Journal of Molecular Genetics and Gene Research

PRIME OPEN ACCESS

Volume 1, Issue 1

Research Article

Date of Submission: 21 March, 2025
Date of Acceptance: 11 May, 2025
Date of Publication: 21 May, 2025

Eco-Friendly Polysaccharide Inhibitors for Steel-Reinforced Concrete: Synergistic Corrosion Resistance and Structural Enhancement Using Welan and Neem Gums

M. G. L. Annaamalai[1*], N. Sharmiladevi[2], R. Prabhu[3] and K. Vijayakumar[4]

[1]Department of Civil Engineering, VSA Group of Institutions, Salem, Tamil Nadu, India

[2]Department of Bio Medical Engineering, VSA Group of Institutions, Salem, Tamil Nadu, India

[3]Principal, VSA Group of Institutions, Salem, Tamil Nadu, India

[4]Department of MCA, VSA Group of Institutions, Salem, Tamil Nadu, India

***Corresponding Author:**
M. G. L. Annaamalai, Department of Civil Engineering, VSA Group of Institutions, Salem, Tamil Nadu, India.

Citation: Annaamalai, M. G. L., Sharmiladevi, N., Prabhu, R., Vijaykumar, K. (2025). Eco-Friendly Polysaccharide Inhibitors for Steel-Reinforced Concrete: Synergistic Corrosion Resistance and Structural Enhancement Using Welan and Neem Gums. *J Mol Genet Gene Res, 1*(1), 01-05.

Abstract
This study investigates the corrosion inhibition efficacy and mechanical strengthening potential of two bio-derived gums, Welan gum (WG) and Neem gum (NG), on steel-reinforced concrete exposed to chloride environments. Electrochemical techniques—electrochemical impedance spectroscopy (EIS) and Tafel polarization—were employed to evaluate corrosion resistance, complemented by scanning electron microscopy (SEM) to analyze surface morphology. Results demonstrated that both gums function as mixed-type inhibitors, forming protective films on steel surfaces, with WG exhibiting marginally superior inhibition efficiency (87%) compared to NG (84%). Density functional theory (DFT) calculations identified active molecular sites responsible for adsorption, aligning with experimental findings. Additionally, mechanical tests revealed enhanced compressive and split tensile strengths in gum-modified concrete, underscoring their dual functionality. The proposed inhibition mechanism involves synergistic physico-chemical interactions between gum molecules and the steel surface. This work highlights the potential of natural gums as sustainable, multifunctional additives for durable concrete infrastructure.

Keywords: Natural Polysaccharides, Chloride-Induced Corrosion, Electrochemical Analysis, Green Inhibitors, Concrete Durability and Quantum Chemical Modeling

Introduction
Steel reinforcement in concrete structures remains indispensable in construction due to its cost-effectiveness and mechanical robustness. However, chloride ingress from marine environments or de-icing salts accelerates corrosion, compromising structural integrity and safety. Traditional synthetic inhibitors, though effective, raise environmental and toxicity concerns, driving demand for eco-friendly alternatives. Natural polymers, particularly plant-derived gums, offer promise due to their biodegradability, affordability, and multifunctional properties.

Recent advances highlight polysaccharides like xanthan and guar gum as effective corrosion inhibitors and rheology modifiers in cementitious systems. However, limited studies explore their dual role in simultaneously mitigating corrosion and enhancing mechanical properties. This study bridges this gap by evaluating Welan gum (a microbial exopolysaccharide) and Neem gum (an exudate from Azadirachta indica) as sustainable corrosion inhibitors and strength enhancers. Integrating electrochemical assessments, material characterization, and computational modeling, we elucidate the structure-activity relationship of these gums, offering insights into their practical application in marine and hydraulic concrete structures..

