

Experimental and Computational Study of Trachyspermum Leaves Extract as a Green Inhibitor for Corrosion Inhibition of Mild Steel in HCl

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ABSTRACT: *The present study investigates the impacts of the extract of Trachyspermum leaves on mild steel corrosion in 0.1M hydrochloric acid (HCl) while highlighting its inhibitory mechanisms. The effects of mild steel corrosion in solutions of HCl were examined using gravimetric and galvanostatic polarization techniques, along with EIS analyses. The EIS data shows the highest coating undamaged index (83 %) after 100 hours of immersion. According to the results, the maximum inhibitory effectiveness corresponding to the minimum corrosion rate could be observed at the highest desirable level of inhibitor concentration equal to 100 ppm, while the corrosion rate decreases with an increase in the extract concentration. The adsorption study promotes that Langmuir isotherm with -31.85kJ/mol in room temperature with $R^2=0.95$ best describes the metal surface interaction with the Trachyspermum leaves extract with the best exposure time for the Trachyspermum to adsorb to the metal surface at all concentrations. SEM, AFM, IR, and XRD showed good coverage of Trachyspermum on the surface of mild steel. Based on the polarization results, the inhibitors can play the role of a mixed inhibitor, which is confirmed by the computational data. The chemical potentials of thymol, cymene, and terpinene are -6.55 , -6.91 , and -6.49 eV respectively.*

KEYWORDS: *Trachyspermum, Corrosion, Mild steel, Hydrochloric acid, Adsorption, Langmuir isotherm.*

INTRODUCTION

One of the important problems faced by various industries is the mild corrosion [1-3] of steel in acids, especially hydrochloric acid. Moderation of such adverse phenomena through the application of organic materials is essential to inhibit corrosion. The collective

work of different scholars has focused on developing efficient inhibitors to secure metallic materials against corrosion [4-6]. Research has shown that the direct and indirect costs of corrosion processes annually account for about 3-4% of the Gross Domestic Product (GDP)

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1021-9986/2023/10/3324-3337 14/\$/6.04

of developed countries. [5, 7]. Several major industrial processes, including steel pickling, oil wells acidification, ion exchanger regeneration, processing of leather, producing organic as well as inorganic compounds, and industrial cleansing use hydrochloric acid (HCl) solution [7-9].

The application of acid inhibitors in different industrial procedures is typically aimed at controlling metal corrosion [10-23], and the use of these inhibitors greatly reduces metal corrosion. [5, 24-28]. Hence, undesirable metal corrosion and acid consumption can be prevented, especially when an acid solution is used [29]. Many acid inhibitors belong to organic molecules, which contain oxygen, nitrogen, or sulfur atoms in a conjugated system, playing an efficient role as corrosion inhibitors. Different inhibitors with N group have been studied by researchers regarding their corrosion inhibitor properties for metals in acid media [30]. These studies show that organic inhibitors that contain N atom prevent metals corrosion in acid solutions [5, 31-35]. Different studies have investigated the effects of plant extracts as green inhibitors for corrosion. The researchers studied the effects of plant extracts because these compounds do not pollute the environment and are eco-friendly, inexpensive, and easy to obtain from nature. Research shows that products taken from nature [36] and coming from plants have different organic substances [5, 26-28] such as alkaloids [37], tannins [38], pigments [39], organic [40, 41] and amino acids [5, 42-44], making them suitable for their inhibitory effects [5, 31, 45-50]. This study aims to provide the *Trachyspermum* [51-60] extract and investigate its corrosion resistance as a corrosion inhibitor for mild steel using a solution of 0.1M HCl according to gravimetric assessments, electrochemical impedance spectroscopy, and potentiodynamic polarization assessments. It also studies the influence of the inhibitors' structural parameters on the effectiveness of the inhibition as well as the adsorption mechanisms on the surface of metal while correlating the experimental data with quantum chemical parameters.

One of the corrosion inhibitors, Ginger extract, which is extracted from natural resources, was previously studied to prevent the corrosion of mild steel in an acid solution. The work illustrates the reduction of corrosion from 8.09 mmpy to 0.72 mmpy in a solution without an inhibitor compared to a solution with 150g/L inhibitor

and inhibition efficiency of up to 91% [39]. In Addition, asafoetida as a corrosion inhibitor has been studied for the effect of inhibiting the corrosion of mild steel [61, 62]. In the other work, *Eruca sativa* seed extract as a green inhibitor was studied to show the inhibition effect for the dissolution of carbon steel in 1 M HCl solution. Excellent inhibition was obtained (94.8%) by a gravimetric method at 0.3 g/L from the extract [63]. The role of the leaf extract of *Pongamia pinnata* as a corrosion inhibitor for mild steel in 1N H₂SO₄ solution was studied by the potentiodynamic polarization, weight loss, and Electrochemical Impedance Spectroscopy (EIS) methods. The results of this work showed that the leaf extract of *Pongamia pinnata* has a good corrosion inhibitor effect for mild steel in 1N sulfuric acid, even in low concentrations of the inhibitor [64]. In this work, *Trachyspermum* leaf extract was studied as a green inhibitor for corrosion inhibition of mild steel in HCl, because of its ability to grow *Trachyspermum* in different places and its high effect of inhibiting the corrosion of mild steel.

