protective properties of AISI 1020 steel surface are enhanced as the concentration of inhibitor copolymer causes an increase in the diameters of the semicircles. Therefore, the adsorbent layer's thickness and the dielectric properties are associated with the capacitive semicircle [25]. Figure 5 illustrates a simple equivalent circuit model that was employed to analyze derived impedance spectra. This model comprised charge transfer resistance (R_{ct}), solution resistance (R_s) and double layer capacitance (C_{dl}) given by.

$$C_{dl} = \frac{1}{2\pi f_{max} R_{ct}} \quad (6)$$

The inhibition efficiency (%IE) from EIS measurements was calculated from the following relation [26]:

$$\%IE = \frac{R_{ct(inh)} - R_{ct}}{R_{ct(inh)}} \cdot 100 \quad (7)$$

where R_{ct} and $R_{ct(inh)}$ are charge transfer resistance without and with inhibitor, respectively. The experimental data and results of computer fitting of the Nyquist plot using the

corresponding equivalent circuit model of 0.1 N HCl containing 45 ppm of PSCOCBDL inhibitor are demonstrated in Figure 6.

Table 1 gives the main parameters obtained from EIS such as charge transfer resistance (R_{ct}), solution resistance (R_s), double layer capacitance (C_{dl}) and inhibition efficiency ($\%IE$). In the presence of various concentrations of the inhibitor copolymer PSCOCBDL, it was observed that the increase in R_{ct} and $\%IE$ and decrease in C_{dl} values were attributable to the formation of a protective film on the metal surface, denoting that adsorption of the inhibitor copolymer was smooth with increasing inhibitor concentration [27, 28].

Table 1. The EIS parameters for AISI 1020 steel at 0.1 N HCl without and with different concentrations of PSCOCBDL inhibitor.

| Name of inhibitor | Conc. (ppm) | R_s ($\Omega \cdot \text{cm}^2$) | R_{ct} ($\Omega \cdot \text{cm}^2$) | C_{dl} ($\mu\text{F cm}^{-2}$) | $\%IE$ |
|-------------------|-------------|--------------------------------------|---|------------------------------------|--------|
| Blank | – | 1.02 | 2.70 | 168.00 | – |
| PSCOCBDL | 15 | 0.77 | 39.00 | 32.50 | 93.07 |
| | 30 | 0.93 | 45.40 | 26.30 | 94.00 |
| | 45 | 0.95 | 49.00 | 24.50 | 94.48 |
| | 60 | 0.98 | 67.50 | 18.30 | 96.00 |

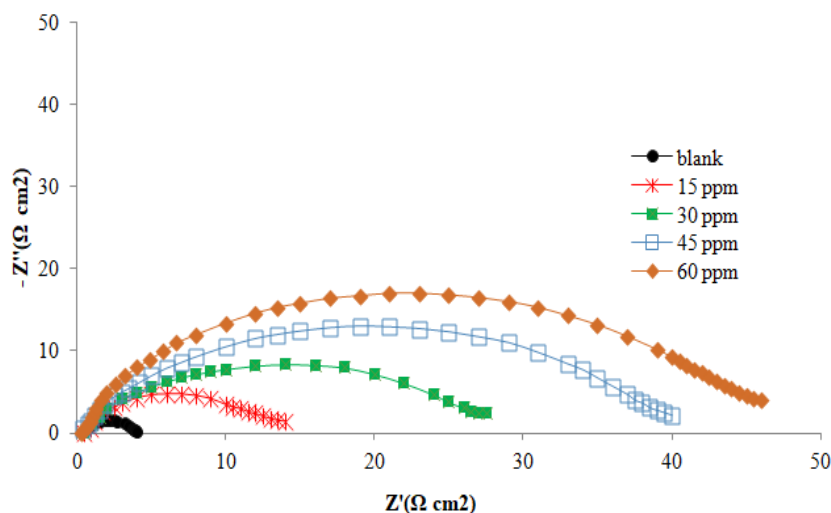


Figure 4. Nyquist plot for AISI 1020 steel in 0.1 N HCl solution without and with different concentrations of PSCOCBDL inhibitor.

