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1186

Evaluation of *N*-piperazinyl-2-furanylketone as a corrosion inhibitor for mild steel in 1 M HCl solution: Combined experimental and theoretical approach

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Abstract

Steel corrosion in acidic environments, poses a formidable challenge with conventional inhibitors, often burdened by issues of toxicity, and environmental impact. This study, addresses this challenge, by investigating the suitability of *N*-piperazinyl-2-furanylketone (NPF) as a green inhibitor for mild steel in 1 M HCl, employing a combined experimental and theoretical approaches. NPF demonstrated an outstanding inhibition efficiency of 93.6% under optimal conditions with an inhibitor concentration of 0.5 mM, at 303 K, showcasing its potential as an environmentally friendly alternative. The efficacy of NPF aligns well with the Langmuir adsorption isotherm indicating a robust and specific interaction between NPF molecules and the steel surface. Further analysis revealed a positive correlation between inhibition efficiency and both immersion time and temperature, suggesting a gradual formation of a protective film on the metal surface. It is worth noting that increasing the temperature enhanced the effectiveness of the tested inhibitor, indicating a thermally activated adsorption process. Theoretical

calculations using density functional theory (DFT) supported the experimental results and provided insight into the molecular interactions at the interface. The calculated electron transfer parameter highlighted the positive interaction between NPF and iron atoms enhancing the observed inhibition mechanism. The study, giving the energy of NPF to be green inhibitor corrosion, among others, depicts a very effective method that can be used for evaluating the mechanism and efficacy of these ecofriendly alternatives. Besides synthetic applications studies can also be designed on real world scenarios hence, also capable of optimizing the performances of NPF for bulk industrial productions.

1. Introduction

Although mild steel may not have the highest strength, formability or its relatively low cost profile, it is definitely in a class of its own and in most, if not all applications in modern industries. In the most simplistic sense, it encompasses telegraph poles and door frames, artistic representations and engineering marvels, and many such varied yet vital implementations. However, this versatility comes with a caveat: a largely corrosion-prone metal, especially in strenuous conditions being factors. Listen to the different molecules flying through space. Nowhere else is the vulnerability of such IT solutions more apparent than in the devices that use 1 M HCl that are prone to the almost non-stop interplay of chemical and electrochemical processes that work in the background and lead to a decay of regolith [1–5]. The effects of steel decay are not mainly visual, but rather than would be impossible to heal the economy as well as the environment. On the economic side, the world is facing a yearly cost of corrosion of an unbelievable \$2.5T which is about 50%, and this cost hits various industries, such as construction, transportation, energy and manufacturing, which are the expense of governments and property. This cost takes into account both direct costs such as that of replacing corroded infrastructure or repairing damaged equipment; and indirect expenses such as that of implementing preventative measures. Yet, there is more than just that difficult financial impact [6–8]. Corrosion being one of the major players of degradation has huge adverse effects on the public safety as well as environment quality. Worn out bridges loosens the integrity of a structure which may trigger an immediate downfall and may prevent vital transportation services as well. Leaking pipes cause polluted soils and running waters, which entails health issues and natural resources damage. The trivialization of the following consequences show the prompt necessity to find proper and effective ways to prevent the corroding of these steels in those critical applications or the environment that is aggressive. Conventional corrosion inhibitors have been the center of attention with regards to abating the associated challenges. Through this means, these coatings act in two ways, meaning they can form a protective film on the steel surface or alter the corrosive nature of the environment, thereby prolonging the life of assets.

Nevertheless, most of the conventional inhibitor classes come with drawbacks as well. They can be extremely detrimental, since they are closely related to oxidative stress, health risks, and the environment. Yet, some of them have limited reliability and require a sufficient amount, which signifies the higher cost and may end up with the wrong properties of the final product [12−17]. Nowadays, the market is highly concerned about environmentally-friendly solutions, and therefore, the manufacturers are more eager than ever to come up with eco-friendly technologies. The emergence of bio-based "gray" corrosion inhibitors, that is, corrosion protectors, made from non-toxic materials and which are easily available, could be the best alternative. Such inhibitors have a capacity not only for effective corrosion hindrance but also for environmental issue and toxicity mitigation [18−23]. Being blessed with the structure similar to the one in Figure 1 and being supported by the successful preliminary test, NPF may become the new star on the environmental friendly and effective protection against mild steel degradation in 1 M HCl where tin(II) chloride is not a good choice. This study is based on a dual experiment and theoretical strategy to deepen the research into the inhibition mechanism of NPF and to evaluate its [validity to be] considered as an environmentally sustainable solution for the protection of a high-value steel asset on poisonous environments.
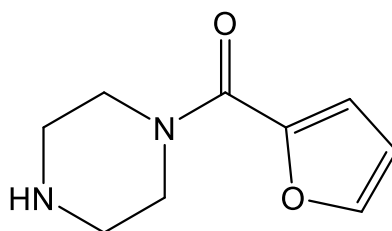
Figure 1. NPF molecular structure.