EXPERIMENTAL SECTION

Preparation of the working electrode

A nominal (wt%) composition of Fe =97.84%, Mn =1.4%, P=0.045%, C =0.17%, N=0.009 % and Si=0.5%. was considered for the mild steel rod (a diameter of 1 cm) in the present work. For electrochemical studies, the mentioned steel samples were soldered to coated Cu-wires for electrical connections with a laid open zone of 1 cm². Mechanical abrasion of the working electrode surface was performed using various grades of emery paper, 600, 800, 1000, and 1500 before measurement. Then, distilled water was used along with acetone to rinse the samples of mild steel, after which drying was done using warm airflow.

Preparation of inhibitor solution and electrode

Distilled water was used to clean *Trachyspermum* leaves from fiery residues of mud. Leaf drying over a 48-74 h period in the thermostat with a temperature of 60 °C. The leaf powder was obtained by grinding 100 mg of dried leaf and then, followed by refluxing and shaking with a mixture of ethanol and water at a temperature of 75 °C over 24 hours. After filtering the refluxed product,

evaporation of the obtained solution was performed to 100 mL of dark brown residue followed by drying in a vacuum drying oven at 60 °C for 48 hours. Procurement of the light brown deposit (about 2.5g material) and its saving in a vacuum desiccator were the next steps. Dilution of the hydrochloric acid to 0.1M HCl was done for preparing the corrosion medium. The brown residue was diluted with 0.1 M HCl solution to obtain different concentrations of *Trachyspermum* leaf extract (30, 45, 70, 100 mg/L). The reagent grade, 37% HCl (from Sigma Aldrich), as well as distilled water, were used to prepare the corrosion solution (0.1M HCl). Different concentrations (30, 45, 70, 100 mg/L) were considered to prepare the inhibitor solution, leading to the highest *Trachyspermum* extract solvency in 0.1M HCl up to 500 mg/L.

Plant material

Leaves of *Trachyspermum* (*Trachyspermum ammi*) were purchased from the traditional herbal market, Tehran, Iran in June 2020. A voucher specimen has been deposited at the Herbarium of the Department of Pharmacognosy, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran (PMP-657).

Gravimetric measurements

Calculations of the mild steel samples were done according to ASTM G 31–72 to perform gravimetric measurements [65] for 24 hours at 298 K. After preparing 0.1M HCl acid blank solution which contained 30, 45, 70, 100 mg/L of the extract of *Trachyspermum* leaves, soaking of the pre-weighted metal samples in the prepared solution was carried out. Removal of the metal samples, deliberate rinsing with acetone, drying with nitrogen flow, and weighing to electronic balance were all performed after drenching. The experimental temperature was kept constant at 298 K, and three replicates were performed in the present work for high precision and accuracy.

Electrochemical measurements

Electrochemical measurements were performed using Emstate Electrochemical Workstation (Metrohm Autolab Nova2). The cell system, an easy three-electrode, contains a mild steel electrode, a platinum electrode, and a Saturated Calomel Electrode (SCE) as the working electrode, the counter electrode, and the reference electrode respectively. A working area of 1 cm² was considered

for the samples to perform electrochemical measurements. A stable Open Circuit Potential (OCP) was initially obtained by immersing the working electrode in the test solution for 1 h. The frequencies of 100 kHz to 0.01 Hz were considered to scan the Electrochemical Impedance Spectroscopy (EIS) considering a signal amplitude perturbation of 5 mV at OCP. Considering OCP at 1 mV/s scan rate, a scan of ± 250 mV against SCE was used to record the potentiodynamic polarization curves. Three replications of the electrochemical measurements resulted in reliable values.