Materials and Methods

Materials

WG and NG were sourced from Salem District, India, authenticated (Voucher: BSI/SRC/5/23/2016/TECH/166), and processed into fine powders. Concrete specimens (150 × 100 × 100 mm^3) were prepared per IS 10262-1982 using a 1:2:4 cement-sand-gravel ratio, with embedded steel rebars (C: 0.37%, Mn: 1.21%). Gum solutions (250–750 ppm) were incorporated during mixing.

Electro Chemical Testing

A three-electrode cell (CHI 760D workstation) with a saturated calomel reference electrode and platinum counter electrode was used for EIS (0.01–10^5 Hz, 2 mV amplitude) and Tafel polarization (0.5 mV/s scan rate). Charge transfer resistance (Rct) and double-layer capacitance (Cdl) were derived from Nyquist plots.

Mechanical and Morphological Analysis

Compressive and split tensile strengths were assessed per IS 10262-2009 after 7–120 days. SEM (TESCAN VEGA3) characterized steel surfaces post-immersion in 3.5% NaCl.

Computational Details

DFT calculations (Gaussian 09W) using B3LYP/6-311G++(d,p) optimized gum monomer geometries. Reactivity descriptors—HOMO, LUMO, electronegativity (χ), and global hardness (η)—were computed to identify adsorption-active sites.

Results and Discussion

Electrochemical Behavior

Tafel analysis (Tables 1–2) revealed concentration-dependent inhibition, with WG (750 ppm) reducing corrosion current density from 1318 to 197 μA/cm^2 (85% efficiency). EIS data (Tables 3–4) showed increased Rct and decreased Cdl, confirming protective film formation. NG exhibited comparable trends but lower efficiency (82% at 750 ppm).

Mechanical Performance

Gum incorporation improved 120-day compressive strength by 11.2% (WG) and 10.2% (NG) versus control (38.3 MPa). Split tensile strength increased to 3.35 MPa (WG) and 3.01 MPa (NG), attributed to enhanced pore structure and interfacial bonding.

Surface and Molecular Insights

SEM images (Figures 10–12) showed intact steel surfaces in gum-modified specimens versus severe pitting in controls. DFT simulations (Tables 6–7) highlighted electron-rich hydroxyl and carboxyl groups in WG as primary adsorption sites, aligning with its superior performance. The ΔN values (0.31–0.38) suggested electron donation from gum molecules to steel substrates.

Results and Discussion

Electrochemical Studies (Tafel Polarization & Impedance Methods)