For long enough, we've been dismantling the steel corrosion in the acidic areas, essentially with the help of typically-used traditional inhibitors. Every one of them comes with the particular advantage, but it only does the good to a certain extent, as the limitations are there. Inorganic options, while inexpensive and readily available, often contain chromates or phosphates, raising toxicity concerns and environmental worries. Stricter regulations further limit their use [24−27]. Organic inhibitors offer greater structural diversity catering to specific environments and some even form protective films. However they can be expensive susceptible to harsh conditions and their effectiveness varies significantly with structure and media composition [28−35]. Surfactant-based inhibitors come with good adsorption and surface coverage sometimes even working synergistically with other inhibitors. Yet their effectiveness is often limited by specific pH ranges can interfere with desired product properties and some raise environmental concerns [36−38]. These limitations become even more prominent when considering the broader impact. The toxicity of chromates and some organic compounds poses health and environmental risks [39, 40]. High costs for specific inhibitors limit their widespread adoption and the limited effectiveness of some in specific environments or at varying temperatures and concentrations

restricts their versatility. These drawbacks have fueled the growing interest in "green" inhibitors. Driven by environmental regulations and sustainability mandates they offer a promising alternative [41–48]:

- Environmentally friendly: Made from readily available renewable resources minimizing environmental impact and toxicity concerns.
- Cost-effective: Often derived from natural sources or synthesized using sustainable methods offering lower production costs.
- Broader applicability: Some green inhibitors demonstrate effectiveness across wider pH ranges and temperatures expanding their potential uses.

The search for effective and sustainable solutions pushes the boundaries of inhibitor development. NPF and its unique structure and early promise represents one such exploration. Investigating its potential as a green inhibitor for mild steel in 1 M HCl aligns with the growing need for environmentally friendly and effective solutions to combat corrosion. This research aims to investigate NPF's performance as a corrosion inhibitor using a combined experimental and theoretical approach. We aim to quantify its inhibition efficiency at different concentrations immersion period and temperatures and elucidate its adsorption behavior on the steel surface in addition to understand the theoretical model of NPF-metal interaction using density functional theory (DFT) calculations. This endeavor could pave the way for a new generation of green inhibitors ensuring a future where protecting our infrastructure and environment go hand in hand.

2. Experimental Methodology

2.1. Materials and reagents

High-quality 37% HCl solution was diluted with double-distilled water to prepare a 1 M HCl solution. The NPF inhibitor obtained from Sigma Aldrich Malaysia was diluted in this 1 M HCl solution to achieve concentrations ranging from 0.1 to 1.0 mM.

2.2. Sample preparation

Mild steel samples underwent X-ray fluorescence spectrometry analysis to determine their chemical composition which was C: 0.21%; S: 0.05%; Mn: 0.05%; Si: 0.38%; P: 0.09%; Al: 0.01%; Fe: balance. Following the ASTM G1-03 protocol these samples were prepared and polished with silicon carbide grits (120 600 and 1200). Before immersion the mild steel coupons were meticulously cleaned with double-distilled water and acetone followed by drying in an oven [49, 50].

2.3. Weight loss measurements

Coupons were immersed in 400 mL of 1 M HCl solution containing varying NPF concentrations (0.1–1 mM) within 500 mL glass beakers. Experiments were conducted at 303 K in a water bath adhering to the NACE TM0169/G31 protocol. Exposure times

included one hour five hours ten hours and twenty four hours in addition to forty eight hours. After each exposure corrosion products were carefully removed from the surface before drying and weighing the coupons. The weight loss (W) and surface area (a) were used to calculate the corrosion rate (C_R) using Equation 1 [50, 51]:

$$C_R \left(\text{mg} \cdot \text{cm}^{-2} \cdot \text{h}^{-1} \right) = \frac{\Delta W}{at} \tag{1}$$

where C_R is the corrosion rate, ΔW is the specimen weight before and after immersion (mg), a refers to surface area of the exposed metal sample (cm²) and t signifies exposure time (h).