Quantum chemical studies

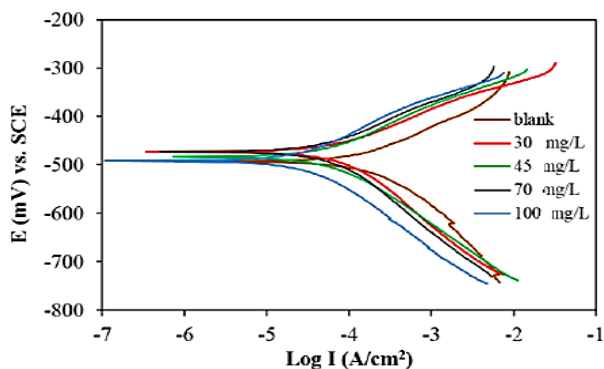
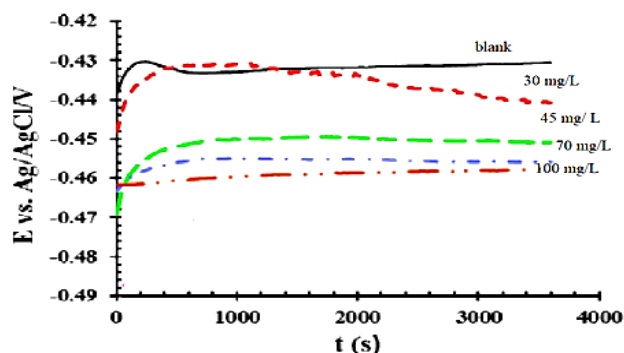
Quantum chemical estimations were performed using the density functional theory (DFT) at a B3LYP function considering 6–311G+ (d, p) basis set for molecules with Gaussian 03 project programming to examine the effects of inhibitor molecular structure as well as electronic features on the effectiveness of inhibition. The optimized structures in the gas phase were considered to obtain the main parameters such as the lowest unoccupied molecular orbital energy (E_{LUMO}), the highest occupied molecular orbital energy (E_{HOMO}), energy gap (ΔE) of the LUMO and HOMO, total energy (T.E.), electronegativity (χ), molecules softness (σ) as well as hardness (η), the energy distinction of the molecule electron exchange and dipole moment (μ), chemical potential (π), the number of transferring electrons (ΔN), etc. The use of the gas phase to perform theoretical estimations is supposed to be a suitable strategy as there are no significant differences in the results of the aqueous phase, while there is a significant decrease in the estimation time [66].

Surface morphology studies (SEM analysis)

The scanning electron microscope was used to observe the samples' surface morphology following the immersion of the pre-treated samples in 0.1M HCl solution in the absence and presence of 500 mg/L *Trachyspermum* leaves extract over 24 hours at 298 K. In order to obtain important information about the surface morphology of mild steel, the surface of the samples was washed with double distilled water and acetone and then dried. SEM instrument MIRA3TESCAN-XMU model with 3-30 kV was used for SEM morphology.

Table 1: Obtained electrochemical data using tafel curves for steel in 0.1M HCl considering various trachyspermum concentrations

C(mg/L)	E(mV)	i_{corr} ($\mu\text{A}/\text{cm}^2$)	β_a (mV/dec)	$-\beta_c$ (mV/dec)	%IE
0	-425	710	99	462	-
30	-459	339	56	310	76.3
45	-477	320	50	109	79.1
75	-483	312	43	214	82.4
100	-490	290	40	243	84.3

**Fig. 1: Tafel curves for steel in 0.1M HCl solutions in the absence and presence of different Trachyspermum concentrations following immersion for five minutes****Fig. 2: OCP of working electrode in 0.1M HCl solutions in the absence and presence of different Trachyspermum concentrations**

RESULTS AND DISCUSSION

Potentiodynamic polarization measurements

Polarization tests were recorded and some electrochemical parameters were attained from the polarization curves containing corrosion current density (i_{corr}), corrosion potential (E_{corr}), anodic and cathodic Tafel slopes (β_a , β_c), and inhibition efficiency (IE, labeled also as η). The IE was calculated using the following equation:

$$\eta(\%) = \frac{i_{corr} - i_{corr}^{(inh)}}{i_{corr}} \times 100$$

In which i_{corr} and $i_{corr}^{(inh)}$ represent the corrosion current densities in blank solution and 0.1M HCl consisting of inhibitor, correspondingly. Fig. 1 indicates the steel polarization plots, taken five minutes following immersion in blank solution and 0.1M HCl consisting of inhibitor. Fig. 2 showed the OCP diagram of the electrode. Table 1 shows the obtained electrochemical data, according to which the greatest IE for both inhibitors can be observed at the maximum concentration of 100 mg/L after 5 minutes of immersion.

When the shift in the E_{corr} is less than 85 mV due to the inhibitor presence, the inhibitor will belong to the mixed-type inhibitor [67, 68], while it will be cathodic or anodic based on the shift direction in other conditions. As the E_{corr} shift was less than 85 mV in this research, the molecule belonged to the mixed-type inhibitor. Nevertheless, as shown in Fig. 1, Trachyspermum functions as a mixed-type inhibitor when it is immersed for five minutes. Meantime, Trachyspermum affected cathodic and anodic reactions significantly. According to Table 1, It is seen that the decrease in i_{corr} value is associated with the increase in Trachyspermum concentration, which indicates that Trachyspermum has very active inhibitory properties.

