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COMPARATIVE STUDIES OF STANDARD STAINLESS STEEL AND IMPROVISED METALLIC IMPLANTS AND CORROSION INHIBITION POTENTIAL OF *GUAIACUM OFFICINALE* VIA ELECTROCHEMICAL AND COMPUTATIONAL APPROACHES

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ABSTRACT

The malleability and fabrication of metal and associated alloys, as well as their vast range of applications, are significantly influenced by their physiochemical characteristics. Gas chromatograph mass spectrometer revealed the presence of eight (8) bioactive components, which are responsible for the inhibitory activities. Having a maximum inhibition efficiency of 85.17 at an inhibitor dose of 0.5g/L, there is a significantly reduction in reaction number in the presence of Guaiacum officinale extract compared to the blank solution. The electrochemical parameters for the improvised metallic biomaterial in 1.0 M HCl solution in the presence and absence of inhibitor concentrations revealed the high polarization region, thus a wide potential range. The addition of the inhibitor affected the anodic and the cathodic partial reactions, which signifies mixed-type mechanism of inhibition. The rate of corrosion mitigation increases in the presence of inhibitors when compared with a blank solution as a result of thin-film formation on metal/solution interface. This work give relevant information on the efficiency of *Guaiacum officinale* as an inhibitor for improvised metallic biomaterial in 1M HCl. The biocompatibility test showed that mechanical and chemical properties are within the recommended values.

Keywords: *Guaiacum officinale,* metallic implants, inhibition

INTRODUCTION

Metal and its alloys have extensive range of utilizations in different industries such as medical, construction, metallurgical among others, due to its physical and chemical features (Ates *et al*. 2020; Vinogradov *et al*. 2019; Yilmaz *et al*. 2020). Metals are characterized by significant changes in their surface properties when exposed to biological, chemical, and biochemical environments, which lead to deterioration of quality as a result of corrosion (Behera *et al*., 2020; Saha and Kang 2022; Yilmaz *et al*. 2020). Corrosion is a viable and thermodynamic favorable process that causes an adverse effect on metallic material (Ameh, 2018). The aggressive media are unavoidably employed in industries, due to manufacture applications that is, oil-well cleaning, industrial acid cleaning, acid pickling, and acid descaling, thus fostered corrosion on metallic substances (Adeniji and Akindehinde 2018; Freer and Powell 2020; Yilmaz *et al*. 2020)

However, researchers have struggled with the negative effects of corrosion on metals over the years. There are corrosion controlling methods such as; paint, plastic, or powder, galvanization, cathodic protection, grease among others. As a result, scientists are seeking corrosion inhibitory methods that are ecofriendly, non-toxic, readily available, applicable at a wide temperature, and cheap. For this reason, a variety of plant materials were employed because of the presence of bioactive components that enhance effective inhibitory activities, cost-effective, and ecofriendly (Dehghani *et al*., 2019).

Advance still, a quantum mechanical modeling technique called density-functional theory (DFT) is used in chemistry to ascertain the electronic structure of various organic components responsible for corrosion inhibition via computational and theoretical knowledge (Hemmerich and Ecker 2020; Liu 2020; Rodriguez *et al*., 2020).

Despite the fact that this plant has been the subject of numerous reports, yet no work was done on inhibitory activities of *Guaiacum officinale* on metal. The objective of this work is to use GC-MS analysis to identify the bioactive ingredients in this plant extract, to investigate their anti-corrosion potential using molecular dynamics simulation, and experimental evaluation of corrosion inhibition efficiency of the extract on a metal surface (Ramezanzadeh *et al*., 2019).

MATERIALS AND METHODS

Plant collection, preparation and extraction

The exudate of *Guaiacum officinale* are recognized in the field using conventional keys and certified at the herbarium unit of the botany section of Ahmadu Bello University, Zaria. Nigeria. The exudate of *Guaiacum officinale* plant were gathered from the farmyard, pounded and sieved into small particle sizes to increase the surface area before the extraction, extraction was carried out using alcohol, filtered and the filtrate is subjected to the rotatory evaporator at 340K to prevent ethanol contaminants and concentrated the extract.

