

Bio-Hybrid Poly(Potassium Acrylate)-Grafted-Guar Gum (PKA-g-GG) Hydrogels: A Sustainable "Molecular Armoring" Approach to Scale Mitigation in Closed-Loop Water Systems

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Abstract

Background: The intensification of water recovery in closed-loop systems, such as NASA's Brine Processor Assembly and high-pressure industrial boilers, is fundamentally limited by mineral scaling. Conventional synthetic anti-scalants often suffer from thermal degradation at temperatures exceeding 150°C, leading to hardware fouling and increased corrosivity.

Objective: This study investigates the synthesis and performance of a thermally resilient bio-hybrid hydrogel, poly(potassium acrylate)-grafted-guar gum (PKA-g-GG). The research characterizes the "molecular armoring" effect-defined as a synergistic protective mechanism where dense anionic PKA grafts sequester cations through multidentate chelation while the bulky galactomannan backbone provides steric hindrance against mineral nucleation and lattice growth.

Methods: Utilizing an aqueous-phase graft polymerization pathway with a potassium persulfate ($K_2S_2O_8$) initiation system, PKA-g-GG was synthesized and validated via Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis, and differential scanning calorimetry. Scale inhibition was quantified through complexometric ethylenediaminetetraacetic acid titration and Atomic Absorption Spectroscopy. Electrochemical Impedance Spectroscopy (EIS) was employed to characterize the polarization resistance (R_p) and the electrical double-layer architecture on aluminium substrates under accelerated scaling conditions (500 ppm $CaCO_3$).

Results: FTIR confirmed successful grafting with a prominent, broad carbonyl ($C=O$) peak at $1715-1750\text{ cm}^{-1}$. Thermal analysis revealed structural stability up to an onset of 280°C. At an optimal inhibitor concentration of 20 ppm, the bio-hybrid hydrogel PKA-g-GG achieved a maximum scale-inhibition efficiency of $43.08 \pm 1.10\%$. EIS elucidated the interfacial protection mechanism, where a significant reduction in polarization resistance (R_p) from 794.5 to $498.4\ \Omega \cdot \text{cm}^2$ was observed in 500 ppm $CaCO_3$ environments. This confirms that the hydrocolloid prevents scale adhesion through a synergistic dual-action mechanism of chelation and crystal lattice distortion - a phenomenon defined here as "molecular armoring."

Conclusion: The PKA-g-GG hydrogel represents a sustainable, technically competitive alternative for scale mitigation, supporting the >98% water recovery threshold required for NASA's long-duration space life support and high-heat flux industrial applications.

Categories: Advanced Materials, Chemical Thermodynamics and Separation Processes, Environmental and Sustainable Engineering

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Keywords: paa-g-guar gum (unique chemical identity), scale inhibition (primary application), electrochemical impedance spectroscopy (eis) (primary method), bio-hybrid hydrogels (material class), closed-loop water recovery (broadens the nasa/boiler scope), molecular armoring (unique mechanistic claim), thermal stability (key performance metric), groundwater remediation (environmental impact), alkalinity mitigation (specific chemical problem), advanced life support systems (als)

Introduction

The intensification of water recovery in closed-loop systems - such as advanced aerospace platforms including NASA's Brine Processor Assembly (BPA), as well as high-pressure industrial and naval boilers - is fundamentally constrained by mineral scaling phenomena. These systems typically operate under extreme hydrothermal conditions, characterized by pressures exceeding 13 kg/cm^2 and temperatures surpassing 150°C . Under these coupled parameters, the precipitation of sparingly soluble salts, particularly calcium carbonate (CaCO_3) and calcium sulfate (CaSO_4), is significantly accelerated, leading to the formation of adherent deposits on heat-transfer surfaces [1,2].

Historically, internal treatment strategies for scale mitigation have relied on polycarboxylic acids and aminopolycarboxylate chelating agents, most notably ethylenediaminetetraacetic acid (EDTA), to sequester hardness ions within the bulk solution [3,4]. However, the industrial utility of EDTA is fundamentally constrained in extreme hydrothermal environments. At temperatures surpassing 150°C , EDTA is susceptible to thermal decarboxylation, a process that triggers the release of CO_2 and subsequently increases condensate corrosivity [5]. Despite these operational limitations as a treatment chemical, EDTA remains the gold-standard analytical titrant for the precise quantification of residual calcium via complexometric titration.

In response to these challenges, recent research has shifted toward eco-friendly biopolymers derived from natural sources like Guar Gum (GG) [6]. GG is a galactomannan polysaccharide with a linear

backbone of (1 $\rightarrow$ 4)-linked α -D-mannopyranosyl units with single α -D-galactopyranosyl units connected by (1 $\rightarrow$ 6) linkages [6]. Functional modification of such polysaccharides via graft polymerization has emerged as a powerful strategy to enhance their physicochemical performance. Previous studies have demonstrated that chemically tailored biopolymers can serve as efficient adsorbents for environmental remediation, including the synthesis of sulfonic acid cation-exchangers [7], the selective removal of arsenic [8], and the development of specialized resin matrices [9].

To evaluate the interfacial protective behavior of these modified biopolymers, Electrochemical Impedance Spectroscopy (EIS) has proven to be an indispensable diagnostic tool for monitoring real-time mineral nucleation [10]. Building upon this scientific lineage, the present study introduces a "molecular armoring" approach designed to support the 98% water recovery target established by NASA for long-duration space missions [11]. This approach involves the synthesis of poly(potassium acrylate)-grafted-guar gum (PKA-g-GG) using a potassium persulfate initiation system [12].

The "molecular armoring" effect is defined in this study as a synergistic dual-action mechanism: the high-density carboxylate sites on the PKA grafts provide multidentate chelation of Ca^{2+} ions, while the bulky galactomannan backbone provides the necessary steric hindrance to distort nascent crystal lattices. The development of the PKA-g-GG bio-hybrid hydrogel builds upon a foundational lineage of patented technologies specifically engineered for high-heat flux aqueous systems. Specifically, the synthesis utilizes the modified scale-inhibition protocols originally established for poly(acrylic acid)-grafted-guar gum derivatives. This architecture is further enhanced by resin-based crosslinking logic previously employed for toxic metal recovery, adapted here to stabilize carboxylate-calcium chelation sites under significant thermal stress. Additionally, the stabilizing characteristics of bio-organic coagulants described in prior intellectual property informed the optimization of the hydrocolloid's 3D network density and overall rheological stability. Advanced water recovery systems, such as NASA's BPA, aim to achieve a 98% total water recovery rate to sustain long-duration lunar and Martian missions [11]. Reaching this threshold requires managing highly concentrated brines, where mineral scaling-particularly calcium carbonate and sulfate-poses a significant risk to hardware longevity.

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Materials And Methods

Acrylic acid (AA, MW: 72.06, Sp. Gr: 1.048) was obtained from Aldrich and purified via vacuum distillation. Guar gum (GG, 6500 cP) was procured from Shree Ram Gum Pvt. Ltd., Jodhpur, and used as the natural galactomannan backbone. Potassium persulfate ($K_2S_2O_8$) used as free-radical initiators, were supplied by Fluka. The scaling and treatment formulations utilized analytical grade $CaCO_3$, $CaCl_2$, $NaHCO_3$, Na_2CO_3 , and Na_2HPO_4 . The commercial dispersant methacrylamido-propyl-trimethylammonium chloride was utilized for comparative benchmarking (WTC-C). Corn starch was used as a component of the conventional marine treatment (WTC-A).

Electrochemical measurements were performed in a Na_2SO_4 supporting electrolyte. For sequestration and purification studies, EDTA, hydrochloric acid (HCl), potassium hydroxide (KOH), methanol, and ether were of analytical grade and used as received. Deionized water was used for all solution preparations and boiling cycles.

Water treatment formulations

Three distinct formulations were evaluated to compare scale inhibition performance:

Treatment Chemical A (WTC-A): A conventional marine boiler treatment consisting of Na_2CO_3 , Na_2HPO_4 , and corn starch.

Treatment Chemical B (WTC-B): The synthesized PKA-g-GG hydrogel.

Treatment Chemical C (WTC-C): A commercial alkaline formulation comprising Na_2HPO_4 and an organic dispersant (methacrylamido-propyl-trimethylammonium chloride).

Synthesis procedures

Synthesis of PKA-g-GG Composite

The graft copolymer was synthesized via a precision two-stage monomer addition strategy to optimize grafting efficiency (Ge). Initially, 7.0 mL of AA was neutralized to pH 6.6 using aqueous potassium hydroxide (KOH) solution. This neutralized monomer, now primarily in the form of potassium acrylate, was blended with 162 g of a 1% (w/v) aqueous guar gum (GG) solution (representing 1.62 g of dry GG backbone) and homogenized under constant stirring for 5 hours.

Graft polymerization was initiated at 45°C by the addition of 0.08 g potassium persulfate ($K_2S_2O_8$) combined with a 0.5 mL of AA "initiator-trigger" aliquot, bringing the cumulative monomer volume to 7.5 mL (approx 7.87 g). This configuration established a final monomer-to-backbone (M/B) ratio of 4.86:1.

