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# AI-Assisted Preparation of *Solanum melongena* Leaf Extract for Mitigating Corrosion of Mild Steel in Acidic Environments

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**Abstract**
Artificial Intelligence (AI) and Chemistry applications are mostly focused on preparation, characterization and applications of extracts of natural products in corrosion inhibition, wastewater treatment, biochemical systems, *etc*. Artificial intelligence can be useful in chemistry and allied field in the areas of compound manufacture and characterization. The present study explores the preparation and unique use of acid extract of *Solanum melongena* (SM) leaves commonly known as garden egg to truncate deterioration of mild steel in hydrochloric acid and tetraoxosulphate (VI) acid. Mild steel of dimensions 30 mm x 30 mm x 1.4 mm was used for the experiment. It was suspended in the corrodents: 1 mol/L hydrochloric acid and 0.5 mol/L tetraoxosulphate (VI) acid. Acid extract of SM was added as 0.4 g/L, 0.4 g/L and 1.6 g/L concentration, to investigate its effects against dissolution of mild steel by making use of mass loss and electrochemical techniques. The result showed that acid extract of SM effectively truncated the dissolution of mild steel in 1 mol/L of hydrochloric acid and 0.5 mol/L of tetraoxosulphate (VI). The result presented more effectiveness as the concentration increased with prolonged time. Mass loss was reduced more in the 1 M HCl system giving 96.65 % while the 0. 5 mol/L $H_2SO_4$ gave 95.85 % inhibitor efficacy, showing good effectiveness for both systems. Polarization experiments revealed a multi-faced character of inhibitor, reducing cathodic, as well as anodic current densities. Surface coverage data using Langmuir adsorption isotherm showed interaction among the adhered substances on the surface of the mild steel with increased surface coverage. The various processes of the preparation, characterization and applications of the leaf extracts are then assigned to AI for any possible relationship in carrying out the processes.

**Keywords:** Corrosion, Mild Steel, Inhibition Efficiency, Electrochemical, Adsorption

## Introduction

Artificial intelligence focuses on the application of machine learning to carry out diverse work requiring the cognitive of man. It reproduces the intelligence of man in the system. (Choudhary et al., 2021). It is the most important aspect of technological world, which assists in collection of raw information, as well as analyzing them in a conducive atmosphere (Kruse et al., 2019). Artificial intelligence has many applications, which includes usage to process speech, inquiry and strategizing (Thakkar et al., 2021). It is capable of changing its objects as required. As we know the syntheses, characterization and chemical reactions of molecules and compounds are the most important task in chemistry. Mild Steel is majorly used in the industry to manufacture vessels, some which carry acidic substances that is utilized in acid pickling processes such as during welding and galvanizing, acid descaling such as in boilers and heat exchangers, oil well acidizing and other acid-treatment activities in the oil sector and in manufacturing industries (Salim et al., 2020). Nevertheless, such activities using acids result in trapping of hydrogen on metal surface and production of acidic gases (Chen et al., 2024) resulting into very destructive and dangerous impacts on gigantic engineering structures, and hence, leading to very huge financial loses. In order to preserve the originality and quality of mild steel, its protective maintenance is very vital. As a way of solving this problem, corrosion inhibitors of various types have been employed (Deyab, 2020). These are substances incorporated on metal surface or added to the corrosive medium to help eliminate the tendency of corrosion on metal surface (Miralrio & Vazques, 2020). However, these inhibitors such as chromates are toxic and not


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biodegradable; REACH (Regulation on the Registration, Evaluation, Authorization and Restriction of Chemicals) laws forbid applying chromates practically as corrosion inhibitors because of its high level of toxicity. (Radha et al., 2024). Due to the increasingly high demand for environmental safety, there has been need to drive towards biocompatible and eco-friendly corrosion inhibitors. Natural plants are sustainable, renewable and environmentally friendly (Okeke et al., 2020). Sulaimon et al. (2023) showed plant extract from Okro to produce high level of inhibitor efficacy (89.98 %) for mild steel dissolution in acids. *Solanum melongena* leaves have been recommended for use in traditional medicine and in other medicinal exploration for treatment of various health disorders (Manh et al., 2022). There has been no record of the use of the acid extract of *Solanum melongena* to inhibit the deterioration of mild steel in acidic media. The present study was carried out to provide an overview on how AI can assist researchers and scientists in demonstrating their usefulness and applicability in the preparation of acid extract of *Solanum melongena* leaves for inhibition of the corrosion of mild steel in acidic environments.