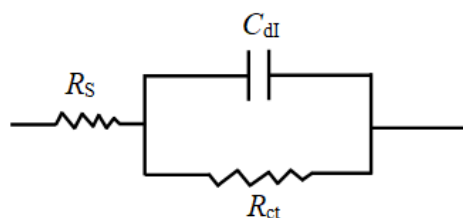


Figure 5. Equivalent circuit diagram for fitting of impedance spectra.

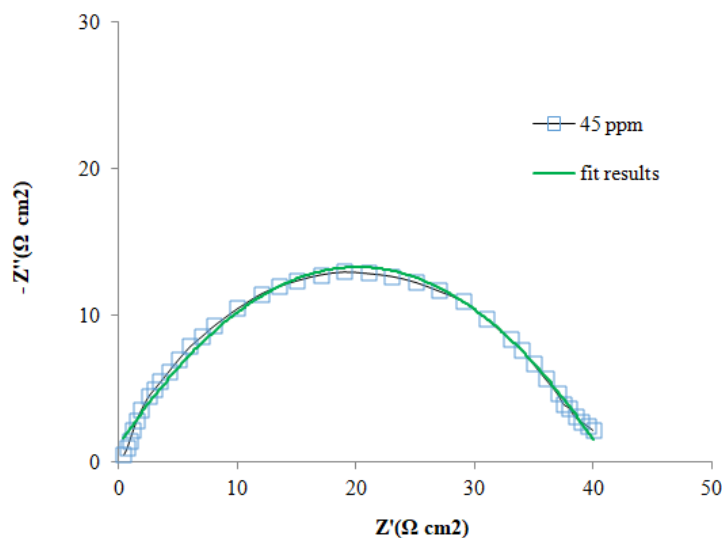


Figure 6. Experimental data and computer fitting results of Nyquist plot in 0.1 N HCl containing 45 ppm of PSCOCBDL.

3.2.3. Potentiodynamic polarization measurements

Potentiodynamic polarization (PDP) studies were performed on AISI 1020 steel samples immersed in 0.1 N HCl solutions containing different inhibitor concentrations at a temperature of 298 K. The potentiodynamic polarization curves thus obtained are presented in Figure 7. Table 2 provides a summary of electrochemical parameters acquired from polarization curves. The corrosion inhibition efficiency (%*IE*) is calculated from the corrosion rate of AISI 1020 steel according to Equation 3 [29].

$$\%IE = \frac{CR_{\text{blank}} - CR_{\text{inhib}}}{CR_{\text{blank}}} \quad (8)$$

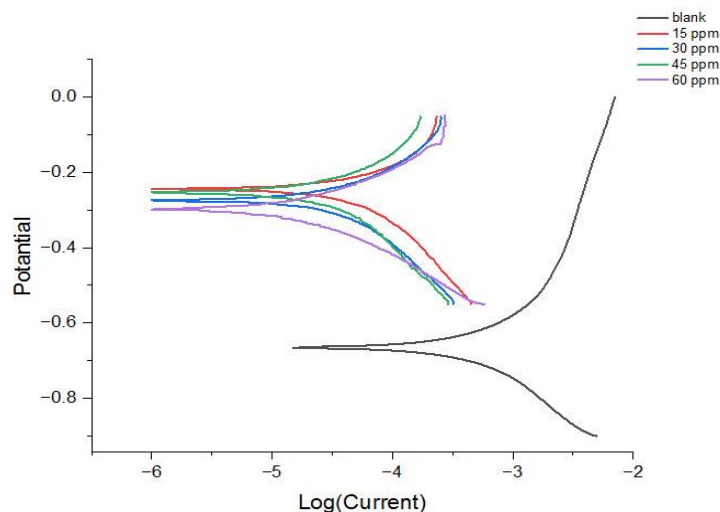


Figure 7. Potentiodynamic polarization curves measured on AISI 1020 steel in 0.1 N HCl solution with and without different concentrations of PSCOCBDL at 298 K.