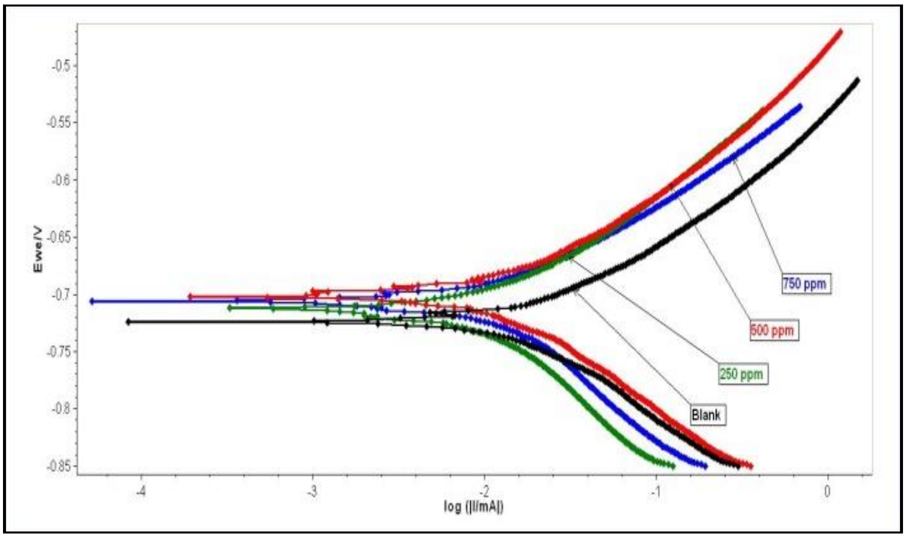

Figure 1: Tafel Plots of Embedded Steel in Concrete Without and With NG120 Days

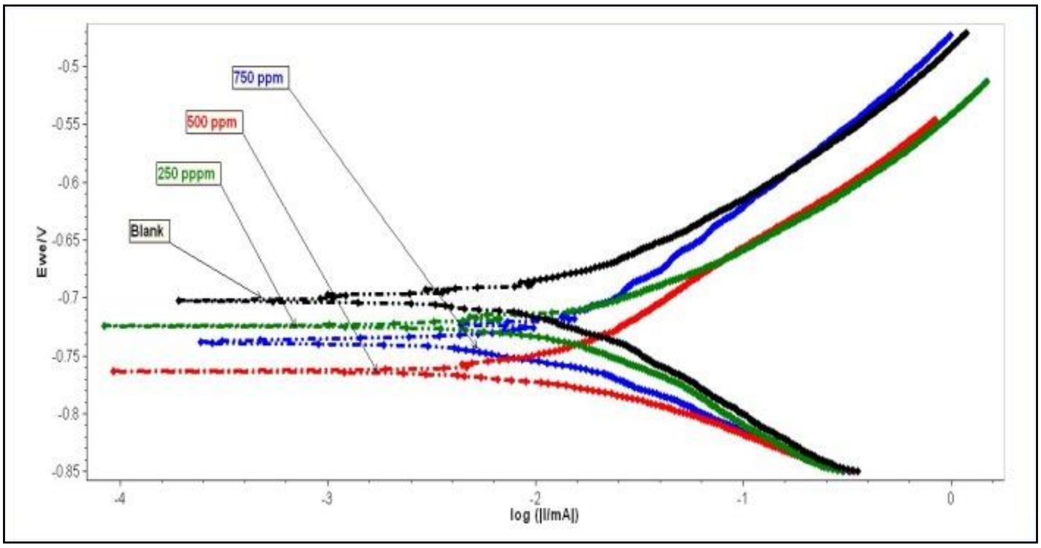

Figure 2: Tafel Plots of Embedded Steel in Concrete Without and With WG 120 Days

The potentiodynamic polarization (PDS) curves were determined with the sweep rate of about 0.5 mVs^{-1}. The potentials were varied from cathodic direction to corrosion potential and simultaneously towards the anodic direction. The PDS curves of reinforced steel without and with various concentrations of Welan and NGs in chloride media are shown in Fig.2.1 and 2.2 and electrochemical parameters viz., corrosion potential (E_{corr}), corrosion current density (I_{corr}), inhibition efficiency (%IE) and Tafel constants (b_a and b_c) of from Tafel curves are given in Table 1 & 2 Inhibition efficiency was calculated by,

$$IE(\%) = \frac{(I_{corr} - I_{corr(1)}) \times 100}{I_{corr}} \text{ --------------- } (8)$$

where, I_{corr} and $I_{corr(i)}$ are the uninhibited and inhibited corrosion current density values, respectively, determined by extrapolation of Tafel lines towards the corrosion potential.