The corrosion rates in the absence and presence of the inhibitor, denoted as C_{R0} and C_{Ri}, respectively, were used to determine the inhibition efficiency (*IE*) according to Equation 2:

$$IE\left(\% \right) = \left[\frac{C_{R0} - C_{Ri}}{C_{R0}} \right] \cdot 100 \tag{2}$$

Surface coverage (θ) for both uninhibited and inhibited solutions was calculated using Equation 3:

$$\theta = 1 - \frac{C_{Ri}}{C_{R0}} \tag{3}$$

To analyze the temperature dependence, coupons were immersed in inhibitor solutions at varying temperatures (303–333 K). Triplicate measurements were performed for each condition, and the average corrosion rate was calculated.

2.4. Adsorption isotherm studies

Langmuir, Temkin, and Frumkin (Equations 4–6 respectively) isotherms were employed to assess the extent of inhibitor coverage on the metal surface. Weight loss measurements were conducted at various inhibitor concentrations to determine the surface coverage [52–54].

$$\theta = K_{ads} \cdot \frac{C}{\left(1 + K_{ads} \cdot C \right)} \tag{4}$$

$$\theta = a \cdot \exp\left(b \cdot \ln\left(K_{ads} \cdot C \right) \right) \tag{5}$$

$$\theta = K_{ads} \cdot C \cdot \exp\left(-\alpha \cdot \theta \right) \tag{6}$$

where θ is the surface coverage fraction (0≤θ≤1), K_{ads} is adsorption equilibrium constant (L/mol), C: inhibitor concentration in bulk solution (mol/L), a is pre-exponential factor, b is constant related to heat of adsorption, and α refers to interaction parameter.

2.5. DFT calculations

Quantum chemical calculations were conducted using ChemOffice software. Gaussian 09 Revision C.01 software was employed for DFT calculations, utilizing the B3LYP method and the 6-31G^{++}(d,p) basis set [55]. The inhibitor structure was optimized in its neutral form. Koopmans theory, along with Equations 7 and 8, was used to determine the ionization potential (*I*) and electron affinity (*A*) [56, 57]:

$$I \text{ (eV)} = -E_{HOMO} \tag{7}$$

$$A \text{ (eV)} = -E_{LUMO} \tag{8}$$

Equations 9−11 were used to calculate the electronegativity (χ), hardness (η), and softness (σ):

$$\chi = \frac{I+A}{2} \tag{9}$$

$$\eta = \frac{I-A}{2} \tag{10}$$

$$\sigma = \frac{1}{2\eta} \tag{11}$$

The electron transfer (ΔN) was evaluated using Equation 12, considering the Fe electronegativity of 7 eV and hardness of 0 eV:

$$\Delta N = \frac{\left(\chi_{Fe} - \chi_{inhibitor}\right)}{2\left(\eta_{Fe} + \eta_{inhibitor}\right)} \tag{12}$$

3. Results and Discussion

3.1. Concentration effect

The investigation explored the impact of inhibitor concentration on the corrosion rate of mild steel in a hydrochloric acid solution, particularly focusing on a 5-hour immersion period. In the absence of the inhibitor, the corrosion rate was found to be high, indicating the aggressive nature of the environment. However, upon introducing the inhibitor, a significant reduction in the corrosion rate was observed, suggesting its effectiveness in inhibiting corrosion. Figure 2 depicts the influence of various concentrations of NPF on the weight loss of mild steel after a 5-hour immersion in a 1.0 M HCl solution at 303 K. This data highlights the corrosion inhibitory effects of NPF under these specific conditions. The figure clearly demonstrates the inverse relationship between inhibitor concentration and the corrosion rate of mild steel. Lower concentrations (0−0.4 mM) result in a gradual reduction in corrosion rate, attributed to enhanced adsorption of inhibitor molecules on the mild steel surface, leading to improved surface coverage [58−61]. As the inhibitor concentration increases