Mechanical and chemical parameters of the improvised metallic implant and standard stainless steel

Improvised metallic biomaterial implant samples were obtained from solid rods of Fan-guard (makers are ORL and China Mainland) at Zaria, Nigeria. The rods have dimensions of 5mm diameter and were cut into 1cm length for material characterization. The chemical compositions were determined using XRF (model +66 EDX1800B Dand USA) for non-destructive analysis while mechanical properties (such as: tensile stress, tensile strain, young modulus, force and area) were determined using Tensiometer for destructive analysis. The mechanical and chemical properties of metallic implants were determined based on American Standard for Testing and Materials ASTM principles (Bolewski *et al*., 2020; Egorov *et al*., 2002; Pandey *et al*., 2021).

Corrosion studies

Thermometric method

Corrosion tests were carried out in an acidic solution. The beakers containing inhibited and uninhibited HCl media, while the steel samples were immersed. The beakers were sited in a thermostat water bath set at 40°C. Corrosion reaction was monitored and the maximum temperatures of the system containing the test solution and the steel sample are recorded when a steady temperature was obtained. Equations (1) and (2) were employed for the determination of inhibition efficiency from the reaction number values.

$$\text{RN } (^{o}\text{CMin}^{-1}) = \frac{T_2 - T_1}{t} \quad (1)$$

Where T_2 and T_1 are maximum and minimum temperature and time interval (t). The inhibition efficiency (% I) of the inhibitor was calculated based on the reaction number:

$$\%I = \frac{RN_a - RN_p}{RN_a} \quad (2)$$

Where RN_a is the reaction number without inhibitors (blank system) and RN_p is the reaction number containing the inhibitor concentrations and aggressive medium that is 1.0 M HCl solution (Shukla and Ebenso 2011).

Electrochemical measurement

Linear polarization determination were carried out via potentiostat (IVIUM, IVIUM XRE Technologies) and three electrodes comprising platinum using as auxiliary electrode, iron employed as the working electrode, saturated calomel electrode (SCE) as reference at a potential range of ± 0.25V for stainless steel in HCl medium containing several concentrations of the test inhibitors ranging from 0.1 to 0.5g/L. The scan rate of 0.33 mV/s at 40ºC, all measurements was performed in triplicate to encourage reproducible results.

The inhibition efficiencies were calculated using equation 3. and 4 respectively:

$$\%I = \left(1 - \frac{i_{cr}}{i_{in}}\right) \times 100 \quad (3)$$

$$\%I = \frac{R_{ct(In)} - R_{ctr}}{R_{ct(In)}} \times \frac{100}{1} \quad (4)$$

where i_{cr} and i_{in} are the corrosion currents in the absence and presence of the inhibitor respectively and R_{ctr} and $R_{ct(in)}$ are the uninhibited and inhibited charge transfer resistance respectively (Oguzie *et al.* 2014).

Computational consideration

Density functional theory (DFT) is used to calculate molecule and structural properties with excellent precision. Computational simulations of the molecular parameters of different components in the plant extract (A to J) were conducted employing DFT (that is density functional theory) in Spartan 14 programme package. The equilibrium geometry of the selected components in plant extract were carried out at functional hybridization of Becke-3-Lee-Yang-Parr with set of polarization d-functions 6-311G(d) at basis set [B3LYP/6-311G(d)] to achieved full geometry optimization. Computational approach is employed to determine the selectivity of an *N*-electron, mimic the molecular properties and predict the reactivity of the system using quantum chemical methods such as: highest occupied molecular orbital (E_{HOMO}), lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE) difference between (E_{LUMO}-E_{HOMO}) energies, ionization energy (I), electron affinity (A), global softness (σ) and global hardness (η) (Awe *et al.* 2015).

RESULTS AND DISCUSSIONS

Table 1: Elemental composition of standard stainless steel and metallic biomaterial employed for the study

S/No	Standard stainless implant	% Elemental Composition A	% Elemental Composition B
1	Fe (93.54)	Fe (98.84)	Fe (98.89)
2	Zn (4.27)	Mn (0.0618)	Ca (0.1203
3	Zr (<0.28)	Zn (<0.001)	Zn (0.2212)
4	Nb (1.3)	Mg (0.0462)	As (<0.042)
5	Pb (0.22)	C (0.1203)	Kr (<0.008)
6		Si (0.0547)	Nb (0.0553)
7		Al (0.0227)	Mo (0.0361)

Table 2: Mechanical properties of selected metallic biomaterial and standard implants