## Material and Methods

### Preparing the mild steel for gravimetric measurements

The mild steel that we used during this research weighed 0.6 manganese, 0.05 carbon, 0.03 silicon, 0.36 phosphorus by elemental composition, the rest is iron. (Okeke et al., 2016) The metal which had thickness of 1.4 mm was cut mechanically to produce coupons which had size 30 mm x 30 mm. The cut coupons were placed in ethanol to remove oily substances and dried in warm air. It was then weighed, and kept secure in desiccators for use.

Preparing mild steel for electrochemical measurements

The working electrode was composed of mild steel, which was enshrined in epoxy resin only to expose 1 $cm^2$ of the metal surface. The exposed area (1 $cm^2$) was polished with emery papers of grades ranging between 200 and 1000 grit. Ethanol was used to remove oil from the metal surface, and as well drying it in warm air.

### Preparing the plant extracts

The leaves of the S*olanum melongena (SM)* used for this experiment were obtained locally and verified in Crop Science department, FUTO. The leaves were washed, shaken free of water droplets, and dried in the sun to a consistent mass. Twenty (20) g of the powdered leaves was weighed with an electronic weighing balance then refluxed in 400 ml of 0.5 M $H_2S0_4$ for three (3) hours to yield the extract. Filtration of the extract was carried out, while the residue was allowed to dry on the filter paper, after which it was weighed and used to evaluate the concentrations of the stock extract solution. The stock solution was used to prepare extract concentrations of 0.4 g/l, 0.8 g/l and 1.6 g/l.

### Mass loss determination

Mass loss procedure was carried out by immersing and suspending the already weighed metal coupon mass loss determination, also known as gravimetric experiment was carried out. Previously weighed metal (mild steel) coupons were completely immersed and suspended in 250 ml of the corrosive medium at temperature of 30 $^0$C. The coupons were drawn from the test solution at 24 h intervals progressively for 168 hrs. Fifty percent of sodium hydroxide was employed to wash it, followed with rinsing in ethanol and drying with warm air, and reweighing. The total mass loss was taken as the change of mass for the total time interval of 168 hours, using the mean of two weighing from two coupons.

### Electrochemical measurements

The electrochemical test was carried out using a three-electrode compartment: saturated calomel electrode as the reference electrode, mild steel as the working electrode, and graphite rod as the counter electrode. The evaluation of potentiodynamic polarization was carried out at ± 0.25 volts and scanned at ±0.333 volts per second.

Prior to the polarization measurement, introduction of the working electrode in the test solution and left for 30 min at that potential for the system to become stable. Triplicate procedures were done to ensure reproducible and reliable measurements. (Okeke et al., 2024)