beyond 0.5 mM, a more pronounced decline in the corrosion rate is observed, accompanied by a remarkable increase in inhibitive efficiency. At concentrations of 0.5 and 1.0 mM, the corrosion rate is significantly suppressed, reaching values of 0.33 mg·cm^{-2}·h^{-1} and 0.31 mg·cm^{-2}·h^{-1}, respectively. The observed trend is consistent with the expected behavior of corrosion inhibitors, wherein higher concentrations lead to greater adsorption and the formation of a protective layer on the metal surface. The significant increase in inhibition efficacy reaching 93.6% and 94.1% at 0.5 and 1.0 mM concentrations respectively which confirms the notable efficiencies of tested inhibitor in mitigating corrosion of mild steel in HCl [45–62].
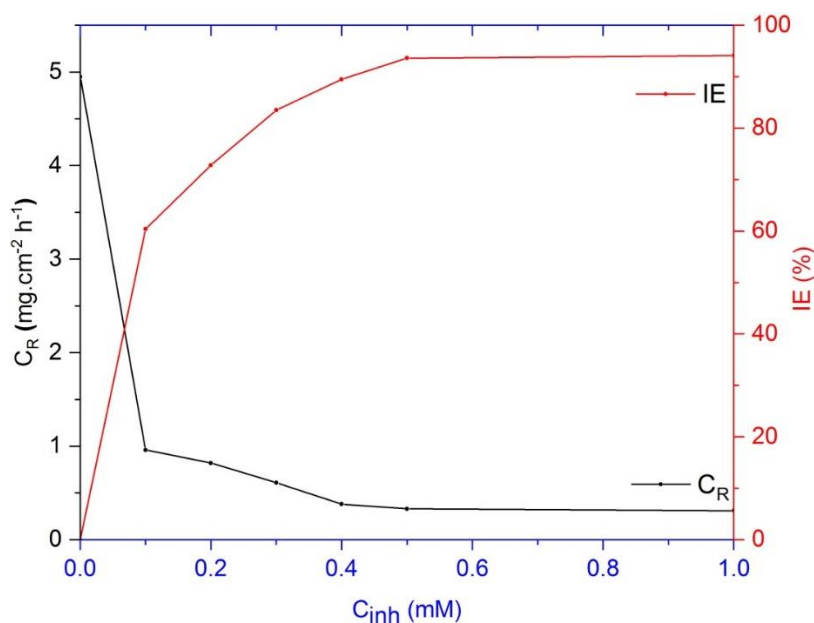

Figure 2. NPF concentrations impacts on the corrosion rate and inhibition efficacy of mild steel in a 1.0 M HCl solution after five hours immersion time at 303 K.

3.2. Effects of immersion time

The research focused on understanding how immersion time affects the corrosion behavior of mild steel in a 1.0 M HCl solution providing important insights into weight loss inhibitory effectiveness and surface coating. Figure 3 provides a visual representation of changes in mass loss over different exposure periods highlighting the dynamic nature of the corrosion process [66–68]. Examining immersion times ranging from 1 to 48 hours yielded a comprehensive view of corrosion development on mild steel when exposed to the NPF inhibitor. As shown in Figure 3 there is a consistent decrease in the corrosion rate with longer exposure times indicating a continuing effect of the inhibitor in reducing the exposure of the metal to corrosion over long periods. Inhibited samples showed reduced weight loss compared to those without inhibition demonstrating the protective role of NPF. The inhibitory effectiveness expressed as percentage reduction in corrosion rate showed an exact relationship with immersion time. While there was a slight increase in inhibitory effectiveness with longer exposure times across all inhibitor concentrations it is important to

note that prolonged exposure can also lead to gradual depletion or desorption of inhibitor molecules due to complex interactions with the mild steel surface [69−71]. It is worth noting that at the optimal inhibitor concentration of 5 mM the inhibition efficiency reached 93.6% after 5 hours of immersion. The highest inhibition activity of 97.5% was observed after 48 hours of immersion with 1.0 mM NPF concentration. Beyond a concentration of 1.0 mM there was no significant difference in inhibition activity within the range tested indicating a possible saturation effect. This trend suggests that NPF exhibits sustained inhibitive performance over prolonged exposure periods, making it a promising corrosion inhibitor for mild steel in aggressive acidic environments [72−75]. Overall, the study show that the inhibitor concentration is very crucial in determining inhibiting ability and the possibility of NPF to be a prospective corrosion inhibitor of mild steel in acidic planetary environments.
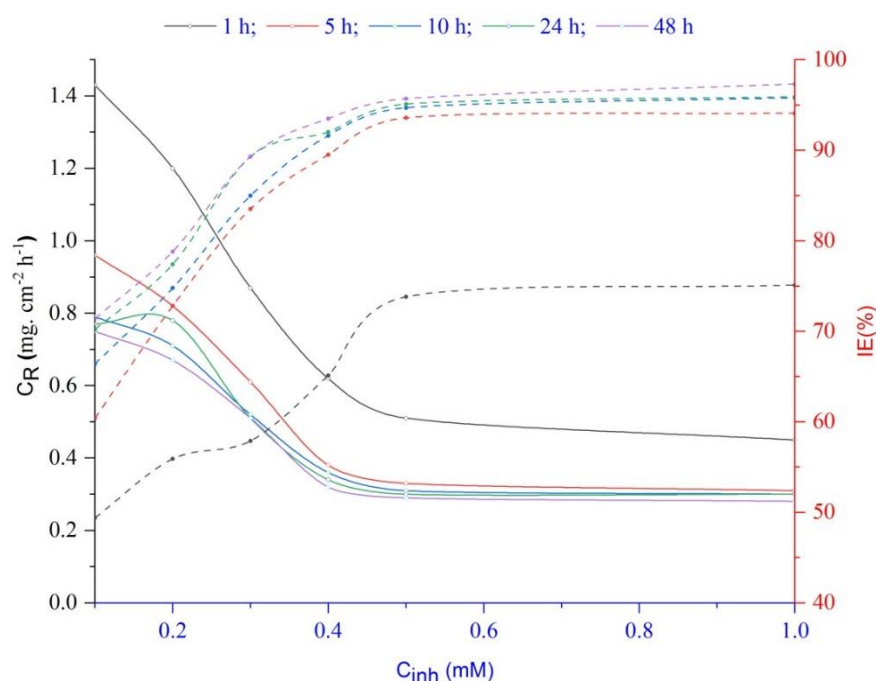