Electrochemical impedance spectroscopy

The Nyquist plots and Bode plots associated with the mild steel in 0.1M HCl solutions are shown in Figs. 3 and 4 in the absence and presence of different inhibitor concentrations following immersion for five minutes. The EIS results were fitted with the equivalent circuit in Fig. 5, in which R_s , R_{ct} , and CPE indicate solution resistance, charge transfer resistance, and the constant phase element, correspondingly. Fig. 3 indicates an increase in the semicircle diameter based on the increase in inhibitor concentration indicating that inhibition efficiency increases with inhibitor concentration. Table 2 indicates Impedance data collected through the test, and the equation below was used to calculate the IE (η):

$$\eta(\%) = \frac{R_{ct}^{(inh)} - R_{ct}}{R_{ct}^{(inh)}} \times 100$$

Table 2: Impedance data were collected using EIS tests for steel in a blank solution and 0.1M HCl considering various concentrations of inhibitors following 5 minutes

C(mg/L)	$R_{ct}(\Omega.cm^2)$	$R_p(\Omega.cm^2)$	CPE($\mu F.cm^2$)	n	$\eta\%$
Blank	242	0.60	94.5	0.842	-
30	785	1.35	76.2	0.854	71
45	940	1.49	62.1	0.868	75
70	1075	1.55	49.01	0.875	78.5
100	1248	1.70	44.0	0.892	83

Table 3: Comparative inhibition effect of several green inhibitors

Green inhibitor	$\eta\%$
This study (100 mg/L)	80 %
Camphor (600 mg/L)	89 %
Magnolia grandiflora (500 mg/L)	85 %
Primrose flower (700 mg/L)	80 %

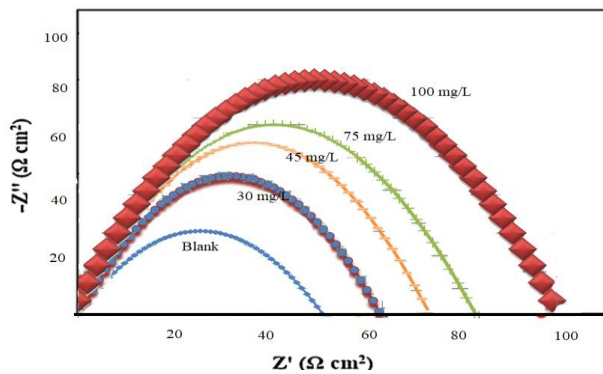


Fig. 3: Nyquist plots obtained for mild steel in 0.1M HCl solution in the absence and presence of different Trachyspermum concentrations

According to Table 2, the R_{ct} values face an increasing trend based on the inhibitor concentration after immersing for five minutes. However, there is a general reduction in the CPE values, reflecting an increasing trend in corrosion inhibition. The reduction of CPE is related to the increment in the protective layer thickness or decline in the local dielectric constant (D) [69]. The findings show similarities between the results obtained by EIS investigations and polarization measurements. Both sets of results indicate that the corrosion inhibition of Trachyspermum is higher, and the highest inhibition of this inhibitor is observed at the concentration of 100 mg/L. The capacitance values of the double-layer were calculated by EIS data $124.8 \times 10^{-5} \mu F/cm^2$ for a concentration of 100mg/L. The comparison between the inhibition effect for Trachyspermum and the other three green inhibitors shows in Table 3.

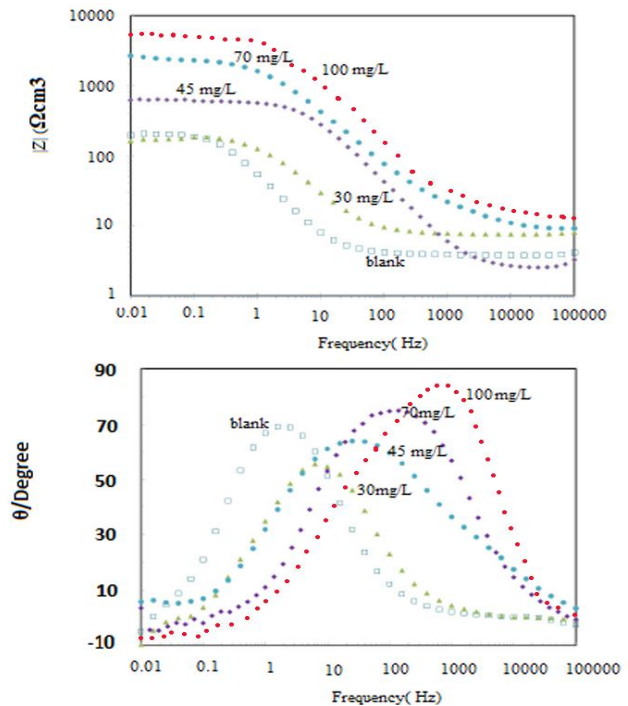


Fig. 4: Bode plots of the for mild steel in 0.1M HCl solution in the absence and presence of different Trachyspermum concentrations