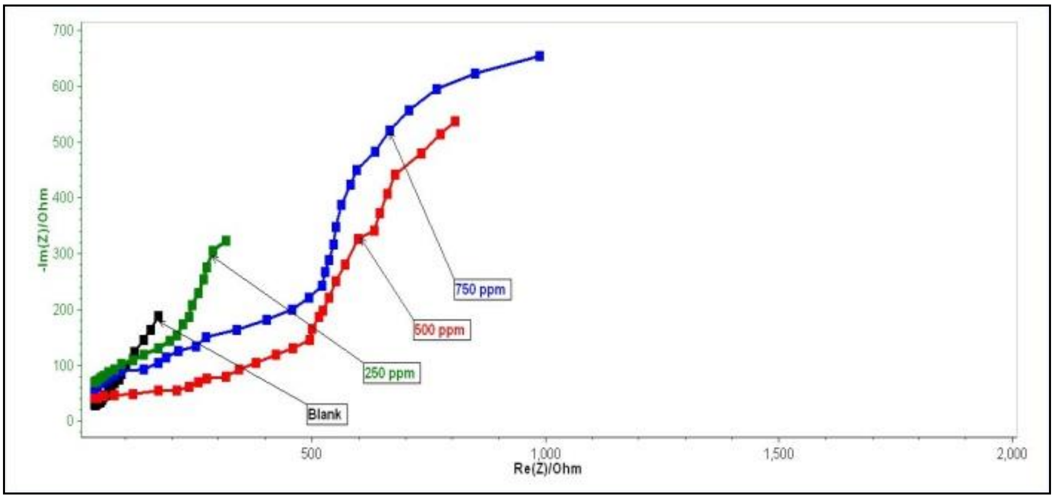

Figure 3: Nyquist Plots of Embedded Steel in Concrete NG 120 Days

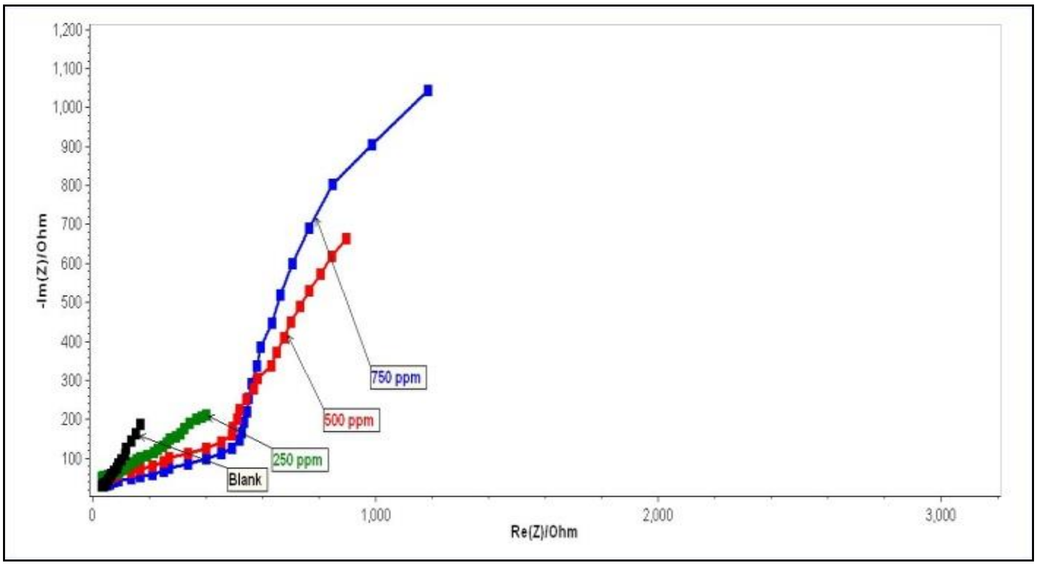

Figure 4: Nyquist Plots of Embedded Steel in Concrete WG 120 Days

The results clearly demonstrate that both Welan gum and Neem gum significantly reduced the corrosion current without causing any notable changes in the corrosion potential values. This observation suggests that the two gums function as mixed-type inhibitors. Additionally, the values of anodic and cathodic Tafel slopes (ba and bc) did not show significant changes, further supporting the conclusion of mixed-mode action for the studied inhibitors. The electrochemical impedance (EIS) response was measured over a frequency range of approximately 0.01 Hz to 100000 Hz at open-circuit potential, using a 1 mV sine wave AC voltage excitation. The equivalent circuit diagram corresponding to the EIS data is illustrated in Figures 1 and 2, where RΩ represents the resistance of the solution, Rt indicates the resistance of the corrosion product film, and Cdl denotes the capacitance of the parallel combination of the resistor and the corroding interface.