Figure 3. The influences of NPF variability on the corrosion rate and the efficiency inhibition of mild steel exposed to a 1.0 M HCl solution comprising different time periods and a constant temperature of 303 K.

3.3. Effect of temperature

The following study was pertinent to determining how temperature influences the corrosion rate and the efficiency of inhibitors on the mild steel in a solution of 1.0 M HCl. Figure 4 presents the results that were found and demonstrating the separated path for the corrosion process in different temperatures environments. Analyzing the impact of temperature on corrosion behavior reveals an interesting trend: the more temperature decreases, the faster the corrosion is to be observed, as it is demonstrated in Figure 4. That is the case with increased chemical interactions, oxygen solution and better oxygen absorption capacity at higher temperatures, a corrosion favorable reaction goes smoothly [76−78]. Nonetheless,

this effect also affects the very efficiency of inhibition as increased temperature goes hand in hand with negative correlation. As the temperatures goes up, the dynamic energy for inhibitor increases as well which may have an effect on those molecules that form the protection paste on the mild steel and make it less protective to the steel. A such, the fiber-optic installation process is complex as the effect or the metal surface temperature varies with the temperature and energy landscape is sensitive to that [79]. Yet, the inhibition efficiency gradually decreases overall, but an intriguing circumstance should be noted concerning the impact of temperature at 10 hours immersion time with 1.0 mM inhibitor concentration – here, the inhibition efficiency rises to 96.4% at 333 K from mere 94.3% at 303 K, demonstrating the interplay between the temperature, As the final words, the impact of temperature on the corrosion properties of mild steel inside an HCl solution is not-single-handed. The method would lead to slag plasticity by modifying chemical interactions with the environment and by concurrently adjusting inhibitor activity. This evidence highlights the importance of carefully assessing the temperature conditions in the corrosion resistance evaluation, as it can, among other things, lead to the dispersion of various corrosion processes.
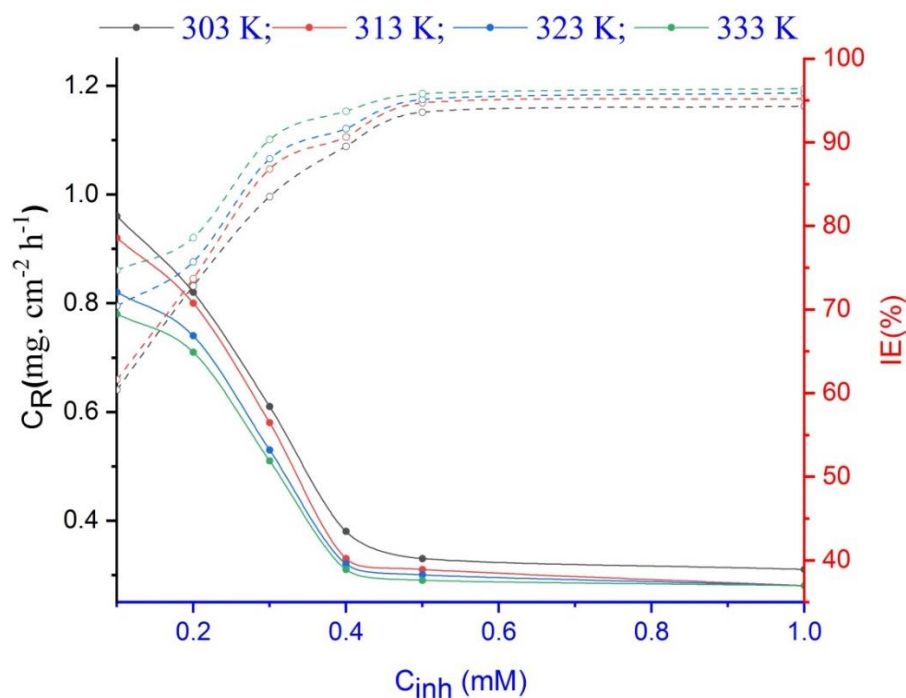

Figure 4. The investigation of NPF concentrations effects to the corrosion rates and efficiency of inhibition of the mild iron in 1 M HCl solution at different temperature with 5-hours immersion time.