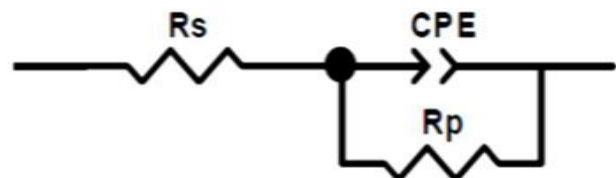


Fig. 5: An electrical equivalent circuit illustration was employed for the analysis of results

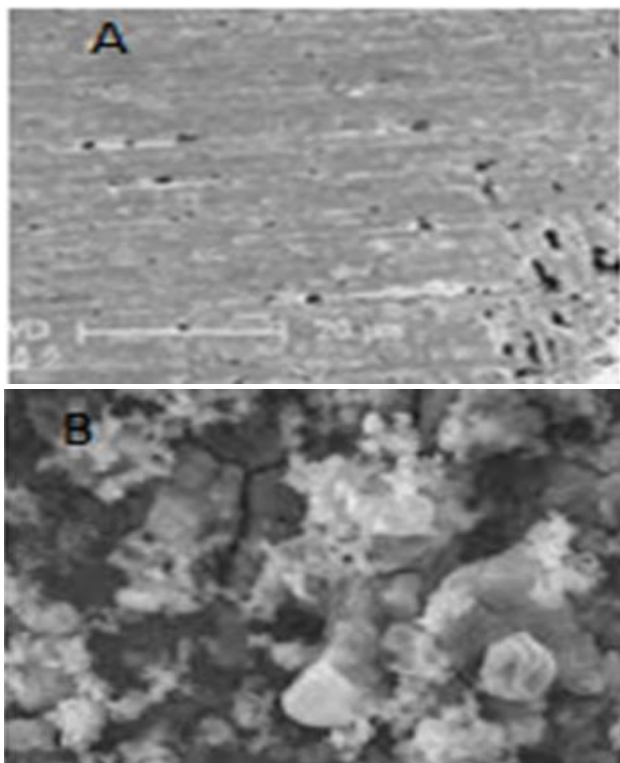


Fig. 6: SEM images for (A) steel samples two hours following immersion in blank solution 0.1M HCl; (B) steel samples two hours following immersion in 100mg/L of Trachyspermum

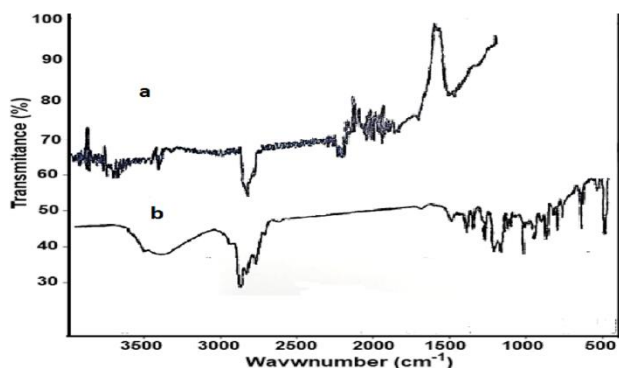


Fig. 7: IR spectrum for (A) steel samples two hours following immersion in blank solution 0.1M HCl; (B) steel samples two hours following immersion in 100mg/L of Trachyspermum

In which $R_{ct}^{(inh)}$ and R_{ct} reflect the charge transfer resistance in the inhibited as well as uninhibited system, correspondingly. The electrical equivalent circuit fitted to experimental results and its fitness is 93%.

Surface morphology

The SEM images of the freshly polished steel specimens and those soaked in 0.1M HCl after two hours

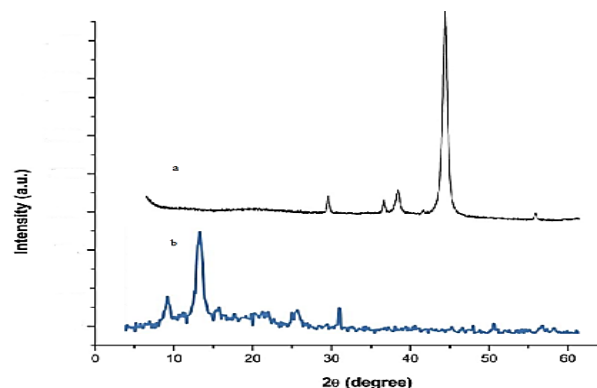


Fig. 8: XRD pattern for (A) steel samples two hours following immersion in blank solution 0.1M HCl; (B) steel samples two hours following immersion in 100mg/L of Trachyspermum

in the absence and presence of inhibitors (100 mg/L Trachyspermum) are displayed in Fig. 6. The damage and pits occur in the absence of an inhibitor, but there is a significant reduction in the damage and pits resulting from corrosion when a 100mg/L inhibitor is added. A protective layer is created on the steel by the inhibitor, preserving it against corrosive attack resulting in the lesser black holes. Besides, as shown in Fig. 6, when Trachyspermum is present, there are no black pits or holes, reflecting that Trachyspermum has better corrosion-inhibitory effects. The findings are completely in line with the data collected through electrochemical measurements. According to the SEM picture Fig. 6(B), the inhibitor covered the whole surface of the steel, and the corrosion site in Fig. 6(A) was covered completely.