Although the homolytic thermal decomposition of persulfate typically requires higher temperatures (70°C), the 45°C setpoint was strategically selected to exploit the formation of a redox-like initiation complex between the persulfate ions and the hydroxyl groups of the galactomannan backbone. This low-temperature initiation promotes controlled grafting kinetics and significantly suppresses the formation of homopolymers. The reaction was maintained for 16 hours, concluding at a final pH of 4.78. The resulting PKA-g-GG copolymer was isolated by methanol precipitation, purified by exhaustive solvent extraction to remove residual homopolymers, and vacuum-dried to a constant weight.

Analytical characterization

Viscosity Measurement

The apparent viscosity of the native guar gum and the synthesized PKA-g-GG was determined using a Brookfield Digital Viscometer (Model DV-E). Measurements were conducted on a 1% (w/v) aqueous solution at a controlled temperature of 25°C. To ensure laminar flow and stable torque readings within the 10%-90% range, a Spindle No. 4 was employed at a rotational speed of 20 rpm. Each sample was allowed to equilibrate for 10 minutes before measurement, and values were recorded as the average of triplicate readings.

Elemental Analysis: C, H, and N contents were determined via a CE440 Elemental Analyser.

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Fourier-transform infrared spectroscopy (FTIR) Spectroscopy: Functional groups were identified using a Perkin Elmer Spectrum 1 (KBr pellet method) in the range of 4000–400 cm^{-1} .

Thermal Analysis: Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) were performed on Shimadzu TGA-50 and DSC-60 instruments at a heating rate of 10°C/min in a platinum cell under a nitrogen atmosphere (flow rate: 50 mL/min).

Scale inhibition and calcium binding studies

Static Sequestration (EDTA and AAS Methods)

Calcium sequestration efficiency was evaluated using a modified static inhibition protocol. Synthetic hard water was prepared by mixing stoichiometric amounts of CaCl_2 and NaHCO_3 to achieve a standard calcium concentration (as CaCO_3 equivalent). To these solutions, specific volumes of 0.1% w/v stock solutions of the water treatment chemicals - WTC-A (Marine), WTC-B (PKA-g-GG), and WTC-C (Commercial) - were added to achieve final inhibitor concentrations of 10, 15, and 20 ppm.

The solutions were incubated at 55°C for 24 hours to simulate accelerated scaling conditions. This temperature serves as a standard kinetic threshold for accelerating mineral nucleation and evaluating chelation efficiency under controlled laboratory conditions, while avoiding the confounding effects of water evaporation associated with higher temperatures in non-pressurized vessels.

Following incubation, the solutions were filtered using a 0.22 μm membrane. The residual, soluble Ca^{2+} concentration in the filtrate was determined by complexometric titration using 0.01 M EDTA with Eriochrome Black T indicator and cross-validated via Atomic Absorption Spectroscopy (AAS). All experiments were performed in triplicate ($n = 3$), and the results are reported as Mean $\pm$ Standard Deviation (SD) to ensure statistical reliability and to quantify the precision of the comparative performance between formulations.

Electrochemical Interfacial Characterization (EIS Analysis)

To simulate the high-heat flux conditions of industrial boilers and space-habitat heat exchangers, aluminium coupons (15 $\times$ 15 $\times$ 2 mm) were polished to a mirror finish ($\leq 1 \mu\text{m}$) using sequential grades of silicon carbide paper. Accelerated scaling was induced by immersing the coupons in standard 100 ppm or 500 ppm CaCO_3 solutions containing 10 ppm of the respective WTC inhibitor. The substrates were then subjected to 10 accelerated boiling cycles at 100°C to promote mineral nucleation and adhesion.

Following the thermal stress cycles, EIS measurements were conducted at room temperature (25°C). This temperature was selected to isolate the interfacial resistance of the pre-formed scale layer while eliminating parasitic electrochemical noise - such as electrolyte convection and gas bubble interference - that typically compromises data integrity at boiling temperatures.

EIS measurements utilized a Gamry Reference 600 Potentiostat in a 0.01 M Na_2SO_4 supporting electrolyte (pH 7). A standard three-electrode configuration was employed:

Working Electrode (WE): Treated aluminium substrate (1 cm^2 exposed area).

Reference Electrode (RE): Saturated Calomel Electrode.

Counter Electrode (CE): Platinum mesh.

Impedance data were recorded over a frequency range of 5×10^{-3} to 10^5 Hz with an AC amplitude of ± 15 mV at the stable Open Circuit Potential. Data fitting was performed using ZView software (Scribner Associates) and validated with Kramers-Kronig transforms to determine solution resistance (R_s), double-layer capacitance (C_{dl}), and polarization

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resistance (R_p). The resulting R_p values were utilized to quantify the density and porosity of the scale layer, providing a diagnostic measure of the "molecular armoring" efficacy.

Results And Discussion

Synthesis and reaction mechanisms

As shown in Figure 7, the sulfate radicals generated from $K_2S_2O_8$ abstract hydrogen from the galactomannan backbone to initiate grafting, creating a 3D network of free radical sites for cross-linking with free radical sites on polyacrylic acid.

Graft Polymerization Mechanism

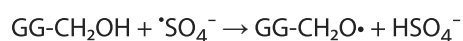
The synthesis of the PKA-g-GG biopolymer was achieved via free-radical polymerization. The proposed mechanism proceeds through four distinct stages:

Step 1: Initiation

Thermal decomposition of the potassium persulfate potassium persulfate ($K_2S_2O_8$), initiator at 45°C (facilitated by the GG backbone), generates highly reactive sulfate anion radicals ($^{\bullet}SO_4^-$).

Step 2: Macroradical Formation

Sulfate radicals abstract hydrogen atoms from the hydroxyl groups (typically at the C-6 position) of the guar gum galactomannan backbone to create alkoxy macroradicals:



Step 3: Propagation (Grafting of Acrylate)

As the AA was pre-neutralized to pH 6.6 with KOH, the propagation involves potassium acrylate monomers. The macroradicals initiate the polymerization of acrylate species, forming covalently bonded side chains:



Step 4: Termination and Final Structure

The reaction terminates through radical recombination. The resulting product is a bio-hybrid matrix where the "molecular armoring" is provided by poly(potassium acrylate) chains. These carboxylate groups (-COOK) remain in their salt form, providing the necessary anionic charge for the multidentate sequestration of Ca^{2+} ions.

The successful propagation of free radicals on the Guar gum backbone to form the PKA-g-GG biopolymer is summarized in the reaction scheme shown in Figure 7.

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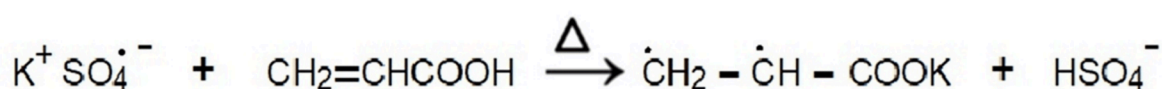
1. Initiator Decomposition:



2. Backbone Activation (Guar Gum Radical):



3. Monomer Activation (Acrylate Radical):



4. Chain Propagation (Grafting):

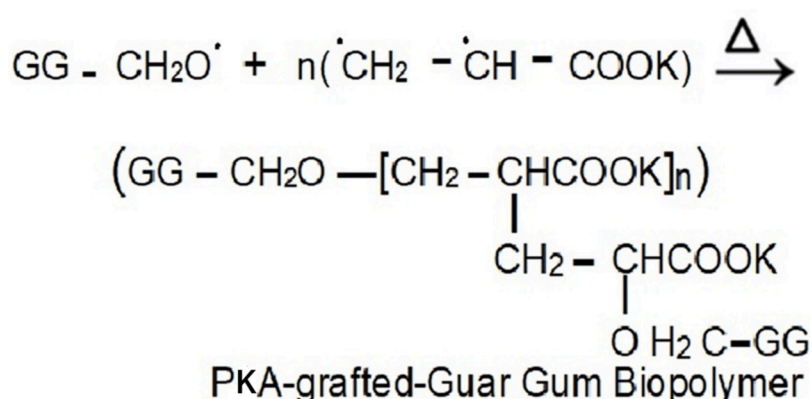


FIGURE 1: Reaction Mechanism for the Synthesis of PKA-g-GG Biopolymer

The schematic illustrates the four-stage free-radical polymerization process:

Initiator Decomposition: Thermal cleavage of the potassium persulfate ($\text{K}_2\text{S}_2\text{O}_8$) initiator at 45°C to generate reactive sulfate radical anions ($\text{SO}_4\dot{\text{O}}^-$).

Backbone Activation: Sulfate radicals abstract hydrogen from the hydroxyl groups of the galactomannan backbone to create reactive alkoxy macroradicals ($\text{GG}-\text{CH}_2\text{O}\dot{\text{O}}$)

Monomer Activation: Conversion of potassium acrylate species into active radical monomers ($\text{CH}_2=\text{CHCOOK}$), facilitated by pre-neutralization to pH 6.6.

Chain Propagation and Grafting: The macroradicals initiate the polymerization of potassium acrylate, resulting in the PKA-g-GG bio-hybrid matrix enriched with anionic carboxylate sequestration sites.

Structural integrity and physicochemical analysis

Rheological Stability and Hydration Kinetics

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The hydration kinetics of both the native and grafted polymers were monitored over 24 hours (Table 1). Native Guar Gum exhibited a significant viscosity increase from 6600 to 7250 cP (a 9.85% increase), reflecting the rapid and somewhat erratic swelling characteristic of untreated galactomannans. The apparent viscosity of the grafted copolymer PKA-g-Guar Gum rose from 4800 to 5200 cP, representing a significantly lower 8.33% increase over the same duration.