Samples	Force	UTS	Area	Strain	Young Modulus	% E
A1	966.67	1230.64	0.788	0.188	6532.06	18.84
A2	1450	820.41	1.767	0.896	915.6	89.60
SI	2375	931.37	2.55	0.57	1757.3	57

Comparative studies of improvised metallic implants and standard stainless steels based on mechanical and chemical properties

Table 1 revealed the X-Ray diffraction evaluate, which is a nondestructive process that offers explicit information about the chemical composition, crystallographic structure and physical properties of the material (Pandey *et al*. 2021). Elemental components such as Ni, Co and V are not toxic or they are elements that cannot cause allergic problems, therefore they acceptable and biocompatible. Cobalt offers continuous phase for basic properties as reported by Shen *et al* (2021). Chromium provides inhibitory effect against metal corrosion via the oxide surface. Molybdenum provides strength and bulk corrosion resistance (Sinnett-Jones, Wharton, and Wood 2005). Nickel and carbon enhance mechanical properties such as ductility. Therefore, elemental component is a critical in the determination of the biocompatibility of improvised metallic implants as reported by (Jadhav *et al*. 2018).

A mechanically compatible metallic material must offer a favourable combination of low elastic and high mechanical resistance as shown in Table 2. Mechanical properties are physical properties that a material exhibits upon the application of forces. and corroborated by Bartlett *et al*., (2017). A higher Young's modulus is considered a high priority when designing implants for biomedical applications, especially if the metallic implants have a modulus that is much higher than that of bone (Abraham and Venkatesan 2023; Bagga *et al*. 2016; Renganathan *et al*., 2021)

Table 3: Thermometric results for the calculation of percent inhibition efficiency and reaction number of *Guaiacum officinale*

C(g/L)	Initial temperature	Max temperature	Reaction number	Percent inhibition
Blank	30	32.6	0.52	-
0.1	30	30.845	0.1690	67.5
0.2	30	30.690	0.1380	73.47
0.3	30	30.482	0.09641	81.46
0.4	30	30.047	0.09069	82.56
0.5	30	30.04	0.07712	85.17

Table 3 clearly revealed that reaction number decreased in the presence of *Guaiacum officinale* extract compared to the blank solution. The inhibition efficiency as expected increased with an increase in the concentration of the inhibitor.

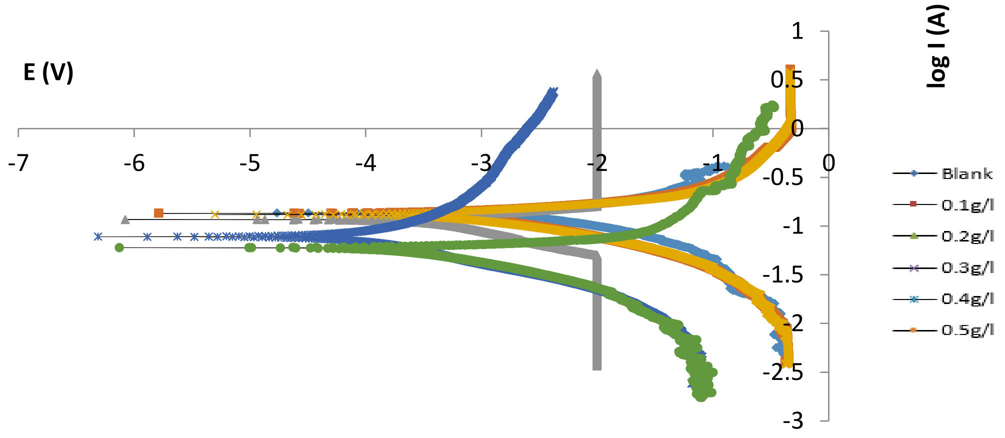

Figure 1: Polarization curve for the corrosion of stainless steel in 1.0 M HCl in the presence and absence of various concentration of *Guaiacum officinale* at 313K

Table 4: Electrochemical parameters and inhibition efficiency values of various inhibitors in the absence and presence of different concentrations of *Terminalia catappa* for the corrosion of improvised biomaterial in 1.0M HCl solution through PDP and LPR methods