XRD pattern and IR spectrum, and AFM analysis show the surface changes after using Trachyspermum. As an inhibitor, the coverage of the surface by Trachyspermum can be found exactly in Figs. 7 to 9. By the IR spectrum, the recognition of the presence of the organic compound on the surface of mild steel after adding the 100 mg/L of Trachyspermum can be confirmed. The sharp and strong peak in 2800 cm^{-1} can refer to the CH Stretching bond of alkyl groups of compounds (Fig 7b). Also, the strong peak in 3500 cm^{-1} illustrates the OH bond of Hydroxyl groups of thymol.

XRD pattern illustrated in Fig. 8 can show the change of mild steel components. As the XRD pattern showed, many compounds changed the composition of mild steel after immersion in Trachyspermum solution. Omitting the peak in $\theta=45^\circ$ for Fig. 8(b) can show the covering of the metal surface.

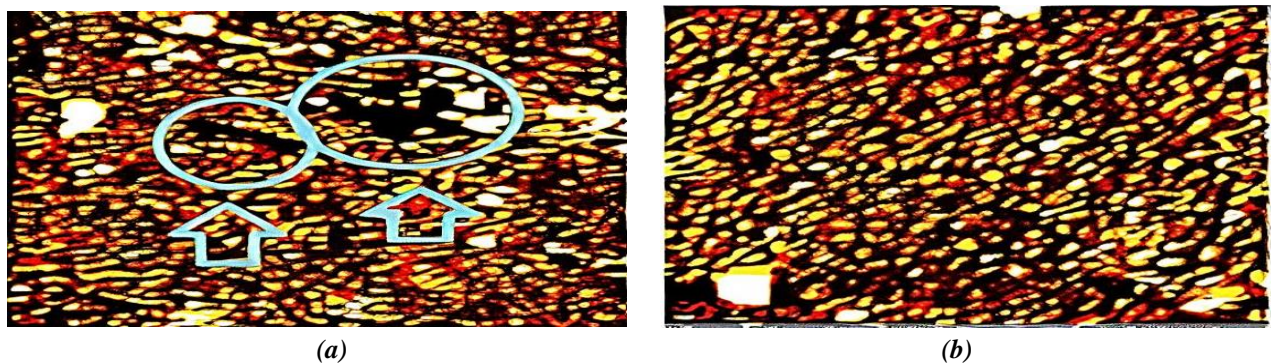


Fig. 9: AFM images for (A) steel samples two hours following immersion in blank solution 0.1M HCl; (B) steel samples two hours following immersion in 100mg/L of Trachyspermum

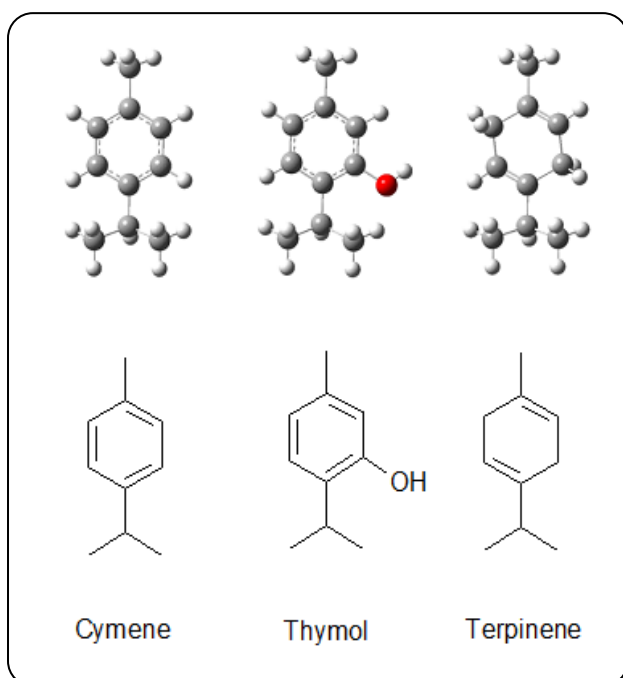


Fig. 10: Structures of important materials in Trachyspermum

AFM imaging is a method of examining surface roughness. Fig. 9 shows the surface of mild steel after 2 hours of immersion in a solution of Trachyspermum extract. As Fig. 9 shows, in the absence of Trachyspermum (HCl 0.1M solution), the mild steel surface has too much roughness and many cuts on the surface, which are covered after immersion in the Trachyspermum solution. The compounds in the Trachyspermum extract solution cover the rough surface of the corrosive mild steel. The roughness of the mild steel surface is about 15.2 micrometers before adding Trachyspermum and after adding Trachyspermum changed to ≈ 3 micrometers. In Fig. 9(a) we can see the black area that refers

to the corrosion surface and in Fig. 9(b) we can see that the same area in part (a) is covered, therefore the AFM shows the inhibition act by Trachyspermum.