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**Results**

**Mass loss against time**

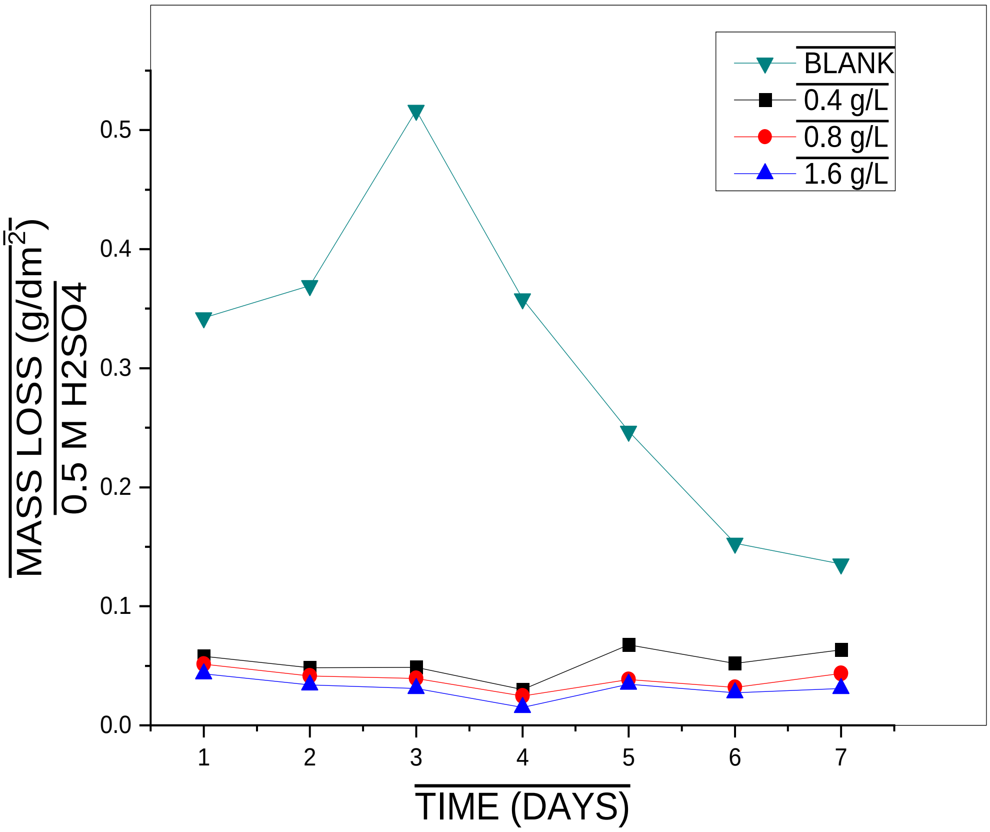


**Fig 1:** Mass loss versus time for mild steel in 0.5 M $H_2SO_4$ with or without 0.4 g/l, 0.8 g//l and 1.6 g/l of SM leaves.

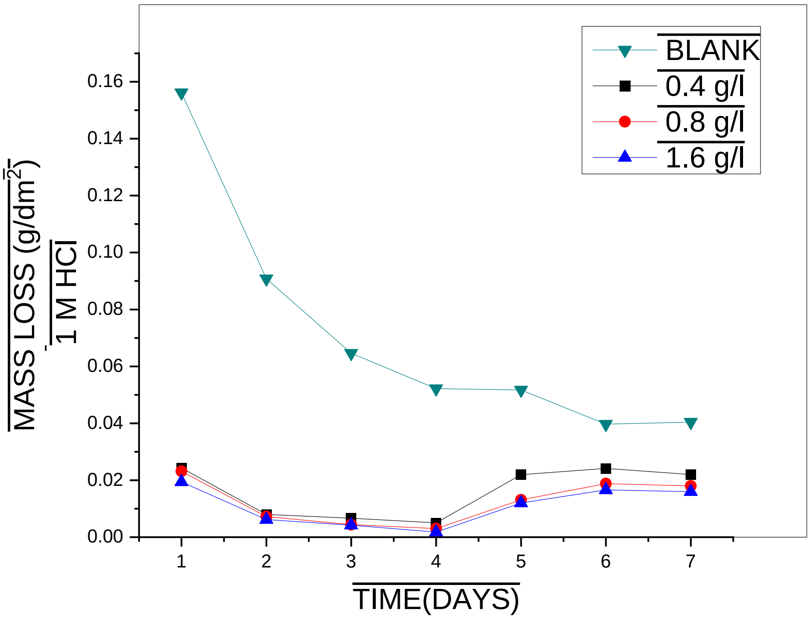


**Fig 2:** Mass loss versus time for mild steel in 1 mol/l HCl with or without 0.4 g/l, 0.8 g/l and 1.6 g/l of acid extract of SM leaves.

**Inhibition efficiency**

The free corrosion behavior of mild steel in various inhibitor/corrodent solutions was done by evaluating the inhibitor efficacy (η%), which is defined as follows:

(Okeke et al., 2019)

For gravimetric test

$$\eta\% = \left(1 - \frac{W_1}{W_2}\right) X100 \qquad (4.1)$$

$w_1$ = rate of corrosion in the inhibited system

$w_2$= rate of corrosion in the uninhibited system

The inhibitor efficacy for the potentiodynamic polarization test was evaluated as follows:

$$\eta\% = \left(\frac{I^{o}_{corrbl} - i_{corrinh}}{i_{corrbl}}\right) X\ 100 \qquad (4.2)$$