Table 2. Electrochemical parameters of AISI 1020 steel in 0.1 N HCl without an inhibitor and with various concentrations of PSCOCBDL at 298 K.

| Conc. (ppm) | $-E_{\text{corr}}$ (mV) | i_{corr} (mA/cm ²) | β_c (mV/dec) | β_a (mV/dec) | CR (mpy) | %IE |
|-------------|-------------------------|---|--------------------|--------------------|----------|-------|
| Blank | 658.600 | 0.485 | 262 | 258 | 5.636 | – |
| 15 | 236.700 | 0.030 | 188 | 107 | 0.352 | 93.75 |
| 30 | 266.900 | 0.028 | 227 | 152 | 0.329 | 94.16 |
| 45 | 236.200 | 0.026 | 270 | 137 | 0.300 | 94.68 |
| 60 | 296.100 | 0.018 | 166 | 145 | 0.212 | 96.23 |

As expected, the data clearly indicate that the corrosion current density (i_{corr}) and corrosion rate (CR) decreased upon addition of different concentrations of PSCOCBDL inhibitor. Because of the adsorption effect of inhibitor molecules, the changes become more evident as the inhibitor concentration increases, providing the metal surface with a significant degree of protection by obstructing the active sites [30]. As seen from Table 4, the shift of the corrosion potential (E_{corr}) value after addition of PSCOCBDL inhibitor exceeds 85 mV, which may suggest cathodic or anodic type of the inhibitor [31, 32]. The E_{corr} values were found to move in the positive direction with increasing concentration of PSCOCBDL. This indicates the anodic type behavior of this prepared copolymer inhibitor at the different concentrations studied [33].

3.3. Simulation of the adsorption isotherm

Surface coverage θ was estimated from the corrosion rate of AISI 1020 steel with and without PSCOCBDL inhibitor (CR_{blank} and CR_{inhib} respectively at 25°C) according to the equation:

$$\theta = \frac{CR_{\text{blank}} - CR_{\text{inhib}}}{CR_{\text{blank}}} \quad (9)$$

In addition, several typical adsorption isotherms (Temkin, Frumkin, Flory Huggins and Langmuir isotherms) were tested. The adsorption behavior was most accurately characterized by the Langmuir isotherm as determined by the correlation coefficient values (R^2). The equation is expressed as [34]:

$$\frac{C_{\text{inhib}}}{\theta} = \frac{1}{K_{\text{ads}}} + C_{\text{inhib}} \quad (10)$$

where K_{ads} is the adsorption equilibrium constant and C_{inhib} is the concentration of the inhibitor. The Langmuir isotherm at 298 K for different concentrations of PSCOCBDL inhibitor in 0.1 N HCl is demonstrated in Figure 8. From Figure 8, the value of intercept is used to determine the K_{ads} value as in Table 3. The larger K_{ads} values indicate a strong adsorption of inhibitor molecules on the surface of AISI 1020 steel [35]. The standard free

energy of adsorption (ΔG_{ads}^0) was determined from the K_{ads} value by using the following equation [36].

$$K_{\text{ads}} = \frac{1}{55.5} \exp\left(\frac{\Delta G_{\text{ads}}^0}{RT}\right) \quad (11)$$

where 55.5 represents the concentration of water in solution in $\text{mol}\cdot\text{L}^{-1}$. The adsorption model is categorized as physisorption when values of ΔG_{ads}^0 are around or lower than $-20 \text{ kJ}\cdot\text{mol}^{-1}$, whilst inhibitors work by chemisorption model when ΔG_{ads}^0 is around or more negative than $-40 \text{ kJ}\cdot\text{mol}^{-1}$ [37]. In this study, the ΔG_{ads}^0 value calculated for PSCOCBDL is $-34.782 \text{ kJ}\cdot\text{mol}^{-1}$. This calculation demonstrates that adsorption of PSCOCBDL on AISI 1020 steel is chemisorption.