Quantum calculation

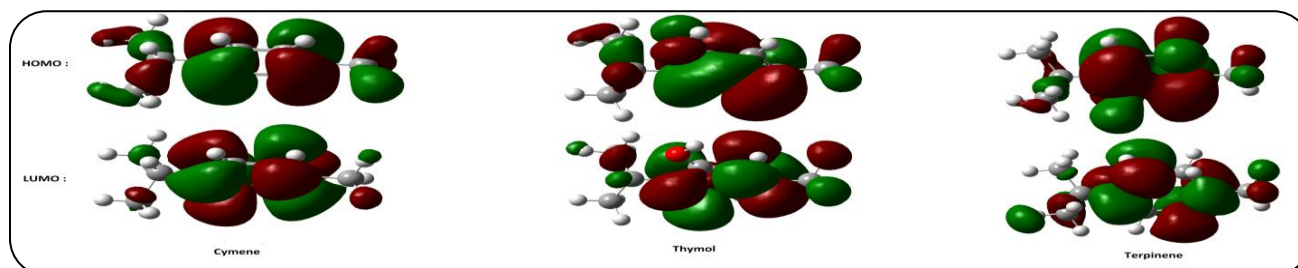
Quantum chemical calculations of electronic parameters and their correlation with the experimentally measured corrosion inhibition efficiency are the most used approach in the corrosion inhibitor studies. Quantum chemical estimations were performed using the Density Functional Theory (DFT) at a B3LYP function considering 6-311G+ (d, p) basis set for molecules with Gaussian 03 project programming to examine the effects of inhibitor molecular structure as well as electronic features on the effectiveness of inhibition (Fig 10). The optimized structures in the gas phase were considered to obtain the main parameters such as the lowest unoccupied molecular orbital energy (E_{LUMO}), the highest occupied molecular orbital energy (E_{HOMO}), energy gap (ΔE) of the LUMO and HOMO (Fig 11), total energy (T.E.), electronegativity (χ), molecules softness (σ) as well as hardness (η), the energy distinction of the molecule electron exchange and dipole moment (μ), chemical potential (π), the number of transferring electrons (ΔN), etc. The use of the gas phase to perform theoretical estimations is supposed to be a suitable strategy as there are no significant differences with the results of the aqueous phase, while there is a significant decrease in the estimation time. Tables 4 and 5 contain information on the energy gap (ΔE), chemical potential (μ), electrophilicity (ω) as well as global hardness (η) of Trachyspermum compounds (Cymene, Thymol, and Terpinene), all of which have been studied in corrosion inhibition research. A critical discussion of the application

Table 4: Some chemical parameters of materials in Trachyspermum

	Thymol	Cymene	Terpinene
E gas(HF)	-464.4051	-389.2362	-390.3000
E water(HF)	-464.6329	-389.4536	-390.5514
μ gas(D)	1.9435	0.0461	0.0691
μ water (D)	2.3923	0.0905	0.1183
HOMO(HF)	-0.3226	-0.3426	-0.3118
LUMO(HF)	-0.1582	-0.1645	-0.1648
H(HF)	-464.4041	-389.2247	-390.2990
G(HF)	-464.4457	-389.2736	-390.3418

Table 5: Molecular electronic parameters(eV) of materials in Trachyspermum

	Thymol	Cymene	Terpinene
IP	8.79	9.34	8.49
EA	4.31	4.48	4.49
χ	6.55	6.91	6.49
μ	-6.55	-6.91	-6.49
σ	0.45	0.41	0.5
η	2.24	2.43	2.00
ω	9.57	9.82	10.53
ΔE	-4.48	-4.86	-4.00

**Fig. 11: The HOMO and LUMO for cymene, thymol, and terpinene**

of this methodology has been provided in another study; it is not possible to provide a straightforward explanation of the corrosion inhibition efficiency just by the use of quantum chemical parameters, reflecting the importance of the nature of the inhibitor effects on the surface. The obtained results represent the estimated electronic parameters along with the relevant discussions on the inhibitors under study. As shown by the specification of the electronic features of isolated molecules, Trachyspermum can play the most efficient role, supported by the experimental data of this study.