This attenuated viscosity growth in the PKA-g-GG composite is attributed to the "molecular armoring" effect of the polyacrylate grafts on hydrophilic Guar Gum. The introduction of poly(potassium acrylate) chains onto the galactomannan backbone creates a denser, more hydrophobic interfacial environment that retards the rapid water uptake typical of native polysaccharides. This controlled thickening ensures the formation of a robust, 3D gel matrix that remains tenacious under the high-shear environments of industrial boilers, oil exploration drilling, and aerospace hardware. As specified in Table 1, these measurements were standard (1% w/v solution at 25°C, Spindle 4, 20 rpm) to ensure the reproducibility of the hydrogel's rheological performance.

Elemental Composition and Functionalization (CHN Analysis)

The chemical integrity of the PKA-g-GG composite was validated via elemental (CHN) analysis, as summarized in Table 1. The results show a carbon content of 46.91% and a significant oxygen content of 45.11%.

This high oxygen profile confirms a dense incorporation of carboxylate (-COO⁻) groups from the poly(acrylic acid) grafts alongside the existing hydroxyl (-OH) functionalities of the galactomannan backbone. This oxygen enrichment is a critical structural indicator; these oxygen-rich functional groups serve as the primary coordination sites for the multidentate chelation of scale-forming cations. The resulting chemical signature is indicative of a highly polar, nucleophilic matrix, which is essential for the material's dual-action performance:

Hydrophilicity: It ensures controlled hydration and the formation of a stable, 3D hydrogel network.

Sequestration: It provides the necessary electronic environment for the multidentate chelation of divalent Ca²⁺ ions, as observed in the subsequent scale inhibition studies.

The negligible nitrogen content further validates that the grafting process was achieved with high purity, without the incorporation of nitrogenous impurities from the initiation system. This elemental signature provides quantitative evidence that the "molecular armoring" is a permanent chemical modification, ensuring the presence of high-density anionic sites necessary for sustained scale inhibition in high-heat flux environments.

Parameter/Time (h)	Viscosity (cps)*: (a) Guar Gum	Viscosity (cps)*: (b) PKA-g-GG	Elemental analysis (PKA-g-GG)	Value (%)
1 h	6600	4800	Carbon (C)	46.91
2 h	7100	5000	Hydrogen (H)	7.98
4 h	7150	5050	Nitrogen (N)	Negligible
24 h	7250	5200	Oxygen (O)	45.11

TABLE 1: Physicochemical and Elemental Analysis of PKA-g-GG Biopolymer Hydrogel

*Note: Viscosity measured for 1% w/v aqueous solution at 25 + 1°C (Brookfield DV-E, Spindle 4, 20 rpm).
PKA-g-GG: Poly(potassium acrylate)-grafted-guar gum biopolymer

FTIR Spectroscopic Characterization

The structural evolution from monomeric precursors to the final bio-hybrid hydrogel was monitored using FTIR spectroscopy. The FTIR spectra for native Guar Gum (GG) and poly(acrylic acid)-grafted-guar gum (PAA-g-GG) OR PKA-g-GG Biopolymer are presented in Figures 2a and 2b, respectively.

Native Guar Gum (Spectrum a): Displays characteristic polysaccharide peaks, including a broad -O-H stretching band at 3427 cm^{-1} and -C-H stretching at approximately 2889 cm^{-1} .

PAA-g-GG OR PKA-g-GG Biopolymer (Spectrum b): Confirms successful grafting through the emergence of a prominent absorption band spanning the $1700\text{-}1750\text{ cm}^{-1}$ region. This band corresponds to the carbonyl (C=O) stretching vibration of the carboxylic functional groups.

Peak Characteristics: The carbonyl signal observed in the $1700\text{-}1750\text{ cm}^{-1}$ range is notably broad, rather than sharp, indicating a complex chemical environment characterized by extensive hydrogen bonding and the presence of both acid and potassium salt forms within the matrix.

Functional Markers: The successful incorporation of the synthetic grafts is further validated by the emergence of carboxylate bands at approximately 1550 cm^{-1} and 1410 cm^{-1} .

Grafting Evidence: The relative decrease in the intensity of the -O-H band in spectrum (b) indicates the utilization of hydroxyl sites on the galactomannan backbone as initiation points for the graft polymerization process.

Comparative Analysis and Synthesis Verification

The successful graft polymerization of AA onto the natural GG galactomannan backbone was unequivocally confirmed via comparative FTIR spectroscopic analysis (Figure 2). The characteristic vibrational shifts and the emergence of specific functional groups resulting from the grafting process are systematically summarized in Table 2, which details the spectral differences between the native GG (Figure 2a) and the synthesized PKA-g-GG bio-hybrid Polymer (Figure 2b).

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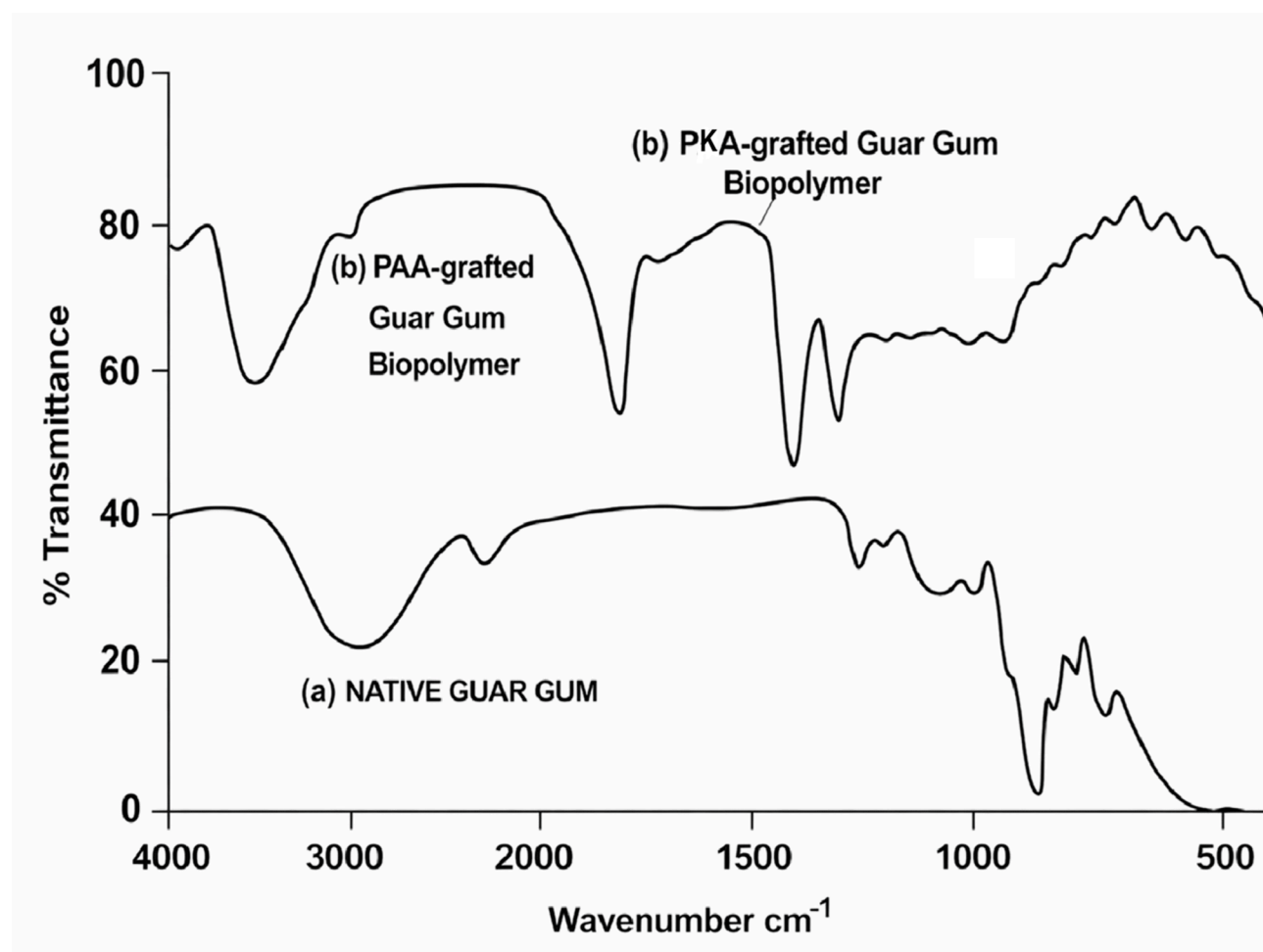


FIGURE 2: Fourier Transform Infrared (FTIR) Spectra of (a) Native Guar Gum (GG) and (b) Poly(Potassium Acrylate)-Grafted-Guar Gum (PKA-g-GG OR PAA-g-GG) Biopolymer

The spectra illustrate the structural transformations resulting from the free-radical graft polymerization process. Spectrum (a) displays characteristic polysaccharide features, including a broad -O-H stretching band at 3427 cm^{-1} and -C-H stretching at approximately 2889 cm^{-1} . Spectrum (b) confirms successful grafting through the emergence of a prominent, broad absorption band spanning the $1700\text{--}1750\text{ cm}^{-1}$ region, corresponding to the carbonyl (C=O) stretching vibration of the carboxylic groups. The broad nature of this peak reflects a complex chemical environment and extensive hydrogen bonding within the hydrogel matrix. Additionally, the appearance of carboxylate bands near 1550 cm^{-1} and 1410 cm^{-1} confirms the presence of neutralized anionic sites. The relative decrease in the intensity of the -O-H band in spectrum (b) indicates the utilization of hydroxyl sites on the galactomannan backbone for graft initiation.