$i_{corrbl}$ =corrosion current density in the uninhibited system

$i_{corrinh}$ = corrosion current density in the inhibited system


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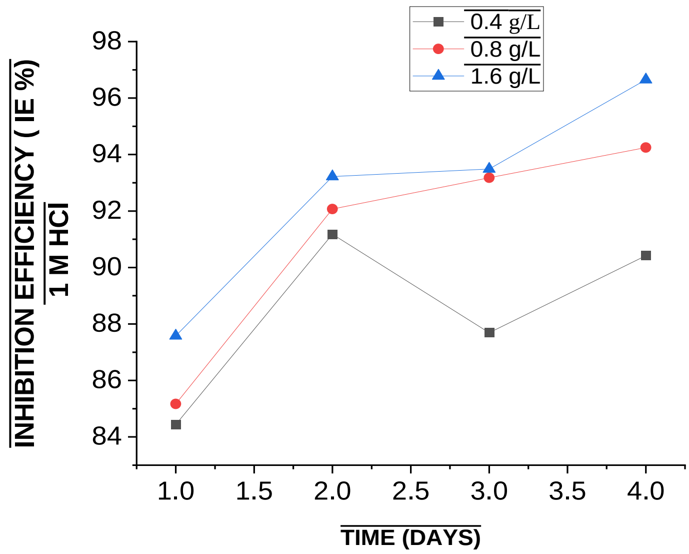


**Fig 3:** Inhibitor efficacy versus time for mild steel in 1 mol/l HCl in 0.4 g/l, 0.8 g/l and 1.6 g/l of acid extract of SM leaves.

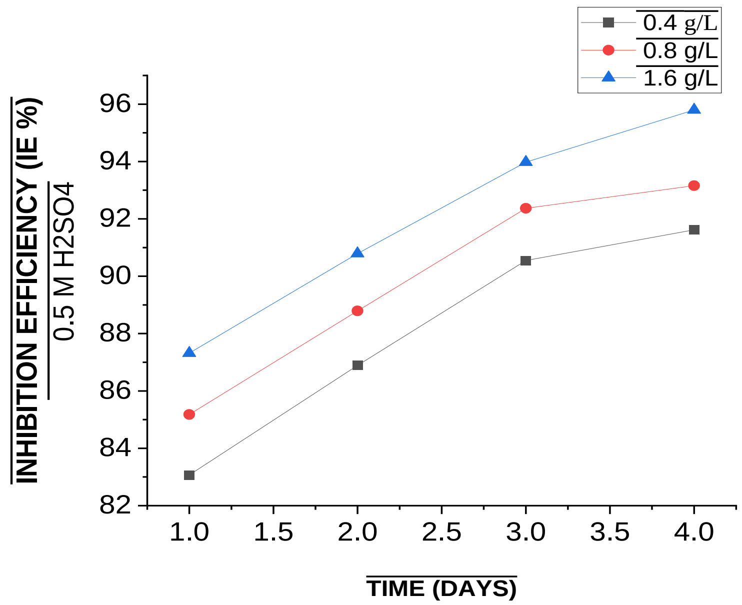


**Fig.4:** Inhibitor efficacy versus time for mild steel in 0.5 M $H_2SO_4$ in 0.4 g/l, 0.8 g/l and 1.6 g/l of acid extract of SM leaves.


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**Electrochemical Result**

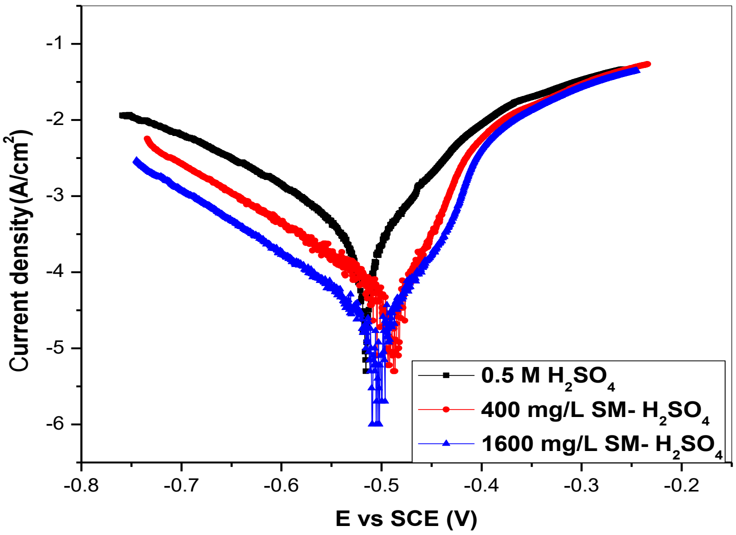


**Fig 5:** Potentiodynamic polarization graphs for mild steel in 0.5 M $H_2SO_4$ with or without 0.4 g/l and 1.6 g/l SM- acid extract.