Tafel polarization parameters					System	Linear polarization resistance (LPR)	
E_{corr} (Mv)	βc (mVdec−1)	βa (mVdec−1)	I_{corr} (μA)	%IE	Concentration	R_p (R/cm^2)	%IE
-851.59	151.2	148.2	1218.0	-	Blank	19.501	-
-856.83	135.5	139.2	596.82	51.91	0.1	59.40	67.17
-941.38	128.6	131.1	377.82	65.98	0.2	75.35	74.12
-1105.8	108.7	125.8	248.47	70.96	0.3	101.15	80.72
-1216.5	101.1	119.6	246.04	79.80	0.4	160.17	87.82
-1412.5	98.5	107.6	183.92	84.90	0.5	256.25	92.39

Potentiodynamic polarization curves for metallic implant in 1M HCl solution in the absence and presence of different inhibitor concentrations at 303K is shown in Figure 1. The electrochemical parameters such as corrosion current density (i_{corr}), corrosion potential (E_{corr}), the cathodic Tafel slope (βc), anodic Tafel slope (βa) and inhibition efficiency (IE %) obtained from the potentiodynamic polarization curve is given in Table 4. The polarization resistance values in the presence of the various inhibitor concentrations are determined, resistance was observed to increase in the inhibited solution compared to the blank, indicating that GO inhibited metallic implants against corrosion in the acid medium. Also, the polarization inhibition values in the presence of the various inhibitor concentrations are determined, resistance was observed to increase in the inhibited solution compared to the blank, indicating that GO and TC inhibited metallic implants against corrosion in the acid medium.t can be deduced from the plots that the nature of the polarization curves are the same in both the uninhibited and inhibited solutions similar to the work of Awe *et al.* (2015), Delfani *et al.* (2021), Lebrini *et al*. 2010 and Umoren *et al*. (2018). However, addition of both *Guaiacum officinale* as inhibitor to the acidic medium reduced the corrosion rate of the metallic implant as evidenced in the shifting of the corrosion current density to regions of lower values in comparison to the blank system, indicating the corrosion inhibiting ability of the plant exudates (Etteyeb and Nóvoa, 2016). This revealed that the corrosion potential (E_{corr}) in the presence of TC shifted to noble values relative to the blank, suggesting that the GC are mixed-type inhibitors (Bentrah, Rahali, and Chala 2014). Both anodic and cathodic current densities are reduced as concentration of inhibitors increased; this is due to the effect of the coating by the active inhibitory compounds of the plant extract on the metal surface, thereby reducing the corrosion rate on the metal surface (Abdullah *et al*. 2019; Awe *et al*. 2015).

It has been reported that the inhibitory corrosion potential of a molecule is a function of electronic properties which can be inferred from its quantum chemical parameters (Xavier *et al*., 2015) such as energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$), electronegativity, polarization surface area, global hardness and global softness These parameters are reported in Table 1. The energy gap is a vital parameter for determining stability of a system. The wider the energy gap, the more stable a molecule is, hence, the less its reactivity. It is the difference between the energies of highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbitals (E_{LUMO}) (Obot, Obi-Egbedi, and Eseola 2011). The ability of an inhibitor to donate electrons into the low-lying vacant orbitals of a metal is a function of its ionization potential (I) which is related to the energy of highest occupied molecular orbital, E_{HOMO}, by the expression: $I = -E_{HOMO}$ Also, the electron affinity (A) of an inhibitor is related to the energy of lowest unoccupied molecular orbital (E_{LUMO}), that is $A = -E_{LUMO}$, which indicates the tendency of the inhibitor to accept electrons. As the energy gap (ΔE) of inhibitors decreases, there is a corresponding increase in their reactivity, hence, an increase in the predictive corrosion inhibition potential. This band gap is related to I and A by the expression: $\Delta E = I - A$. The energy gap elucidates the ultimate charge transfer interaction inside the molecule; and it is useful in evaluating molecular electrical properties. According to the frontier molecular orbital theory (FMO), the energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) is related to the inhibition efficiency of inhibitor molecule. It has been reported that low values of ΔE will provide good inhibition efficiency, because the energy for removing an electron from the last occupied orbital will be low (Ameh 2015; Arukalam 2014). For instance, compounds that have a high energy gap are stable, and hence are chemically harder than compounds having a small energy gap (Leila *et al*., 2018; Madkour *et al.*, 2018; Ruiz-Morales and Mullins, 2009). The shapes and symmetries of the organic compounds are employed in predicting the corrosion inhibition reaction, the reactivity of the organic compound and predicting the chemical reaction product (Eddy *et al*., 2011). Both molecular and structural properties have great correlation with corrosion inhibition efficiency (Khaled, Babić-Samardžija, and Hackerman 2005). The dipole moment (μ) parameter is a vital parameter which is connected with the molecular stability in polar environments. In this research, the experimental dipole moment is not identified. The calculated dipole moments in gaseous phase are shown in Table 5. The influences of the polar environment (i.e. acetone, toluene, ethanol among others) are not considered in comparison the dipole moment values but carried out only in gas phase. Among the considered compounds 1,2 -benzisothiazol-3-amine has the highest dipole moment in the gas phase among the selected aromatic based compounds in the plant exudates, because it has a higher dipole interaction, therefore, it indicate strong dipole–dipole interaction between the inhibitor molecule and the iron surface.