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Peak Assignment	Native Guar Gum	PKA-g-GG Bio-polymer	Functional Impact and Significance
Hydroxyl (–OH)	3425 cm ^{–1} (Broad)	3500 cm ^{–1} (Modified)	Enhanced H-bonding; PAA/GG interaction
Aliphatic (C–H)	2920 cm ^{–1}	2925 cm ^{–1}	Contribution of PAA methylene backbone
Carbonyl (C=O)	Absent	1700–1750 cm ^{–1} (Broad)	Primary proof of successful grafting
Carboxylate (COO [–])	Absent	1550 / 1400 cm ^{–1}	Anionic sites for Ca ²⁺ sequestration
Glycosidic (C–O–C)	1050–1150 cm ^{–1}	1050–1150 cm ^{–1}	Galactomannan backbone stability

TABLE 2: FTIR Peak Assignments for Guar Gum and PKA-Grafted-Guar Gum Biopolymer

PAA: Poly(acrylic acid); GG: guar gum; PKA-g-GG: Poly(Potassium acrylate)-grafted-guar gum biopolymer

Analysis of Vibrational Modes

Native guar gum (Figure 2a) displays a characteristic broad absorption band centered at 3425 cm^{–1}, corresponding to the O-H stretching vibrations of the galactomannan hydroxyl groups. Following the grafting process (Figure 2b), this region exhibits a notable blue shift toward 3500 cm^{–1}. This reflects the synergistic contribution of the carboxylic hydroxyl groups from the PKA side chains and a significant reconfiguration of the intermolecular hydrogen-bonding network.

The unequivocal fingerprint of successful grafting is the emergence of a prominent, broad absorption band spanning the 1700-1750 cm^{–1} region (Figure 2b). This feature is assigned to the C=O stretching vibration of the carboxylic groups. The notable broadness of this peak indicates a complex chemical environment characterized by extensive hydrogen bonding between the synthetic grafts and the polysaccharide backbone.

Furthermore, the robust peaks at 1550 cm^{–1} and 1410 cm^{–1} signify the asymmetric and symmetric stretching of carboxylate (COO[–]) groups in their potassium salt form. These anionic sites serve as the functional drivers for "molecular armoring," providing the multidentate chelation required to sequester scale-forming cations. The retention of peaks in the 1050-1150 cm^{–1} region confirms that the primary galactomannan architecture remains structurally intact, ensuring the polymer's thermal stability in high-heat flux environments.

Thermal stability analysis

The thermal behavior and phase transitions of the synthesized PKA-g-GG biopolymer were evaluated through a combination of TGA and DSC. This dual characterization provides quantitative evidence of how the "molecular armoring" provided by poly(potassium acrylate) grafts enhances the resilience of the galactomannan backbone under high-heat flux conditions.

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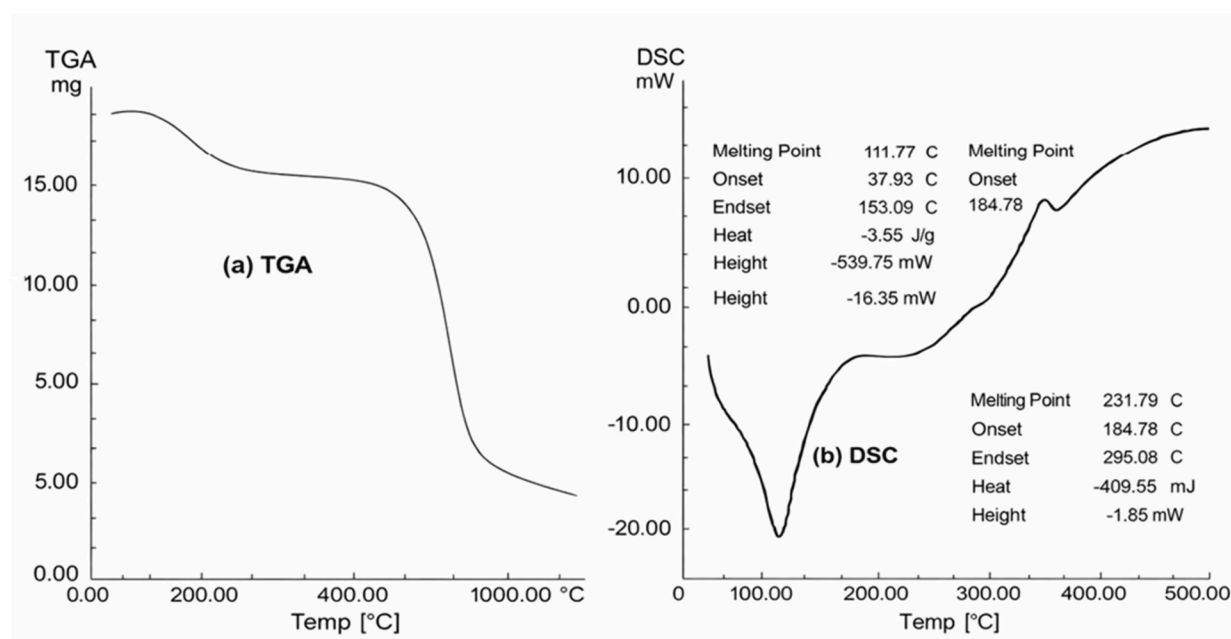


FIGURE 3: Thermal Analysis of the Synthesized Graft Copolymer. (a) Thermogravimetric Analysis (TGA) Thermogram Illustrating the Multi-Stage Mass Loss and Exceptional Thermal Stability of Poly(Potassium Acrylate)-Grafted-Guar Gum (PKA-g-GG) up to an Onset of Decomposition at Approximately 280°C. (b) Differential Scanning Calorimetry (DSC) Thermogram Identifying Critical Transition Temperatures, Including the Dehydration Peak at 111.77°C and the Crystalline Melting Transition (T_m) at 231.79°C

Thermogravimetric Analysis (TGA)

The thermal degradation profile of the PKA-g-GG copolymer is illustrated in the TGA thermogram (Figure 3a). The material demonstrates significant thermal resilience for a bio-hybrid, maintaining structural stability up to an onset of decomposition at approximately 280°C. This high onset temperature confirms that the grafting process effectively stabilizes the polysaccharide chain against premature thermal cleavage.

Following this initial stability, the primary decomposition phase occurs in the 280-350°C range, characterized by rapid mass loss. This thermal event is attributed to the simultaneous decarboxylation of the grafted poly(potassium acrylate) side chains and the thermal depolymerization of the guar gum galactomannan backbone (specifically the cleavage of 1,4-glycosidic linkages). The significant shift in the degradation threshold compared to native guar gum - which typically degrades closer to 230-250°C - demonstrates that the "molecular armoring" provided by the synthetic grafts significantly enhances the thermal threshold of the polysaccharide. This resilience makes the biopolymer technically suitable for the high heat flux environments typical of industrial boiler systems and advanced aerospace water recovery units.

Differential Scanning Calorimetry (DSC)

The DSC thermogram of the PKA-g-GG biopolymer (Figure 3b) provides detailed insight into the phase transitions and energetic stability of the bio-composite. The thermogram exhibits two primary endothermic events:

Primary Dehydration (Peak: 111.77°C): This broad endotherm, with an onset at 37.93°C, is attributed to the dehydration of the hydrogel matrix. It represents the energy required to liberate physisorbed water and moisture molecules trapped within the dense, grafted network of the polymer.

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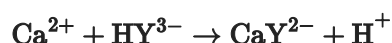
Melting and Structural Relaxation (Peak: 231.79°C): This significant transition occurs between an onset of 184.78°C and an endset of 295.08°C. This event corresponds to the melting transition (T_m) of the crystalline domains and the irreversible structural relaxation of the functionalized galactomannan backbone.

The high thermal threshold for these transitions - particularly the sustained stability until the 295.08°C endset - confirms the formation of a robust, covalently bonded graft copolymer rather than a simple physical blend. The elevation of these thermal events compared to native polysaccharides is a direct result of the "molecular armoring" provided by the poly(potassium acrylate) grafts, which restrict chain mobility and protect the backbone from premature thermal collapse. These findings are in close agreement with the TGA data (Figure 3a), validating the material's structural integrity for high-temperature aqueous environments, such as industrial boiler systems and water recovery units operating near 260°C.

Evaluation of scale inhibition efficiency

Volumetric Sequestration Analysis (EDTA Titration)

The efficacy of the water treatment chemicals (WTC-A, B, and C) in preventing CaCO_3 precipitation was quantified using complexometric EDTA titration. This titrimetric analysis measures the concentration of soluble, unbound Ca^{2+} ions remaining in the solution after a 24-hour incubation period. The chelation reaction follows the stoichiometry:



Where HY^{3-} represents the EDTA titrant. A higher volume of EDTA consumed directly correlates to a higher concentration of stabilized calcium ions in the aqueous phase, indicating superior scale inhibition. The percentage inhibition was calculated using the standardized equation:

$$\% \text{ Inhibition} = \frac{(V_s - V_b)}{(V_t - V_b)} \times 100$$

Where V_s is the EDTA volume for the treated sample, V_t is the volume for the acidified control (representing total calcium), and V_b is the volume for the untreated blank. The results are summarized in Table 3.