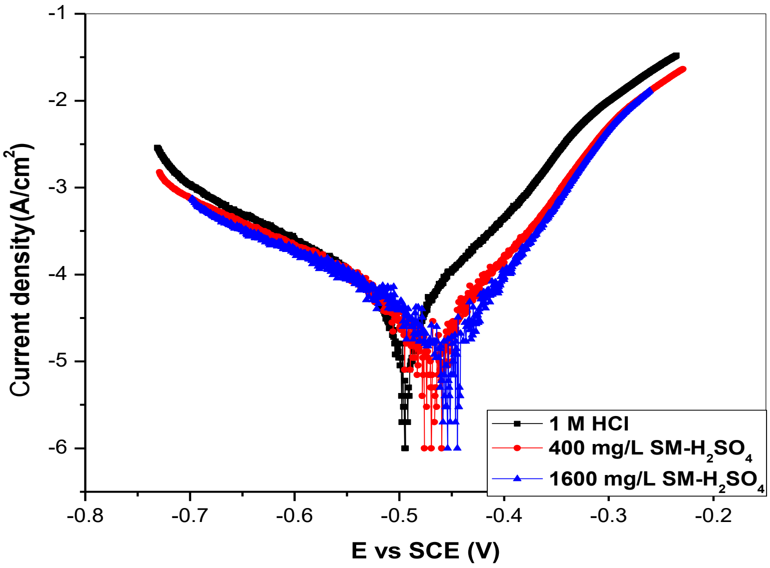


**Fig 6:** PDP graph for mild steel in 1 mol/l HCl with or without 0.4 g/l and 1.6 g/l-acid extracts


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**Table 1:** Potentiodynamic polarization results for mild steel in 0.5 M $H_2S0_4$ and I M HCl

| System | $E_{corr}$ | $I_{corr}$ | $β_a$ | $β_c$ | IE (%) |
|---|---|---|---|---|---|
| **0.5 M $H_2SO_4$** | -515 | 462.6 | 115.9 | 167 | |
| 400 mg/L SM-$H_2SO_4$ | -490.6 | 63.5 | 80.2 | 129.9 | 86.3 |
| 1600 mg/L SM- $H_2SO_4$ | -501.1 | 13.15 | 67.2 | 100.6 | 97.0 |
| **1 MHCl** | -493.5 | 148.9 | 163.3 | 645 | |
| 400 mg/L SM-$H_2SO_4$ | -470.9 | 37.6 | 87.0 | 118.8 | 74.7 |
| 1600 mg/L SM- $H_2SO_4$ | -501.5 | 12.9 | 70.3 | 151.0 | 91.3 |

**Adsorption considerations for mild steel**

Surface coverage data play a crucial role in determining the adsorption characteristics of inhibitors. These data are used in constructing adsorption isotherms and provide valuable insights into the adsorption mechanism. Mass loss determinations could be applied to evaluate adsorption behaviour of SM on mild steel in acid media using Langmuir equation: (Nleoun et al., 2022)

$$\frac{C}{\theta} = \frac{l}{b} + C$$

$\frac{l}{b}$= intercept

C = concentration of inhibitor

Ɵ = surface coverage.