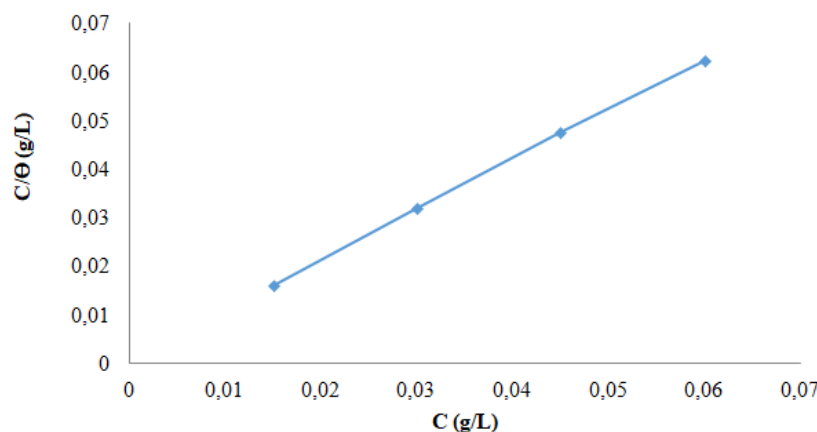


Figure 8. Langmuir adsorption for AISI 1020 steel in 0.1 N HCl solution with different concentrations of PSCOCBDL at 298 K.

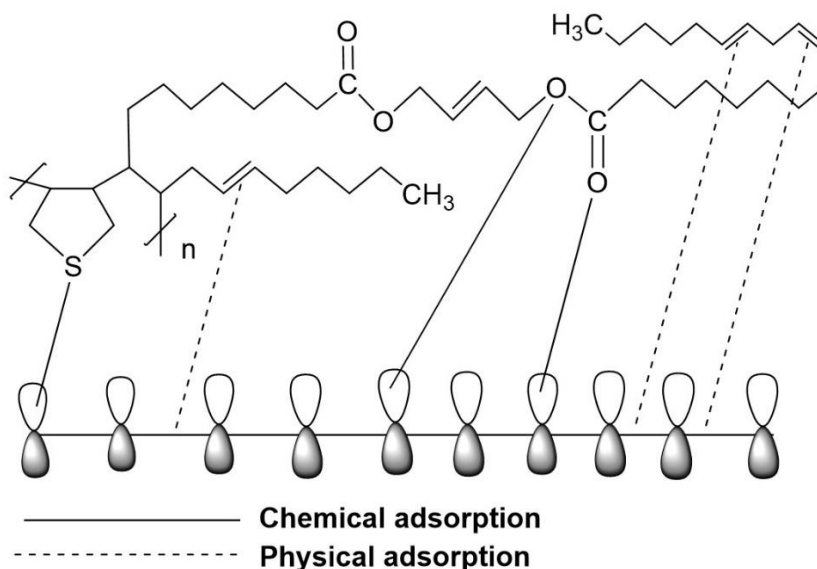


Figure 9. Suggested inhibition mechanism of PSCOCBDL of AISI 1020 steel in the acid environment.

Table 3. Adsorption equilibrium constant, correlation coefficient and standard free energy of PSCOCBDL adsorption on AISI 1020 steel in 0.1 N HCl.

| Inhibitor | K_{ads} ($\text{L}\cdot\text{g}^{-1}$) | R^2 | ΔG^0 ($\text{kJ}\cdot\text{mol}^{-1}$) |
|-----------|---|--------|--|
| PSCOCBDL | 1250 | 0.9998 | -34.782 |

Figure 9 provides particular adsorption mechanisms that contribute to PSCOCBDL inhibitor's corrosion inhibition properties. This understanding helps to unravel the corrosion prevention function of PSCOCBDL.