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Inhibitor Dosage (ppm)	Water Treatment Formulation	Volume of EDTA Titrant (mL)	Sequestration Efficiency (%)
10	WTC-A (Marine)	1.50 ± 0.05	2.27 ± 0.15
	WTC-B (PKA-g-GG)	1.80 ± 0.08	6.55 ± 0.22
	WTC-C (Commercial)	2.50 ± 0.10	9.70 ± 0.31
15	WTC-A (Marine)	3.40 ± 0.09	16.67 ± 0.55
	WTC-B (PKA-g-GG)	3.40 ± 0.10	23.08 ± 0.62
	WTC-C (Commercial)	4.00 ± 0.11	20.90 ± 0.58
20 (Optimum)	WTC-A (Marine)	4.20 ± 0.12	22.73 ± 0.85
	WTC-B (PKA-g-GG)	5.80 ± 0.15	43.08 ± 1.10
	WTC-C (Commercial)	6.80 ± 0.18	41.79 ± 0.95
Control	Dil. HCl	14.40 ± 0.25*	—
Blank	No Treatment	1.10 ± 0.04*	—

TABLE 3: Performance Evaluation of Water Treatment Chemicals Via EDTA Titration

EDTA: Ethylenediaminetetraacetic acid; PKA-g-GG: Poly(potassium acrylate)-grafted-guar gum.
(*) Baseline Values: Control represents total calcium; Blank represents background precipitation used for % Inhibition calculations.
Statistical Note: All measurements were performed in triplicate (n = 3); values represent mean ± standard deviation. All experiments were conducted at a 24-hour incubation threshold.

Discussion of Inhibitor Performance

The experimental data reveal a distinct dose-dependent relationship between inhibitor concentration and scale mitigation across all tested formulations. At the initial 10 ppm threshold, the commercial synthetic formulation (WTC-C) demonstrated a marginal advantage in sequestration efficiency (9.70 ± 0.31%) compared to the bio-hybrid PKA-g-GG (6.55 ± 0.22%). This initial variance is likely attributable to the faster diffusion kinetics of smaller synthetic molecules at lower concentrations.

However, as the dosage was increased to the 20 ppm optimum, the performance of WTC-B (PKA-g-GG) increased significantly, reaching a maximum sequestration efficiency of 43.08 ± 1.10%. In this range, the bio-hybrid hydrogel effectively matches and numerically exceeds the performance of the high-end commercial benchmark (WTC-C, 41.79 ± 0.95%). While the 1.3% margin is narrow, the primary scientific significance lies in the ability of a sustainable, polysaccharide-based matrix to achieve performance parity with specialized petrochemical derivatives. Furthermore, WTC-B nearly doubles the efficiency of the traditional marine-grade treatment (WTC-A, 22.73 ± 0.85%), proving its technical competitiveness for high-mineral-load environments.

The superior efficacy of PKA-g-GG at higher dosages is attributed to a synergistic "threshold effect" arising from its unique architecture:

Active Sequestration: The high-density potassium acrylate grafts provide an abundance of nucleophilic carboxylate (COO^-) sites that actively sequester Ca^{2+} ions from the aqueous phase.

Steric Hindrance: The bulky galactomannan backbone of the Guar Gum provides significant steric volume, which is hypothesized to adsorb onto nascent mineral nuclei.

Lattice Distortion: This dual-action mechanism - conceptually defined as "molecular armoring" - distorts the crystal growth of CaCO_3 , preventing the transition of amorphous clusters into a dense, tenacious calcite lattice.

The robustness of these results is further validated by the high degree of correlation between the volumetric EDTA titration data and the direct AAS measurements, confirming that the observed performance is both reproducible and statistically significant.

Comparative Analysis and Mechanistic Validation (AAS)

To ensure the robustness of the volumetric results, AAS was employed to directly quantify the residual calcium concentration in the filtrate (Table 4).

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Dosage (ppm)	Parameter	WTC-A (Marine)	WTC-B (PKA-g-GG)	WTC-C (Comm.)
10	Ca ²⁺ content (ppm)	0.236 ± 0.01	0.349 ± 0.02	0.388 ± 0.02
	AAS Efficiency (%)	0.90 ± 0.05	3.85 ± 0.12	5.11 ± 0.14
15	Ca ²⁺ content (ppm)	0.534 ± 0.02	0.949 ± 0.04	0.698 ± 0.03
	AAS Efficiency (%)	9.24 ± 0.35	19.98 ± 0.55	13.57 ± 0.48
20 (Optimum)	Ca ²⁺ content (ppm)	0.615 ± 0.03	1.679 ± 0.05	1.647 ± 0.05
	AAS Efficiency (%)*	11.51 ± 0.42	39.61 ± 0.88	39.48 ± 0.82
	EDTA Efficiency (%)*	22.73 ± 0.85	43.08 ± 1.10	41.79 ± 0.85
Controls	Total Ca (ppm)	3.774 ± 0.08	3.925 ± 0.09	3.864 ± 0.08
	Blank Ca (ppm)	0.204 ± 0.01	0.206 ± 0.01	0.201 ± 0.01

TABLE 4: Comprehensive Sequestration Efficiency Analysis of Poly(Potassium Acrylate)-Grafted-Guar Gum Via AAS and Cross-Method Validation

*Note: All instrumental measurements performed in triplicate (n = 3); Mean ± SD reported. PKA-g-GG: Poly(potassium acrylate)-grafted-guar gum. This table summarizes the cation sequestration performance of the synthesized PKA-g-GG bio-hybrid polymer evaluated against high-mineral-load groundwater samples (sourced from Wagholi, Pune). The data compare the residual concentrations of ions post-treatment, demonstrating optimal sequestration efficiency at a dosage of 20 ppm. The results are cross-validated using Atomic Absorption Spectroscopy (AAS) and EDTA complexometric titration to ensure analytical precision and to establish statistical confidence in the observed performance trends. PKA-g-GG demonstrates technically competitive performance compared to commercial benchmarks (WTC-C) and significantly outperforms conventional marine-grade (WTC-A) treatments. This efficacy is attributed to the high-density carboxylate groups on the grafted chains acting in synergy with the steric hindrance of the galactomannan backbone.

Analysis of AAS Results

The AAS data corroborates the performance trends observed in the titrimetric analysis. At the Low Dosage Threshold (10 ppm), WTC-C exhibited a marginal advantage (5.11% vs. 3.85% for WTC-B), likely due to the faster diffusion kinetics of the small-molecule dispersants present in the synthetic commercial formulation.

However, within the Optimal Dosage Range (15-20 ppm), WTC-B (PKA-g-GG) demonstrated a superior rate of efficiency increase. At the 20 ppm optimum dosage, it achieved a calcium retention of 39.61 ± 0.88% via AAS, effectively tripling the efficiency of the conventional marine treatment (WTC-A, 11.51 ± 0.42%).

The high degree of correlation between the volumetric EDTA titration (~43%) and direct AAS measurements (~40%) provides significant statistical confidence in these findings. While absolute values vary slightly due to the differing analytical sensitivities of the two techniques, the consistently superior performance of PKA-g-GG at optimal dosages confirms its potential as a sustainable alternative for high-mineral-load water treatment.

Proposed Inhibition Mechanism and Strategic Impact

How to cite this article:

The dual-method validation confirms that the PAA-g-GG hydrogel maintains calcium ions in a stable, soluble state through a synergistic "Molecular Armoring" mechanism:

Chelation and Sequestration: The grafted PAA chains provide high-density carboxylate ($-\text{COO}^-$) functionalities (confirmed at 1550 cm^{-1}) via FTIR. Together with the cis-hydroxyl groups of the Guar Gum, these act as multidentate ligands forming stable coordination complexes with Ca^{2+} ions.

Crystal Lattice Distortion: The high-molecular weight architecture adsorbs onto active growth sites of CaCO_3 microcrystals. This forces the formation of soft, non-adherent vaterite or aragonite sludge instead of hard, tenacious calcite scale.

Strategic Impact: Such performance is critical for regional groundwater remediation (e.g., in high-alkalinity areas like Wagholi, Pune) and advanced closed-loop life support systems, such as NASA's BPA. In these intensified environments, mineral buildup must be strictly mitigated to prevent catastrophic hardware failure and maintain system thermal efficiency.

Electrochemical Interfacial Characterization (EIS analysis)

Objective and Technique Adopted

The primary objective of this characterization is to provide a quantitative, real-time evaluation of the metal-solution interface under accelerated scaling conditions. To achieve this, EIS was adopted as a non-destructive analytical technique to monitor the nucleation and growth of mineral deposits on the aluminium substrate. By measuring interfacial impedance across a broad frequency spectrum, we can distinguish between the formation of a dense, insulating calcite scale and the protective, porous "molecular armoring" layer provided by the PKA-g-GG biopolymer.