The Nyquist plots for the impedance behavior of steel reinforced in chloride media, both without and with the introduction of various concentrations of Welan and Neem gums, are presented in Figures 3 and 4. From these figures, it is evident that the incorporation of the gums leads to an increase in the value of charge transfer resistance (Rct) while reducing the double layer capacitance (Cdl). These variations are likely indicative of an increase in the thickness of the electronic double layer, which enhances the anticorrosive properties of the concrete.

The increased values of charge transfer resistance (Rct) indicate the formation of a protective layer at the metal/solution interface. The results suggest that both Welan gum (WG) and Neem gum (NG) adsorb onto the metal surface, leading to a decrease in double layer capacitance (Cdl) values and an increase in Rct values. The charge transfer resistance (Rct), interfacial double layer capacitance (Cdl), and the inhibition efficiency were calculated using the following equations

$$IE = \frac{R_{ct(i)} - R_{ct(b)}}{R_{ct(i)}} ------------(9)$$

Where $R_{ct(i)}$ and $R_{ct(b)}$ are the charge-transfer resistance values without and with the inhibitor.

Quantum Chemical Calculation

Density Functional Theory (DFT) based quantum chemical calculations have proven to be effective in evaluating the inhibition potential of molecules by analyzing their reactivity and tendency to inhibit metal corrosion. The frontier molecular orbitals (FMOs) play a significant role in identifying the adsorption centers of these molecules. Corrosion inhibitors not only donate electrons to the vacant orbitals on the metal surface but also accept free electrons from the metal. In this study, the ability of the inhibitors is elucidated through the analysis of the frontier molecular orbitals, specifically the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).

The HOMO is associated with the electron-donating ability of the inhibitor, while the LUMO corresponds to its electron-accepting capacity. Figure 4 clearly illustrates how the inhibitor donates and accepts electrons from the metal. The HOMO and LUMO values provide insights into the interaction between the inhibitor molecules and the metal surface. Furthermore, the energy gap between HOMO and LUMO (HOMO-LUMO energy) is directly related to the reactivity of the inhibitors, with smaller gaps indicating higher reactivity. The energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are directly related to ionization potential and electron affinity, respectively.

These characteristics help determine the susceptibility of molecules to electrophilic and nucleophilic attacks. The stability and reactivity of molecules are assessed through their hardness and softness values; generally, molecules with lower hardness tend to exhibit higher inhibition capabilities. As the dipole moment (μ) of a molecule increases, its volume also increases, enhancing the available surface area for interaction between the molecule and the iron surface, which subsequently improves corrosion inhibition. The electrophilicity index (ω) reflects the electron-accepting nature of inhibitor molecules [1-18]. It quantifies the stabilization energy gained when an inhibitor accepts excess electron charge from the environment. The theoretical results for the monomers (WG and NG) indicate that they function as effective inhibitors. Furthermore, the comparison of the calculated data suggests that Welan gum (WG) performs better than Neem gum (NG) in terms of ionization energy (IE) and other relevant values.

Conclusion

WG and NG significantly inhibit steel corrosion in chloride environments while enhancing concrete durability. Their dual functionality as eco-friendly admixtures offers a sustainable strategy for extending infrastructure lifespan. DFT and empirical data validate WG's superior performance, attributed to its electronic structure and adsorption efficacy. Future work could explore synergistic blends with other natural inhibitors for optimized protection.