It is noticed that some dipole moments determined in the selected organic compounds in the plant exudates were higher than the dipole moment of water that is 1.88Debye (Li *et al.*, 2022). This implies that some of the organic compounds in the plant exudates will displaced the water molecules from the metal surface, get chemically adsorbed onto the metal surface thereby inhibit in metallic implants surface against corrosion (Ameh, 2015; Dehdab *et al.*, 2016). In this work, higher dipole moment values were observed in the compounds possessing in electron donor (i.e. N, O, Cl, S) compared to those with electron- acceptor groups (i.e. H, C, H) in the studied gas phase (Aigbogun and Adebayo, 2021; Miar *et al*., 2021). The global electrophilicity index (ω), introduced by (Parr *et al*., 1999) is based on thermodynamic properties and measures the favorable change in energy when a chemical system or compound attains saturation by the addition of electrons. It can be defined as the decrease in energy due to the flow of electrons from the donor (E_{HOMO}) to the acceptor (E_{LUMO}) in molecules. It also plays an important role in determining the chemical reactivity of a system. Compounds having greater values of chemical potential are more reactive than those with small electronic chemical potentials (Ayers *et al.,* 2006).

Table 5: DFT at B3LYP/6-311G(d) at level theory to validate quantum chemical calculations of plant extract components

Compounds	E_{HOMO} ev	E_{LUMO} ev	DM debye	MW (amu)	MA (Å^2)	MV (Å^3)	PSA (Å^2)	Pol	Ovality	Log P
$C_{16}H_{12}O_5$	-9.18	-0.93	5.22	284.27	289.61	274.97	62.32	61.73	1.42	1.66
$C_{23}H_{46}$	-9.17	1.5	0.58	322.62	489.54	434.29	0	74.09	1.77	9.54
$C_{16}H_{30}O_2$	-10.8	0.57	5.03	254.41	346.3	308.07	34.48	63.69	1.57	5.19
$C_{16}H_{34}O$	-9.46	0.54	1.83	282.46	397.41	351.46	34.78	67.53	1.65	6.29
$C_{18}H_{34}O2$	-9.59	2.3	1.62	242.45	357.83	318.05	6.74	64.38	1.59	5.8
$C_{14}H_{11}C_{l2}NO_2$	-8.67	-0.61	4.25	296.15	278.83	266.57	42.83	61.1	1.39	3.6
$C_{22}H_{44}O_2$	-1.73	0.5	2.38	340.59	489.31	430.66	34.87	73.67	1.77	8.28
$C_{20}H_{34}O_2$	-9.5	0.51	1.57	306.49	413.82	378.58	33.43	69.73	1.64	6.48

CONCLUSION

Corrosion inhibition of improvised metallic implants using *Guaiacum officinale* in 1M HCl solution was measured by thermometric and electrochemical methods at different temperatures. The result showed that corrosion rate was considerably declined in presence of the *Guaiacum officinale* extract and inhibition efficiency increased with increasing the concentration of extract. 85.17% inhibition efficiency was found in 1M HCl at 0.5g/L inhibitor concentration of plant extract. The condition of mixed inhibitor adsorption on the implant surface was displayed by potentiodynamic polarization. Computational investigations revealed a remarkable report that supported by experimental results. All the theoretical parameters ensure that *Guaiacum officinale* extract can act as an effectual blanket layer and minimise the corrosion process.

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