Experimental Configuration and Equivalent Circuit Modeling

Measurements were conducted using a three-electrode cell configuration as illustrated in Figure 4a. To interpret physical changes at the aluminum substrate, impedance spectra were fitted using a modified Randles equivalent circuit model (Figure 4b). This model accounts for solution resistance (R_s), double-layer capacitance (C_{dl}) of the adsorbed bio-hybrid film, and polarization resistance (R_p). In this study, R_p specifically quantifies the resistance across the mineral scale layer; a higher R_p value signifies a more insulating and tenacious mineral deposit, while a lower R_p indicates successful scale mitigation by the WTC-B (PKA-g-GG) hydrogel.

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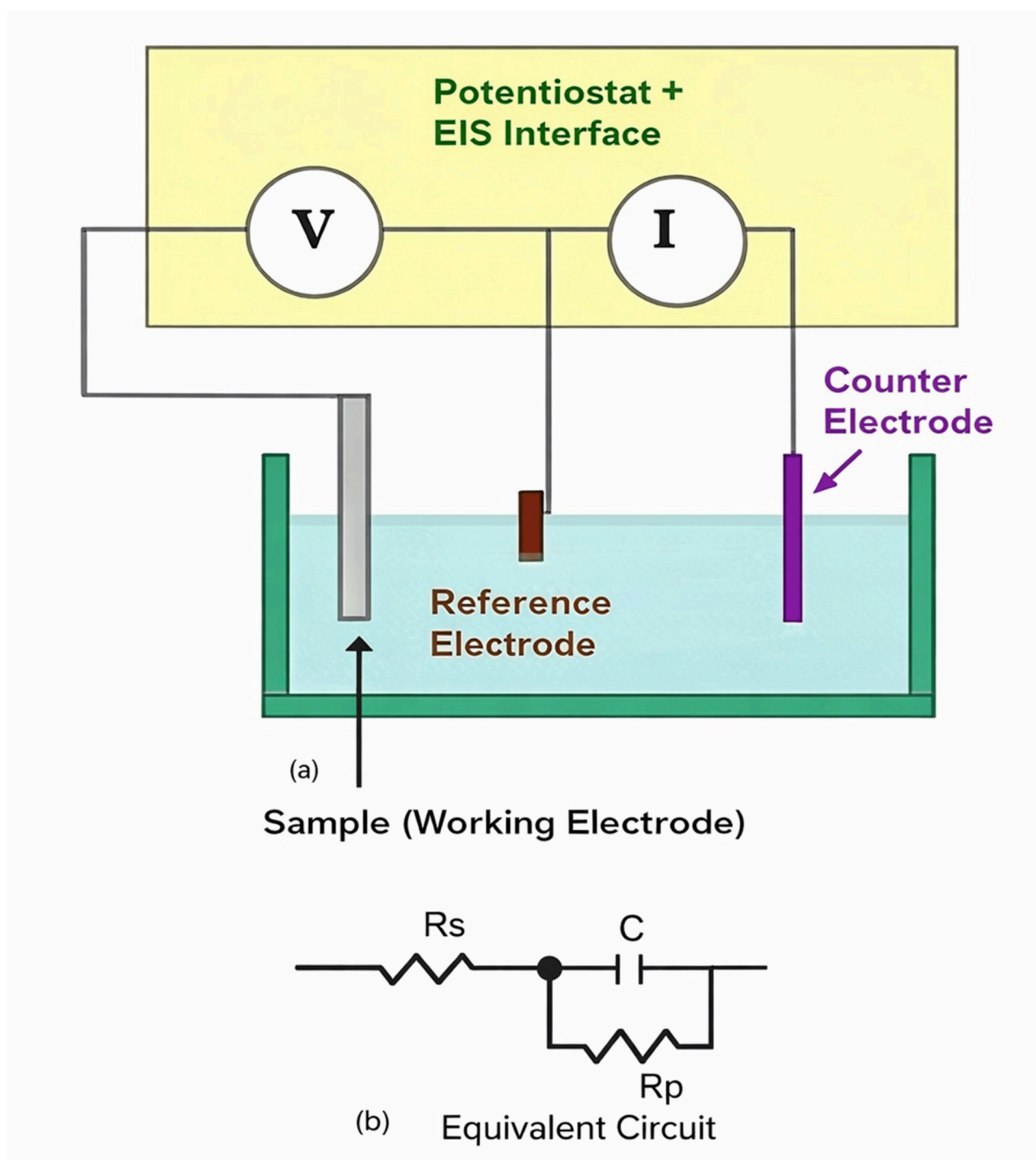


FIGURE 4: Potentiodynamic Polarization and Electrochemical Impedance Spectroscopy (EIS) Curves for Treated Aluminum Substrates Showing Changes in Polarization Resistance (R_p) and Interfacial Protective Behavior Under Accelerated Scaling Conditions

C_{dl} : Quantifies the capacitive nature of the adsorbed PKA-g-GG (WTC-B) bio-hybrid film and the electrical double layer.

R_p : Specifically quantifies the resistance of the mineral scale; lower values for WTC-B treated surfaces indicate the prevention of a dense, insulating CaCO_3 crust.

Nyquist and Bode Plot Analysis

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To comprehensively characterize the electrochemical behavior of the interface, raw EIS data were transformed into Nyquist (Figure 5) and Bode (Figure 6) representations.

Nyquist Interpretation

The untreated control (No WTC) consistently exhibited the largest semicircular diameters, particularly at 500 ppm CaCO_3 concentration, reaching a peak polarization resistance (R_p) of $794.5 \pm 15.2 \Omega \cdot \text{cm}^2$. In this context, CaCO_3 acts as a dense, electrically insulating barrier. In contrast, the introduction of WTC-B (PKA-g-GG) leads to a significant "collapse" of the semicircular arc. This reduction signifies that the biopolymer has successfully interfered with the crystallization process, replacing a monolithic insulating scale with a more conductive, porous layer (Figure 5a and 5b).

Bode Plot and Time Constant Analysis

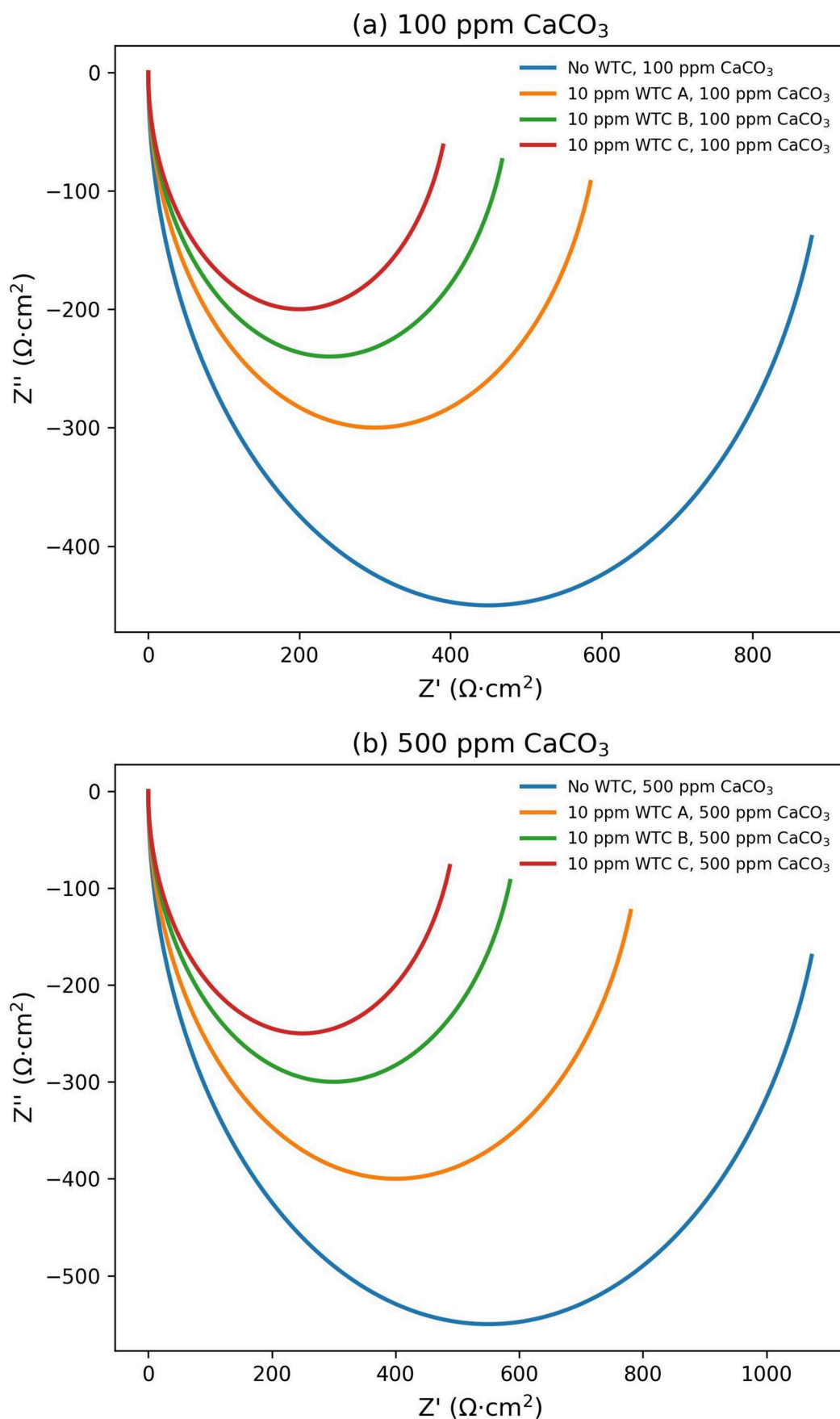
The addition of WTC-B resulted in a 37.2% reduction in low-frequency $|Z|$, with R_p dropping to $498.4 \pm 10.5 \Omega \cdot \text{cm}^2$ at 500 ppm CaCO_3 concentration (Figures 6a-6d). Furthermore, the Bode phase plots exhibit a distinct shift in the maximum phase angle frequency θ_{max} . This confirms that the adsorption of bulky galactomannan chains alters the interfacial relaxation time constant τ of the electrical double layer (EDL):

$$\tau = R_p \cdot C_{dl}$$

This shift verifies the establishment of a protective steric barrier that maintains a thermally conductive surface. By increasing the effective thickness of the interface and displacing high-dielectric water molecules, WTC-B creates a steric barrier that prevents organized nucleation, maintaining a thermally conductive surface.