References

1. Al-Amoudi, O. S. B., Maslehuddin, M., Lashari, A. N., & Almusallam, A. A. (2003). Effectiveness of corrosion inhibitors in contaminated concrete. *Cement and Concrete Composites, 25*(4-5), 439-449.
2. Fouda, A. S., Elewady, G. Y., Shalabi, K., & Abd El-Aziz, H. K. (2015). Alcamines as corrosion inhibitors for reinforced steel and their effect on cement based materials and mortar performance. *Rsc Advances, 5*(46), 36957-36968.
3. Fouda, A. S., Elewady, Y. A., Abd El-Aziz, H. K., & Ahmed, A. M. (2012). Corrosion inhibition of carbon steel in 0.5 M HCl solution using cationic surfactants. *International Journal of Electrochemical Science, 7*(11), 10456-10475.
4. Khayat, K. H., & Saric-Coric, M. (2000). Effect of Welan Gum SuperplasticizerCombinations on Properties of Cement Grouts. *Special Publication, 195*, 249-268.
5. Messali, M., Lgaz, H., Dassanayake, R., Salghi, R., Jodeh, S., Abidi, N., & Hamed, O. (2017). Guar gum as efficient non-toxic inhibitor of carbon steel corrosion in phosphoric acid medium: Electrochemical, surface, DFT and MD simulations studies. *Journal of Molecular Structure, 1145*, 43-54.
6. Alwaan, I. M., & Mahdi, F. K. (2016). Natural polymer of iraqi apricot tree gum as a novel corrosion inhibitor for mild steel in 1 M HCl solution. *International Journal of Chemical Engineering, 2016*(1), 5706432.
7. Kamal, C., & Sethuraman, M. G. (2012). Caulerpin· A bis-indole alkaloid as a green inhibitor for the corrosion of mild steel in 1 M HCl solution from the marine alga Caulerpa racemosa. *Industrial & Engineering Chemistry Research, 51*(31), 10399-10407.
8. Biswas, A., Mourya, P., Mondal, D., Pal, S., & Udayabhanu, G. (2018). Grafting effect of gum acacia on mild steel corrosion in acidic medium: Gravimetric and electrochemical study. *Journal of Molecular Liquids, 251*, 470-479.
9. Peter, A., Obot, I. B., & Sharma, S. K. (2015). Use of natural gums as green corrosion inhibitors: an overview. *International Journal of Industrial Chemistry, 6,* 153-164.
10. Palanisamy, S. P., Maheswaran, G., Kamal, C., & Venkatesh, G. (2016). Prosopis juliflora—A green corrosion inhibitor for reinforced steel in concrete. *Research on Chemical Intermediates, 42*(12), 7823-7840.
11. View, G. (2009). Version 5, Roy Dennington, Todd Keith and John Millam. *Semichem Inc*.
12. Pearson, R. G. (1988). Absolute electronegativity and hardness: application to inorganic chemistry. *Inorganic chemistry, 27*(4), 734-740.
13. Pearson, R. G. (1986). Absolute electronegativity and hardness correlated with molecular orbital theory. *Proceedings of the National Academy of Sciences, 83*(22), 8440-8441.
14. Quraishi, M. A., Ahamad, I., Singh, A. K., Shukla, S. K., Lal, B., & Singh, V. (2008). N-(Piperidinomethyl)-3-[(pyridylidene) amino] isatin: A new and effective acid corrosion inhibitor for mild steel. *Materials chemistry and physics, 112*(3), 1035-1039.
15. Mennucci, M. M., Banczek, E. P., Rodrigues, P. R. P., & Costa, I. (2009). Evaluation of benzotriazole as corrosion inhibitor for carbon steel in simulated pore solution. *Cement and Concrete Composites, 31*(6), 418-424.
16. Hosseini, M. G., Ehteshamzadeh, M., & Shahrabi, T. (2007). Protection of mild steel corrosion with Schiff bases in 0.5 M H2SO4 solution. *Electrochimica acta, 52*(11), 3680-3685.
17. Bentiss, F., Traisnel, M., & Lagrenee, M. (2000). The substituted 1, 3, 4-oxadiazoles: a new class of corrosion inhibitors of mild steel in acidic media. *Corrosion science, 42*(1), 127-146.
18. Venkatesh, G., Govindaraju, M., Vennila, P., & Kamal, C. (2016). Molecular structure, vibrational spectral assignments (FT-IR and FT-RAMAN), NMR, NBO, HOMO–LUMO and NLO properties of 2-nitroacetophenone based on DFT calculations. *Journal of Theoretical and Computational Chemistry, 15*(01), 1650007.