$$Ɵ = \frac{(IE\ \%)}{100}$$


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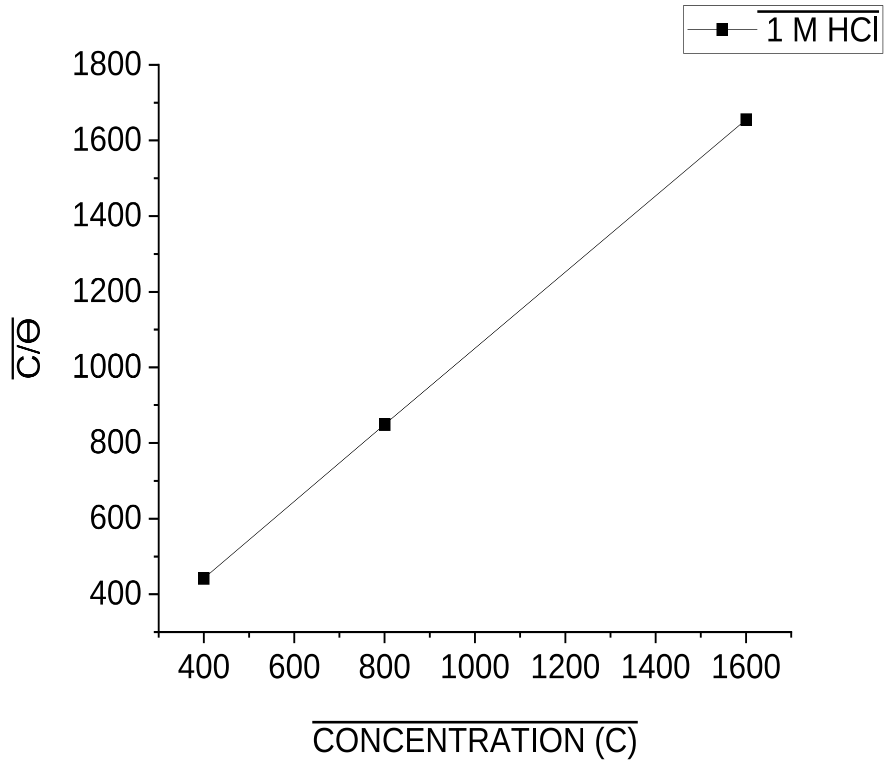