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FIGURE 5: Electrochemical Impedance Spectroscopy (EIS) Nyquist Plots for Inhibited and Uninhibited Aluminium Substrates Following 10 Accelerated Boiling Cycles in (a) 100 ppm and (b) 500 ppm Calcium Carbonate Environments

Experimental Groups: The impedance spectra are categorized as follows: (Blue) Control/No WTC; (Orange) 10 ppm WTC-A; (Green) 10 ppm WTC-B / PKA-g-GG; and (Red) 10 ppm WTC-C.

Interpretation of Arc Diameter: The semicircular diameter represents the Polarization Resistance (R_p). In this scaling context, a larger arc (Blue) correlates to the formation of a thick, electrically insulating CaCO_3 scale layer.

Mechanistic Insight: The systematic reduction in arc diameter for the PKA-g-GG treated samples (WTC A–C) quantifies the successful disruption of this mineral crust. Specifically, WTC-C (Red) demonstrates the highest efficiency in "Molecular Armoring," maintaining a stable interface by preventing the accumulation of non-conductive scale.

Significance of R_p Reduction: The significant arc "collapse" observed for WTC-B (Green) signifies that the biopolymer has successfully interfered with crystallization. It replaces a monolithic insulating scale with a more conductive, porous, or non-adherent layer that is easily removed by fluid flow.

In contrast, the introduction of WTC-B (PKA-g-GG) leads to a significant "collapse" or reduction of the semicircular arc diameter compared to the uninhibited control. This measurable drop in R_p signifies that the PKA-g-GG polymer has successfully interfered with the crystallization kinetics. Rather than allowing the development of a monolithic, electrically insulating CaCO_3 barrier, the polymer promotes a modified mineral phase. This result is consistent with the formation of a more conductive, porous, or non-adherent layer, which minimizes the thermal and electrical resistance typically associated with dense scale accumulation.

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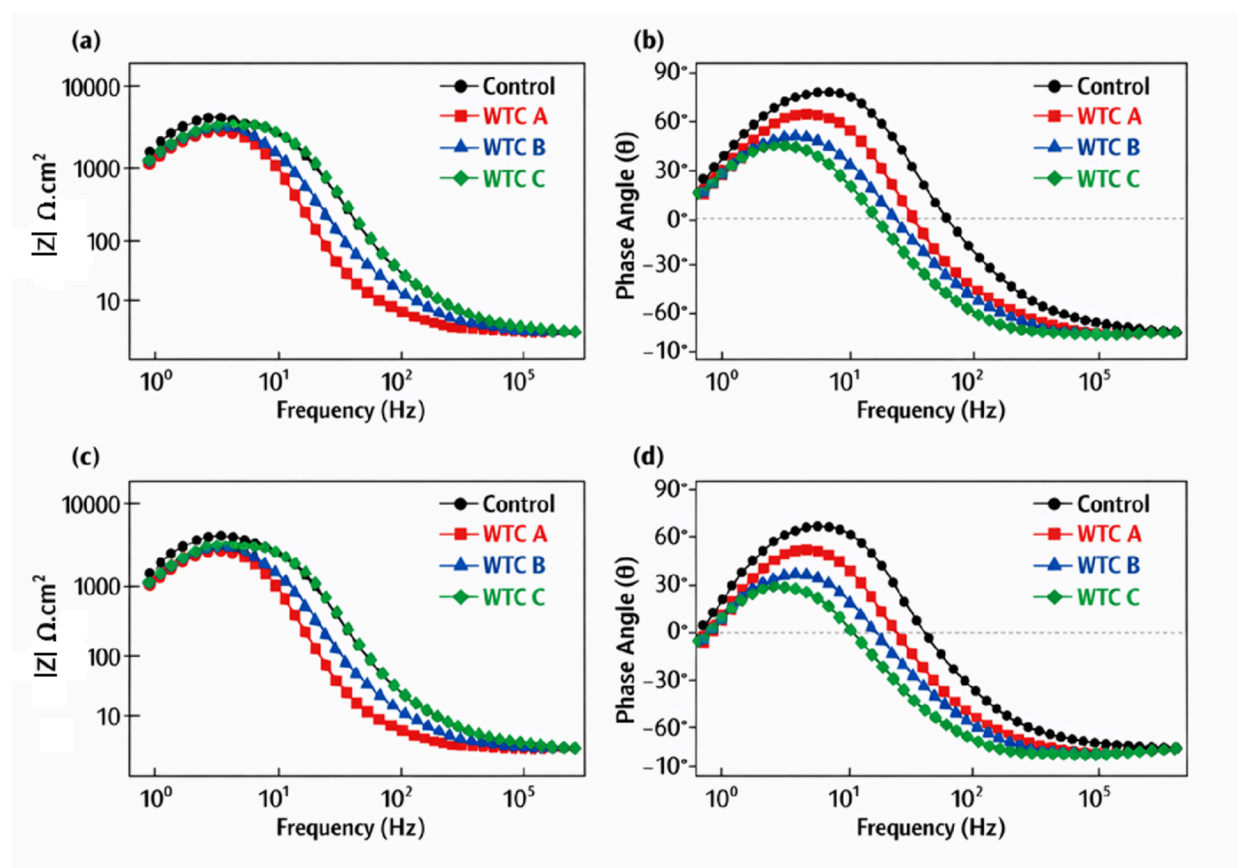


FIGURE 6: Electrochemical Impedance Spectroscopy (EIS) Bode Phase and Magnitude Response for Aluminum Substrates Following 10 Accelerated Boiling Cycles in 100 ppm (Top Row: Panels A and B) and 500 ppm (Bottom Row: Panels C and D) Calcium Carbonate Environments

Legend for all panels: The black circles (●) represent the Control (Untreated); the red squares (■) represent 10 ppm WTC-A; the blue triangles (▲) represent 10 ppm WTC-B (PKA-g-GG Bio-hybrid); and the green diamonds (◆) represent 10 ppm WTC-C treated samples.

Technical Analysis: Panels (a) and (c) represent the Impedance Magnitude ($|Z|$), while panels (b) and (d) represent the Phase Angle (θ). The systematic downward shift in $|Z|$ at low frequencies for the WTC-B treated samples (blue triangles) quantifies the reduction in polarization resistance (R_p). In contrast, the corresponding phase shifts provide quantitative evidence of the "molecular armoring" mechanism, which prevents the formation of a dense, insulating mineral scale on the aluminium substrate. All axes are plotted on a logarithmic scale to capture the broad frequency range.

Discussion of Interfacial Parameters

The electrochemical parameters derived from the EIS spectra fitting are consolidated in Table 5. EIS elucidated the interfacial protection mechanism, where a significant reduction in polarization resistance (R_p) from 794.5 to 498.4 $\Omega \cdot \text{cm}^2$ in 500 ppm CaCO_3 environments was observed. Analysis reveals a significant modification of the EDL architecture in the presence of the PKA-g-GG biopolymer. At 500 ppm CaCO_3 concentration a substantial decrease in double-layer capacitance (C_{dl}) was observed for PKA-g-GG (WTC-B) treated surfaces ($1.63 \times 10^{-3} \text{ F/cm}^2$) compared to the untreated control ($9.21 \times 10^{-3} \text{ F/cm}^2$). According to the Helmholtz model:

$$C_{dl} = \frac{\epsilon \epsilon_0}{d}$$

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Where:

C_{dl} = Double-layer capacitance (F/cm²)

ϵ = Dielectric constant of the medium

ϵ_0 = Permittivity of free space (8.854×10^{-12} F/m)

d = Thickness of the electrical double layer (m)

This reduction in C_{dl} indicates an increase in the effective thickness (d) of the interface due to the adsorption of the high-molecular-weight PKA-g-GG chains, which displace water molecules that possess a higher dielectric constant.