3.4. Adsorption isotherm investigations

The linear relationship observed in the plot of C_{inh}/θ against C_{inh} at 303 K provides confirmation of Langmuir's suitability for describing the adsorption process. The high linear regression coefficient reinforces Langmuir's adequacy compared to alternative isotherm

models. From the intercept of the straight line in Figure 5 the adsorption equilibrium constant (K_{ads}) is determined indicating the strength of interaction between the adsorbate and adsorbent. A higher K_{ads} value signifies more effective adsorption correlating with higher inhibition efficiency [80–82].
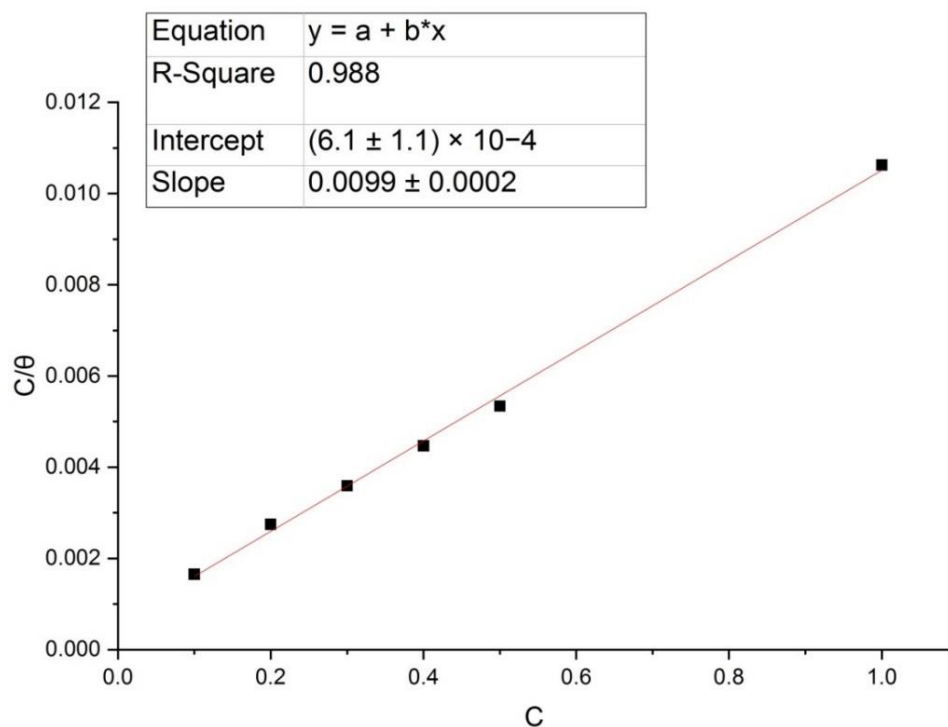
Figure 5. NPF Langmuir Isotherm for the surface of mild steel in a 1.0 M HCl solution at 303 K.

Adsorption free energy $\left(\Delta G^0_{ads}\right)$ as in Equation 13, serves as a crucial indicator of adsorption interactions. A ΔG^0_{ads} value less than or equal to -20 kJ/mol suggests physisorption, indicating a weaker interaction where inhibitor molecules adhere to the surface through physical forces. Conversely, an extremely negative ΔG^0_{ads} value exceeding -40 kJ/mol implies chemisorption, involving the formation of coordination bonds between iron atoms on the coupon surface and the inhibitor molecules [83–85].

$$\Delta G_{ads} = -RT \ln\left(55.5 K_{ads}\right) \tag{13}$$

The calculated value of ΔG_{ads} as -25.75 kJ/mol suggests a mixed interaction type involving both chemisorption and physisorption. This highlights the diverse nature of interactions between the inhibitor and the metal surface which contributes to a comprehensive understanding of the inhibition mechanism. In conclusion adsorption isotherm studies confirm the effectiveness of Langmuir isotherm in characterizing the adsorption behavior of NPF on mild steel in hydrochloric acid. The mixed reaction type involving both chemisorption and physical adsorption enriches the understanding of the

inhibition mechanism demonstrating the potential of NPF as a corrosion inhibitor with versatile reaction modes.