Weight loss

The inhibition degree of surface coverage (θ) at each concentration of Trachyspermum was calculated by

comparing the corrosion loss in the absence (W_u) and presence of inhibitor (W_i) using the relationships:

$$\eta(\%) = \frac{W_u - W_i}{W_i} \times 100$$

$$\theta = \frac{W_u - W_i}{W_i}$$

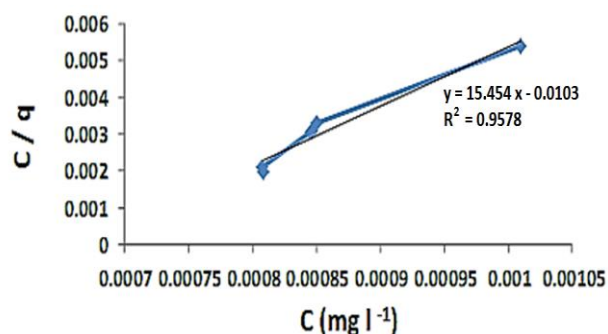
The increased efficiency observed for the inhibition based on the concentration can be explained by considering the extent of adsorption of the inhibitor molecules on the metal surface. It is supposed that the formation of the film by the inhibitor molecule adsorption on the surface of the metal is the only criterion to lower the surface area of the cathodic and anodic reactions. At any instant, a fraction (θ)

Table 6: The surface coverage area of mild steel in 0.1M HCl containing Trachyspermum for 24 hours

C(mg/L)	0	30	45	70	100
θ	0.7750	0.8210	0.8536	0.8625	0.8954

Table 7: Results of Langmuir adsorption for investigated inhibitors on the steel in 0.1M HCl were obtained from polarization and EIS

Inhibitor	method	R ²	K _{ads} (M ⁻¹)	ΔG°_{ads} (kJ/mol)
Trachyspermum	polarization	0.9578	2225	-32.2
Trachyspermum	EIS.	0.9586	1851	-31.85

**Fig. 12: Langmuir adsorption plots of Trachyspermum on the steel in 0.1M HCl were obtained from the polarization results**

of the metal surface is covered by the inhibitor molecules and the uncovered fraction ($1-\theta$) reacts with acid as it does in the absence of the inhibitor. It is possible to deduce the inhibitor adsorption features according to the nature of the inhibitor interaction with the corroding surface. The adsorption features can be also explained using the values of the surface coverage (Table 6).

Adsorption isotherm

In general, it is possible to explain the adsorption behavior of inhibitors using adsorption isotherms, indicating critical information on the interactions between metals and inhibitors [70]. As shown by simplifying assumptions, inhibition efficiency can be considered proportional to surface coverage [71]. Examination of Frumkin, Temkin, and Langmuir adsorption isotherms as well as the El-Awady kinetic-thermodynamic model [72] aims at fitting the inhibitors' adsorption. Fig. 12 shows the curve with a good fitness to Langmuir adsorption isotherm obtained using the equation below [73]:

$$\frac{C}{\theta} = \frac{1}{k_{ads}} + C$$

In which, K_{ads} , C , θ , indicate the equilibrium constant used in the adsorption process, the inhibitor's molar concentration, and the surface coverage, respectively.

The equation below was used to calculate the free energy of adsorption (ΔG°_{ads}) [74]:

$$\Delta G^{\circ}_{ads} = -RT \ln (55.5 K_{ads})$$

In which, T and R represent the absolute temperature and universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), respectively, while water molar concentration is considered to be 55.5. When ΔG°_{ads} has a value ranging from -20 to -40 kJ/mol , there is evidence of both physical and chemical adsorption types [75-79]. Table 7 indicates the values of ΔG°_{ads} (-32.2 and -31.85) which shows that both types of chemical and physical adsorption occur.

CONCLUSIONS

Evidence showed that the extract obtained from Trachyspermum had inhibitory effects on mild steel using HCl, while there was an increase in the inhibitory efficacy as the extract concentration increased. The highest value of inhibitory effectiveness was 98%, obtained at a concentration of 100 ppm. Based on the Potentiodynamic polarization curves, the extract of Trachyspermum leaves could be considered a mixed inhibitory agent. The adsorption isotherms follow the Langmuir adsorption isotherms. According to the EIS data, the highest coating undamaged index (83 %) was obtained after 100 h of immersion. According to the results, the maximum inhibitory effectiveness corresponding to the minimum corrosion rate could be observed at the highest desirable level of inhibitor concentration equal to 100 ppm, while the corrosion rate decreases with an increase in the extract concentration. The absorption examinations indicated the best description of the metal surface interaction by Langmuir isotherm with -31.85 KJ/mol , while obtaining the best exposure time for the Trachyspermum leaves extract adsorption into the surface of the metal in different concentrations. SEM, AFM, IR, and XRD showed good coverage of Trachyspermum on the surface of mild steel. Based on the polarization results, Trachyspermum can play the role of a mixed inhibitor, which is also confirmed by the computational data.

Acknowledgments

The authors gratefully acknowledge the financial support from the Research Council of Islamic Azad University Kerman branch.

Received : Dec.19, 2022 ; Accepted : Apr.3, 2023

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