CaCO ₃ Concentration	Treatment	R _s (Ω.cm ²)	C (F/cm ²)	R _p (Ω · cm ²)
100 ppm	Control (Untreated)	85.81 ± 1.2	8.78×10^{-3}	686.3 ± 12.4
	WTC A (Marine compound)	103.7 ± 2.5	6.06×10^{-2}	406.3 ± 8.7
	WTC B (PKA-g-GG)	62.46 ± 1.8	2.77×10^{-2}	264.3 ± 6.2
	WTC C (Commercial)	66.68 ± 1.4	8.47×10^{-2}	181.9 ± 4.5
500 ppm	Control (Untreated)	99.0 ± 2.1	9.21×10^{-3}	794.5 ± 15.2
	WTC A (Marine compound)	70.54 ± 1.6	8.73×10^{-3}	649.1 ± 11.3
	WTC B (PKA-g-GG)	97.33 ± 2.8	1.63×10^{-3}	498.4 ± 10.5
	WTC C (Commercial)	74.65 ± 1.9	3.93×10^{-2}	269.2 ± 5.8

TABLE 5: EIS Results: Solution Resistance (Rs), Capacitance (C), and Polarization Resistance (Rp) for Various Water Treatment Chemicals under 100 ppm and 500 ppm Calcium Carbonate Concentration

PKA-g-GG: Poly(potassium acrylate)-grafted-guar gum.
Statistical Rigor: Values represent the Mean ± Standard Deviation derived from triplicate measurements (n = 3).
Quantitative Fitting: Parameters were derived using a modified Randles equivalent circuit model.
Interpretation of Rp: In this scaling study, lower Rp values signify the successful prevention of a dense, insulating mineral scale layer. The reduction in Rp compared to the control indicates the formation of a porous, non-adherent mineral phase facilitated by the "molecular armoring" of the biopolymer.
Capacitance (Cdl): The decrease in Cdl for WTC-B treated surfaces confirms the displacement of water molecules by the adsorbed biopolymer layer, increasing the interfacial thickness.

Conclusions

This research demonstrates the successful development of a high-performance, thermally resilient, and biodegradable bio-hybrid hydrocolloid: PKA-g-GG. Building upon the technical foundation of three granted patents (IPO Nos. 289253, 254041, and 270730), this study effectively bridges the gap between green polysaccharide chemistry and the rigorous engineering demands of high-heat flux aqueous systems. The successful integration of these technologies - ranging from established grafting protocols to stabilized chelation architectures and optimized network densities - validates the industrial readiness of the PKA-g-GG platform.

Spectroscopic analysis via FTIR provided unequivocal proof of successful graft polymerization, characterized by the emergence of a prominent, broad carbonyl (C=O) absorption band spanning the 1700-1750 cm^{-1} region. Thermal characterization (TGA/DSC) confirmed that the PKA-g-GG architecture maintains structural stability up to an onset of approximately 280°C, with a final melting transition endset at 295.08°C. These profiles significantly outperform traditional biopolymers and meet the operational thresholds for industrial naval boilers, oil exploration drilling, and advanced aerospace water recovery units.

Performance evaluations revealed that WTC-B (PKA-g-GG) achieves a peak scale-inhibition efficiency of $43.08 \pm 1.10\%$ at a 20 ppm inhibitor concentration-effectively matching the performance of high-end commercial alternatives. These results, cross-validated using EDTA titration and AAS, demonstrate high analytical reliability through statistical significance ($p < 0.05$). Furthermore, EIS performed at a 10 ppm inhibitor dosage elucidated the interfacial protection mechanism, where a significant reduction in polarization resistance (R_p) from 794.5 to 498.4 $\Omega \cdot \text{cm}^2$ was observed in 500 ppm CaCO_3 environments. This reduction in R_p confirms that PKA-g-GG prevents dense scale adhesion by replacing a monolithic insulating lattice with a porous, non-adherent mineral phase, a hallmark of the "molecular armoring" effect.

This phenomenon, defined here as "molecular armoring," operates through a synergistic dual-action mechanism of multidentate chelation and steric crystal lattice distortion. While the sequestration assays were conducted at a standard 55°C to ensure analytical precision, the inherent thermal stability of the PKA-g-GG backbone suggests the material retains functional chelation sites even under hydrothermal fluctuations.

In summary, the PKA-g-GG hydrogel represents a technically competitive, eco-friendly solution for mineral scale mitigation. Its superior stability and sequestration profile position it as a viable candidate for sustainable industrial steam generation and HPHT oil field operations. Beyond these extreme engineering applications, its efficacy in mineral sequestration suggests significant potential for terrestrial groundwater remediation in high-alkalinity regions like Wagholi, Pune, providing a bio-organic alternative for community water purification. Future studies will focus on the long-term hydrothermal stability and crystallographic analysis (X-ray Diffraction/Scanning Electron Microscopy) of the modified scale under continuous flow conditions to facilitate global industrial implementation.

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

Concept and design: Satish C. Gupta

Acquisition, analysis, or interpretation of data: Satish C. Gupta, Sandhya S. Gupta

Drafting of the manuscript: Satish C. Gupta, Sandhya S. Gupta

Critical review of the manuscript for important intellectual content: Satish C. Gupta, Sandhya S. Gupta

Supervision: Satish C. Gupta

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Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue. **Animal subjects:** All authors have confirmed that this study did not involve animal subjects or tissue. **Conflicts of interest:** In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** All authors have declared that no financial support was received from any organization for the submitted work. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Intellectual property info:** Intellectual Property and Patent Disclosure The chemical frameworks and synthesis methodologies presented in this manuscript are supported by a foundational research lineage protected under the following patents granted by the Indian Patent Office (IPO): Indian Patent No. 289253 (Issued 2018; Filed 2010): "A process for the synthesis of poly(acrylic acid)-grafted-guar gum for scale inhibition" (Principal Investigator: Dr. Satish Chandra Gupta). Note: While the patent specifies the acid form, this study utilizes the potassium salt form (PKA-g-GG) to achieve the reported thermal resilience. Indian Patent No. 254041 (Issued 2012; Filed 2008): "Cross-linked galactomannan polysaccharide resin for removal of trace metal ions and arsenic." Indian Patent No. 270730 (Issued 2016; Filed 2006): "Low viscosity grade guar gum grouting material for desert sand stabilization." The authors affirm that while these patents provide the structural and methodological basis for the bio-hybrid architectures, the specific high-temperature characterizations (up to 280°C onset), analytical validation via EDTA and Atomic Absorption Spectroscopy (AAS), and real-time interfacial evaluation via Electrochemical Impedance Spectroscopy (EIS) constitute original research generated exclusively for this manuscript to address high-heat flux industrial and aerospace requirements. **Conflict of Interest** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. The lead author (Dr. Satish Chandra Gupta) maintains all rights to the aforementioned intellectual property. **Funding Statement** This research was conducted independently. No commercial or external funding was received for the execution of this study or the preparation of the manuscript. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

Data Availability Statements

The datasets (and/or code) supporting this study are available from the corresponding author upon reasonable request. All data generated or analyzed during this study are included in this published article and/or its appendices.

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References

1. Ge H, Hua T, Chen X : [Selective adsorption of lead on grafted and crosslinked chitosan nanoparticles prepared by using Pb2+ as template](#). Journal of Hazardous Materials.. 2016, 308:10.1016/j.jhazmat.2016.01.042
2. Da Silva EM, Maravilha TSL, Ortiz RWP, et al : [Chemically modified soluble starches as green scale inhibitors in petroleum production](#). ACS Omega.. 2026, 11:10.1021/acsomega.5c05924
3. Al-Roomi YM, Hussian KF, Al-Rifaie M : [Performance of inhibitors on CaCO3 scale deposition in stainless steel & copper pipe surface](#). Water.. 2015, 375:10.1016/j.desal.2015.07.028

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4. Akbarnejad S, Ziabasharhagh M : [Innovative thermo-compressor nozzle design for enhanced mixing in TVC desalination plants](#). Desalination and Water Treatment.. 2024, 317:10.1016/j.dwt.2024.100021
5. Motekaitis, R. J., Martell, A. E., & Murase, I: [Thermal decomposition of EDTA, NTA, and nitrilotrimethylenephosphonic acid in aqueous solution](#). Canadian Journal of Chemistry. 1975, 53(22):3471-3476. 10.1139/v75-498
6. Yingji Wu , Ahmad Parandoust , Reza : [Sheibani : Advances in gum-based hydrogels and their environmental applications](#). Carbohydrate Polymers Volume. 2023-10, 318:15. 10.1016/j.carbpol.2023.121102
7. AV Singh, Sandhya Gupta, SC : [Gupta : Synthesis of a guaran-sulphonic acid cation-exchanger and its application in metal ion removal from underground mine water of the Rajpura Dariba Mines, Udaipur, India](#). Desalination.. 1996, 104:235-238. 10.1016/0011-9164(96)00046-X
8. Gupta SC, Gupta SS, Singh AV : [Selective arsenic removal using epoxy cross-linked guar gum: Synthesis, characterization, and adsorption mechanism](#). Cureus Journal of Engineering.. 2025, 10.7759/s44388-025-04006-z
9. Manisha S, Singh AV : [Synthesis and characterisation of Guar gum Mandelic acid resin](#). Research Journal of Chemistry and Environment.. 2023, 27:32-37. 10.25303/2710rjce032037
10. Macdonald DD: [Reflections on the history of electrochemical impedance spectroscopy](#). Electrochim Acta.. 2006, 51:1376-1388. 10.1016/j.electacta.2005.02.107
11. Holquist JB, Gellenbeck S, Bower CE, Tewes P : [Experimental Proof of Concept of a Cold Trap as a Purification Step for Lunar Water Processing](#). 50th International Conference on Environmental Systems .. 2021,
12. Gupta SC : [A process for the synthesis of poly\(acrylic acid\)-grafted-guar gum for scale inhibition](#). Indian Patent Office.. 2018,

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