3.5. Computational studies

Experimental results supported by computational analysis provide valuable insights into the corrosion inhibition mechanism of NPF on mild steel. The low values of ΔE (energy gap) and hardness coupled with high softness indicate a physical adsorption mechanism consistent with experimental observations. High HOMO energy is associated with high inhibition efficiency consistent with adsorption isotherm data $\left(\Delta G_{ads}^0\right)$. In addition molecular structure affects adsorption as evidenced by the electron density of the active sites especially oxygen and nitrogen atoms which are vulnerable to electrostatic attacks. Electronegativity plays a crucial role in predicting inhibitory efficacy with electron transfer values decreasing as inhibitory electronegativity increases [86–88]. Positive ΔN values confirm the electron donation potential of the inhibitor further validating the E_{HOMO} trends. These computational insights advance the understanding of the molecular interaction of NPF and its efficiency in corrosion inhibition on mild steel. The negative dipole moment of NPF indicates a polar nature indicating the direction of charge distribution along a specific axis. This polarity which is likely influenced by the orientation of the functional groups within the molecule enhances electrostatic interactions with the mild steel surface facilitating adsorption and formation of the protective layer. The quantum chemical parameters summarized in Table 1 support the experimental insights as NPF shows high HOMO energy and strong electron donating ability consistent with the observed physical absorption mechanisms and inhibition efficacy. The LUMO energy highlights NPF's electron-accepting ability while low energy gap (ΔE) values confirm its high inhibitive efficiency.

Table 1. Quantum chemical calculations for NPF molecule.

| Parameter	Value
HOMO Energy (eV)	-10.290
LUMO Energy (eV)	-0.868
Energy Gap (ΔE) (eV)	9.422 eV
Hardness (eV)	4.711 eV
Softness (eV)	0.212 eV^{-1}
Electronegativity	-5.579 eV
ΔN (Electron Transfer)	1.335
Dipole moment (μ) (Debye)	-5.1505

Analysis of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) as in Figure 6 reveals concentration of HOMO populations around piprazin and carbonyl groups, indicating significant electron donation capability. This alignment with physisorption mechanisms further validates experimental findings and underscores the molecular features influencing NPF's performance as a corrosion inhibitor.

Optimum Structure   HOMO   LUMO
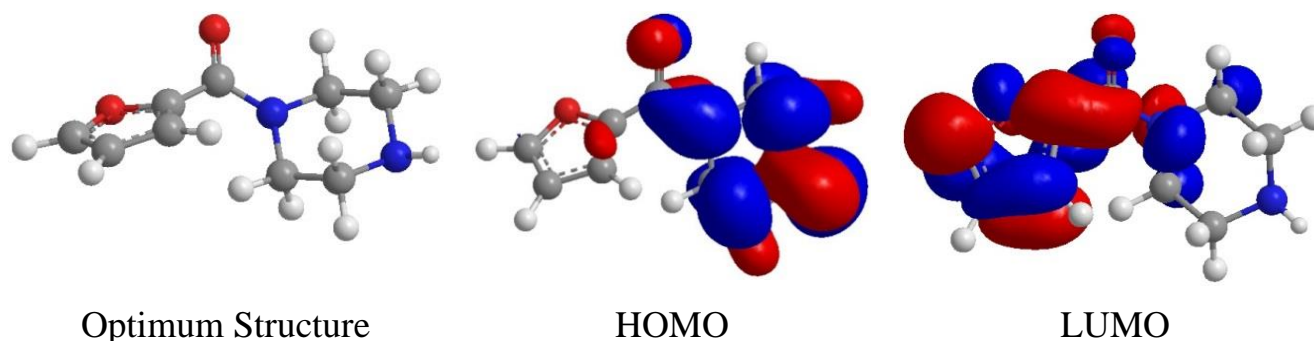
Figure 6. Molecular Orbitals of NPF.