3.4. Atomic force microscope analysis (AFM)

AFM is a strong technique to examine surface morphology. It has become a new option for studying the impact of an inhibitor on the generation and progression of corrosion in acid media [38]. Two dimensional (2D) and three dimensional (3D) AFM morphologies of AISI 1020 steel surface immersed in 0.1 N HCl (blank) and AISI 1020 steel surface immersed in 0.1 N HCl containing different concentrations of inhibitor copolymer PSCOCBDL are given in Figure 10(a)–(f). In AFM analysis, S_q as the root mean square, S_a as the average roughness, S_p as the maximum peak height, and S_v as the maximum pit depth are the most utilized metrics for describing the surface roughness. The results in Table 4 indicate that roughness increased in the acid medium (0.1 N HCl) because of the corrosion reaction, but in the presence of inhibitor copolymer PSCOCBDL the roughness was reduced because of adsorption of the inhibitor copolymer on AISI 1020 steel surface to form a protective layer [39]. The reduced roughness value of the PSCOCBDL copolymer at 60 ppm concentration compared to that at 45 ppm reveals that the PSCOCBDL inhibitor at 60 ppm concentration protects the AISI 1020 steel surface more efficiently than at 45 ppm concentration in 0.1 N HCl solution.

Table 4. AFM parameters of AISI 1020 steel at 0.1 N HCl with and without different concentrations of PSCOCBDL inhibitor.

| Name of the inhibitor | Conc. (ppm) | S_q (nm) | S_a (nm) | S_p (nm) | S_v (nm) |
|-----------------------|-------------|------------|------------|------------|------------|
| blank | – | 324.5 | 266.9 | 883.2 | 816.1 |
| PSCOCBDL | 45 | 266.5 | 207.7 | 786.9 | 787.6 |
| | 60 | 133.0 | 106.9 | 395.8 | 461.3 |