**Fig 7:** Langmuir adsorption isotherm for acid extract of SM on mild steel in 1 M HCl

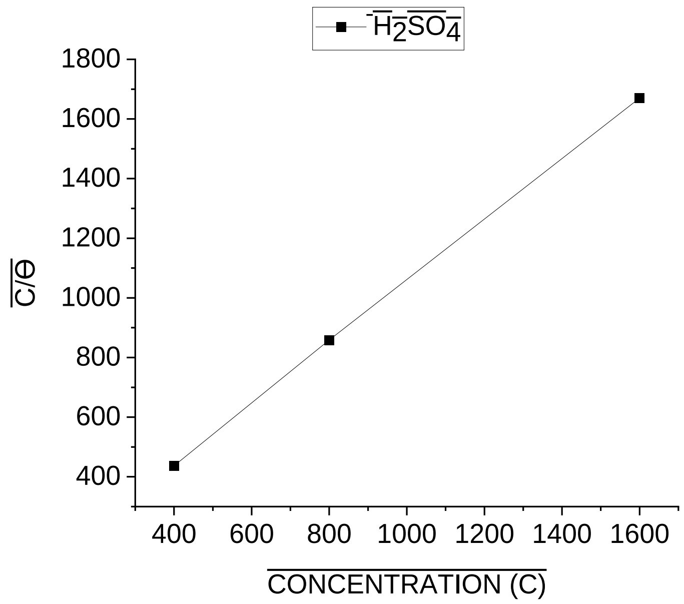


**Fig 8:** Langmuir adsorption isotherm for acid extract of SM on mild steel in 0.5 M $H_2SO_4$

**Discussion**

Figure 1 is a graph of evaluation of mass loss of the metal, which was carried out for 7 days, with the results showing increase between 0.34 g and 0.51 g for day 3, and later going down to 0.14 g, for the system without the inhibitor. Figure 1 showed significant reduction in mass loss in 0.4 g/l of SM between 0.058 g to 0.030 g on day 4, gets to a peak for 1.6 g/l between 0.043 g to 0.015 g for day 4. By the $5^{th}$, $6^{th}$ and $7^{th}$ day, mass loss still decreased in comparison to compared to the value of the corrodent. In figure 2 loss in mass of the uninhibited acid decreased steadily with exposure time from 0.16 g to 0.04 g. While in the inhibited acid, the 0.4 g/l concentration of the inhibitor decreased the mass loss from 0.02 g to 0.005 g on day 4, and peaked for 1.6 g/l concentration from 0.019 g to 0.0017 g on day 4. By the $5^{th}$, $6^{th}$, and $7^{th}$ day, weight loss still decreased in comparison to the corrodent system as reflected in Figure 2, which shows retardation of mid steel dissolution. In fig 3 we evaluated inhibition efficiency for mild steel for 4 days, the values for the inhibition efficiency is quite high in the presence of 0.4 g/l concentration of the inhibitor from 84.44 % to 90.42 % by the fourth day, and is highest in the 1.6 g/l concentration from 87.58 %- 96.65 % by the fourth day. The impact of concentration on the inhibition of mild steel corrosion was notice throughout with elevated inhibitor efficacy as seen in Figure 3. Fig 4 shows inhibitor efficacy for mild steel for 4 days, which is significantly high for the 0.4 g/l concentration of SM, in the range of 83.07 % to 91.62 % on day 4, getting to a peak for 1.6 g/l in the range of 87.32 % to 95.80 % by the fourth day. Impact of concentration on the inhibition of mild steel was notice all through the duration as seen in fig 4 showing high inhibition efficiency. In Fig 5 the 0.4 g/l and 1.6 g/l concentrations of the acid extract of SM in 0.5 M $H_2SO_4$ showed values of corrosion potential, $E_{corr}$ as -490.6 mV and -501.1 mV respectively as revealed in Figure 5 and in Table 1. The matching $i_{corr}$ figures are 63.5 mA/cm$^2$ and 13.15 mA/cm$^2$ for the 0.4 g/l and 1.6 g/l systems as well. From the results, it can be deduced that the introduction of SM lowered the cathodic and anodic corrosion current densities. This implies a reduction in of the mild steel's deterioration rate, in comparison with the blank with $E_{corr}$ as -515 mV and $I_{corr}$ as 462.6 mA/cm$^2$. Also, the $E_{corr}$ of the 1.6 g/l became more negative (cathodic) when compared with the 0.4 g/l, with higher inhibitor efficacy in 1.6 g/l as 97.0 % 86.3 %. For 0.4 g/l, as has been studied by (Oguzie et al., 2011).

In 1 mol hydrochloric acid environment, as seen in Figure 6, $E_{corr}$, for 0.4 g/l as well as 1.6 g/l concentrations of the acid extract of SM containing mild steel are -501.5 mV and -470.9 mV respectively as shown in Figure 6 and in Table 1. The corresponding $i_{corr}$ values are 37.6 mA/cm$^2$ and 12.9 mA/cm$^2$ for the 0.4 g/l and 1.6 g/l concentrations. The result depicts that the presence of the inhibitor reduces both the cathodic and the anodic corrosion current densities, as evident in Table 1. The deterioration rate of mild steel was retarded when compared with the corrodent system, which was evident in the lowering of the cathodic and anodic current densities, with the blank values as is -493.5 mV for $E_{corr}$ and 148.9 mA/cm$^2$ as $I_{corr}$. Also, the higher concentration of 1.6 g/l gave a higher value of I.E as 91.3 %, while the lower concentration of 0.4 g/l gave a lower value of I.E as t 74.7 %, thus showing the impact of increase in concentration on inhibitor efficacy. Figure 7 and 8 is a graph of C/Ө versus C, and it demonstrates Langmuir adsorption isotherm for acid extract of SM on mild steel in 1 M HCl and 0.5 M $H_2SO_4$. The graph is linear, having a slope of 1.04, with intercept 48.8 for 1 M HCl system and a slope of 1.05 and intercept of 55.16 for 0.5 M $H_2SO_4$ system, showing that the plant extract contained some organic substances, whose adsorption on the metal surface obeyed the Langmuir adsorption isotherm. The slope of the graph deviated from unit, which suggest that the adsorbed species has some interaction with the surface of the metal, and the heat of adsorption changed with increase in surface coverage.

The different stages of this work could be related to artificial Intelligent systems as follows: For the preparation of the mild steel; chemists can use computer- aided software such as molecular dynamics (MD) simulations to design the mild steel surface as Fe (110) surface (Okeke et al., 2024). Preparation of plant extract and the corrosion inhibition of mild steel, the researchers made use of Radia Distribution Functions (RDFs) of atoms from the acid extract of SM on mild steel surface in the two acid media: for 1 mol/l hydrochloric acid and 0.5 mol/l of tetraoxosulphate (VI), MD simulations can be used, this provides details of atom distribution of the extract on surface of the metal.