3.6. Mechanism of inhibition

The corrosion inhibition mechanism of mild steel in a corrosive solution containing NPF revolves around the adsorption of NPF molecules onto the steel surface. This adsorption exploits the unpaired electron pairs within NPF, effectively interacting with the unoccupied d-orbitals of iron (Fe) atoms on the surface [90–92]. Heteroatoms, particularly oxygen, and nitrogen, serve as crucial reaction sites during this process, strategically positioned within the molecular configuration of NPF to facilitate targeted interaction with the metal surface. The computed adsorption free energy ($\Delta G_{ads}^0 = -25.75$ kJ/mol) indicates a spontaneous process, implying a combination of physisorption (electrostatic interactions) and chemisorption (chemical reaction) mechanisms. Figure 7 illustrates the diverse adsorption modes of NPF molecules at the steel/HCl interface, forming a protective shield on the steel surface that impedes corrosive attacks. This versatile inhibitive mechanism, incorporating both physical and chemical interactions, enhances the efficacy of NPF as a corrosion inhibitor for mild steel in acidic environments [93–95]. The suggested mechanism further elucidates the complex interactions between NPF and the steel surface, detailing the initial adsorption, physisorption, chemisorption and the pivotal role of heteroatoms as reaction sites. The protective layer formed as a result of these processes acts as a barrier against corrosive elements, as depicted in Figure 7. The visual representation of the inhibition mechanism highlights the multifaceted nature of NPF's interaction with the mild steel surface, showcasing its potential effectiveness in mitigating corrosion in acidic environments [96–100]. Overall, the proposed mechanism provides valuable insights into the protective action of NPF and underscores its promise as a corrosion inhibitor.
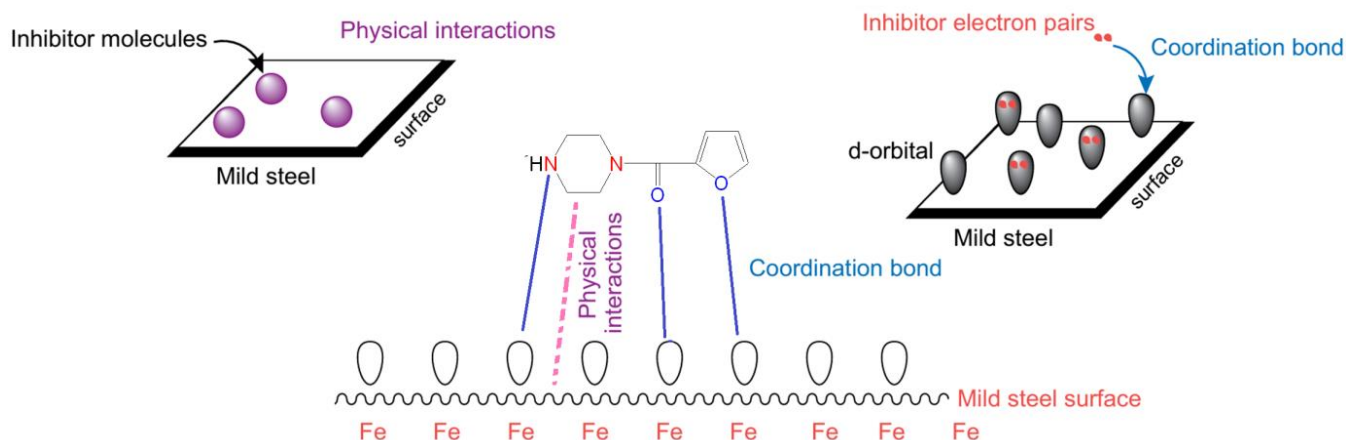
Figure 7. Postulated mechanism of NPF molecules adsorption on steel surface.

4. Conclusion

Finally, this study presents the complete examination of the efficiency of NPF precursor as a corrosion inhibitor for mild steel in 1 M HCl solution by a simultaneous process of the experimental and theoretical method. The obtained result manifested a very high inhibition impact of NPF with the efficiency reaching 93.6% under optimal conditions that proves the applicability of NPF for environmental replacement of traditional inhibitors. The Langmuir adsorption isotherm analysis enlightens the strong and specific interaction between NPF molecules and steel surface through which the theoretical calculations using DFT support also fulfill the process. Moreover, we also inferred that inhibition measure showed a positive correlation with immersion time as well as temperature. The prolonged exposure to an electrolyte causes all inhibitors to become more effective. Seemingly, their effect is known to be related with the gradual formation of a protective film on the metal surface. Furthermore, higher precipitation temperature may increase NPF efficiency, which interprets an activated sorption mechanism. The DFT calculations theoretically provide important information on the molecular interactions interfacial which the calculated electron transfer parameter show a positive relation constituting an electronic donor and iron atom behavior, supporting the observed mechanism of action. In summary, this research illustrates this NPF as being a realistic efficient and environmentally friendly corrosion inhibitor and strongly establishes a reliable methodology for identifying the potential and mode of action of green alternative corrosion inhibitors. Having said that, further study might target on looking to the limits in how appropriate and practical NPF to be applied to real-world cases and improving its performance parameters for wider industrial purposes.

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