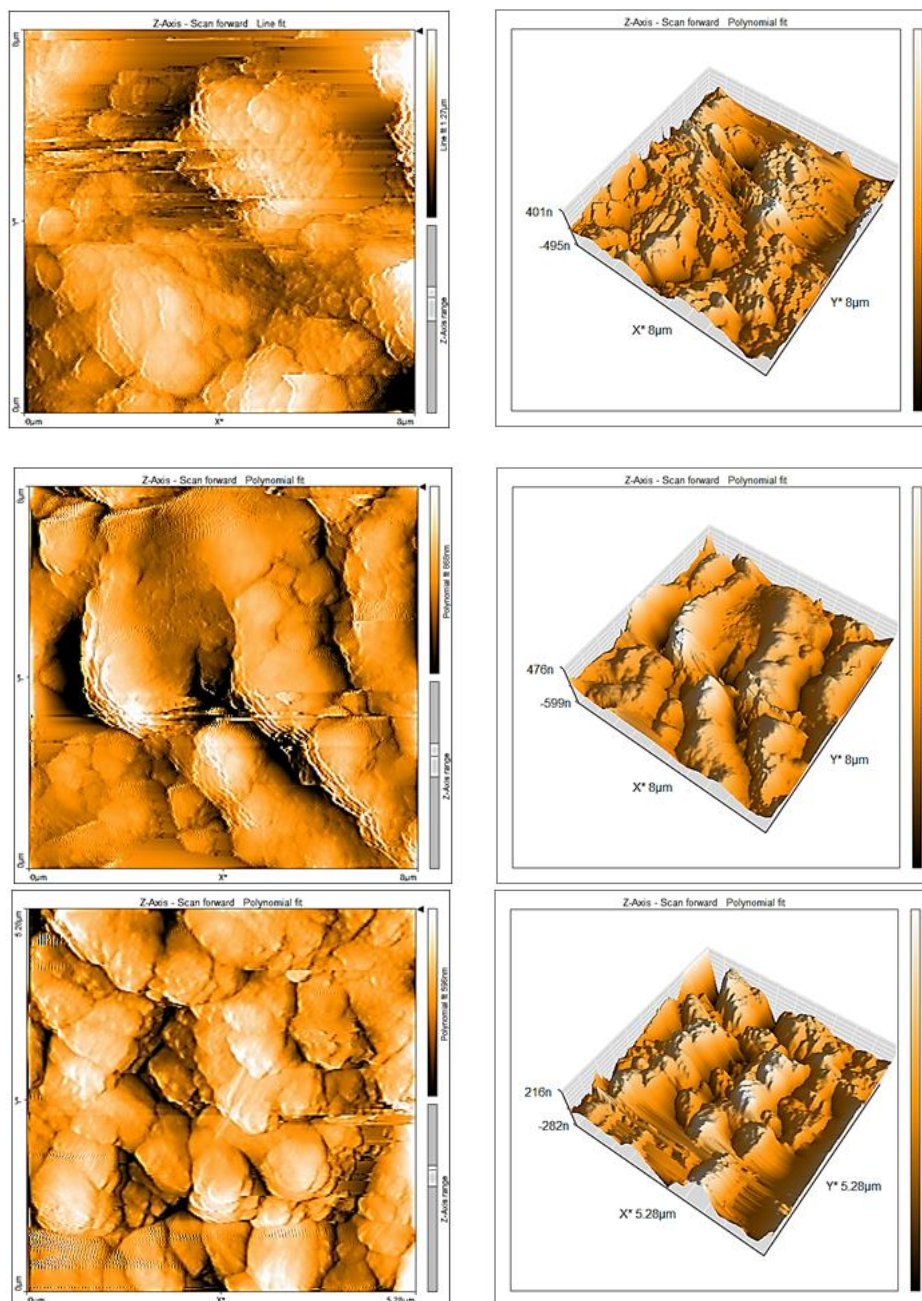


Figure 10. AFM 2D & 3D images of AISI 1020 steel in 0.1 N HCl (a) and (b) in the absence of inhibitor, (c) and (d) in the presence of 45 ppm PSCOCBDL, (e) and (f) in the presence of 60 ppm PSCOCBDL.

3.5. Theoretical results

The optimized geometry, HOMO and LUMO of the synthesized copolymer (PSCOCBDL) determined in this work are presented graphically in Figure 11. The parameters of this copolymer such as E_{HOMO} , E_{LUMO} , ΔE , E_{Total} , ionization potential (I), electron affinity (A), electronegativity (χ), hardness (η), softness (S), and chemical potential (μ) determined by quantum chemical calculations are listed in Table 5.