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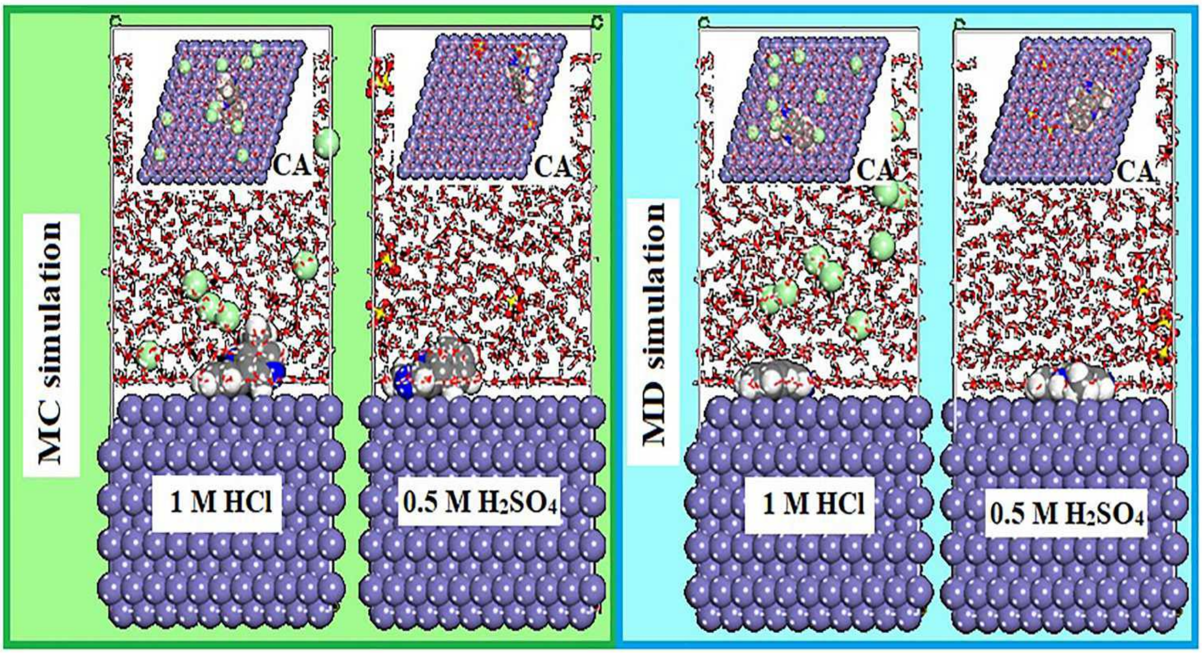


**Fig 9:** diagram showing molecular conductivity (MC) simulation, molecular dynamics (MD) simulation, the mild steel surface, the inhibitor molecules and the acidic environments (Okeke et al., 2024).

There could also be a modeling of the PDP tests in this study based on artificial intelligence system, the distribution of the adsorption energies (Eads) can be obtained via the Molecular Conductivity (MC) simulations, and prediction of the binding energy (Adindu et al., 2024) via molecular docking can be achieved. The system of artificial intelligence could be used to gather and disseminate information, to provide enlightenment on methods and expected outcomes of research studies, so that people can follow the rules properly, to regulate their experiments and to share research data (Segler et al., 2018).

**Conclusion**

Corrosion can badly degrade the functional properties and the appearance of mild steel structures; natural products are considered more because they can be synthesized easily and they are eco-friendly in nature. The results obtained from this work indicated that the acid extracts of *solanum melongena* is a good retardant of mild steel corrosion in acidic media. The extract revealed high inhibitor efficacy for the 1 mol/l HCl system giving 96.65 % while the 0. 5 mol/l of tetraoxosulphate (VI) acid gave 95.85 % inhibitor efficacy for gravimetric analysis. The Potentiodynamic polarization results showed that both systems were hybrid inhibitors of mild steel corrosion in acidic media inhibiting the anodic, as well as the cathodic reactions, 1.6 g/l concentration of 0.5 M $H_2SO_4$ acid extract of SM gave the highest inhibitor efficacy of 97.0% with 0.5 M $H_2SO_4$ corrodent. The surface coverage data indicated that the adherence of organic material from the extract obeyed the Langmuir adsorption isotherm. However, the departure of the slope from unity propose association between the adsorbed species on the metal surface and variations in the heat of adsorption as surface coverage increases on mild steel. This artificial intelligence system is very less time consuming and provides an output within lesser period of time based on input given. This machine-based software can also help in solving various other problems related to chemistry. The AI system is highly time-efficient, delivering output within a shorter period with regards to the given input. Additionally, machine-based software can assist in providing answers to diverse chemistry-related problems.

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