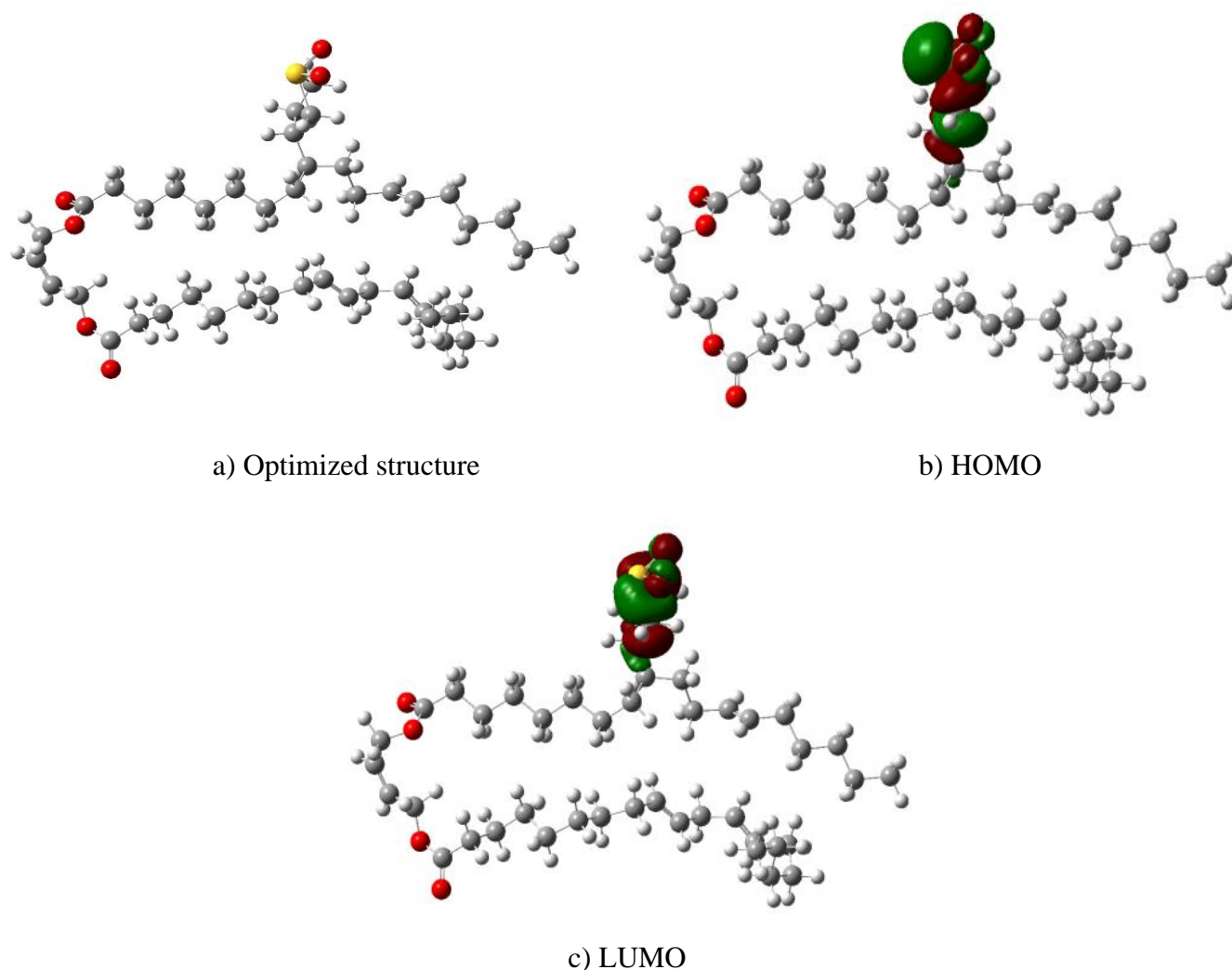


Figure 11. Optimized structure (a), HOMO (b) and LUMO (c) of PSCOCBDL copolymer.

Table 5. Quantum chemical characteristics of PSCOCBDL inhibitor molecule.

| E_{HOMO} (eV) | E_{LUMO} (eV) | ΔE_{gap} (eV) | E_{Total} (eV) | I (eV) | A (eV) | χ (eV) | η (eV) | S (eV) | M (eV) |
|---------------------------|---------------------------|---------------------------------|----------------------------|----------|----------|-------------|-------------|----------|----------|
| -8.568 | -2.503 | 6.065 | -5.562 | 8.568 | 2.503 | 5.535 | 3.032 | 0.165 | -5.535 |

According to Koopman's theorem, the ability of molecules to donate electrons can be reliably predicted using these energies. Literature study indicates that adsorption of inhibitor on the metal surface can occur due to donor–acceptor interactions between lone pairs and/or π electrons of the inhibitor molecules with the d-orbitals of metal surface atoms, leading to stronger adsorption of inhibitor molecules on the surface, thus the protective layer is formed [40, 41]. A molecule with a higher E_{HOMO} can speedily take electrons from a suitable acceptor molecule with a lower-energy vacuous molecular orbital [42], while the E_{LUMO} value indicates how well the molecule can donate electrons. Hardness (η) is defined as a

measure of variation in chemical potential over the overall number of atoms, one of key specifics in corrosion investigations [43]. As hardness (η) increases, the molecule becomes more stable, while softness (S) is the opposite of hardness. These results are in good agreement with experimental ones.

Conclusions

In this investigation, poly(3-sulfolene-co-*cis*-2-butene-1,4-dilinoleate) (PSCOCBDL) inhibitor prepared was sturdy in inhibiting corrosion of AISI 1020 steel. The electrochemical techniques demonstrate that the inhibition efficiency amounts to 96% at 298 K in the presence of PSCOCBDL inhibitor at a concentration of 60 ppm. The corrosion inhibition efficiency was shown to increase with the concentration of the copolymer inhibitor. Potentiodynamic polarization measurements detected that PSCOCBDL was an anodic type corrosion inhibitor. The PSCOCBDL copolymer adsorption on the metal was shown to occur as chemisorption and fit the Langmuir adsorption isotherm. The AFM investigation denoted that PSCOCBDL inhibitor molecules are adsorbed on AISI 1020 steel surface and protect AISI 1020 steel against corrosion. The results acquired from the experiments agree with those of the theoretical study.

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