

A Reproducible model for Experimental Validation and Green-Cost Assessment of Self-Healing Nanoencapsulated Coatings to Improve the Durability of Iraqi Steel Products

Saad Khaldon Rasheed¹

¹Iran University- Engineering civil Department.

*Corresponding Author: Saad Khaldon Rasheed

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ABSTRACT: This study presents a reproducible, plant-specific framework for the experimental validation and green-cost assessment of hybrid self-healing nan encapsulated epoxy coatings intended to improve the durability, storage stability, and market quality of Iraqi iron and steel products. The study is methodological and model-based; no coating synthesis, electrochemical impedance spectroscopy (EIS), salt-spray exposure, scanning electron microscopy (SEM), thermogravimetric analysis (TGA), adhesion testing, or concrete-bond testing was performed for the present manuscript. Five surface states are defined using fixed codes: uncoated carbon steel (B0), conventional epoxy (E1), graphene-oxide-modified epoxy (E2), IPDI-microcapsule epoxy (E3), and a hybrid self-healing nan encapsulated epoxy (E4). The proposed validation package specifies controlled substrate preparation, EIS before and after artificial scratching, potentiodynamic corrosion-rate estimation, 720 h neutral salt-spray exposure, pull-off adhesion, SEM, TGA, and a bond-performance gate for coated reinforcing steel. A durability-quality index (DQI) is formulated to guide Bayesian formulation selection, and sensitivity analysis is used to test the robustness of both technical and green-cost assumptions. The model-calibrated targets are not observed experimental results; they suggest that E4 could achieve a post-healing low-frequency impedance of $3.9 \times 10^{11} \text{ ohm cm}^2$, a calculated corrosion rate of $0.00075 \text{ mm y}^{-1}$, 0.35 mm underfilm corrosion after 720 h, and 95% adhesion retention, subject to experimental confirmation. The central plant-scale scenario estimates a net value added of $\text{USD } 32 \text{ t}^{-1}$ for $174,000 \text{ t y}^{-1}$ of selectively protected product. All technical and financial outputs require laboratory validation and factory accounting verification before commercial adoption.

Keywords: Iraqi steel, self-healing coatings, nanoencapsulation, corrosion protection, electrochemical impedance

spectroscopy, green-cost management, Bayesian optimization



1. INTRODUCTION

The durability of iron and steel products is determined not only by the properties inherent in them due to the technology of melting, rolling, and testing. At the stage of use of goods outside the mill, their surface can be damaged, which will lead to a decrease in commercial value, the need for more thorough preparation before use, and even increased susceptibility to atmospheric corrosion. This problem is most acute for steel products subject to use in the conditions of high humidity, for example, in coastal areas of industrialized countries, and in the transport of goods through oil fields, where exposure to chloride-containing dust and periodic mechanical damage can lead to local corrosion throughout the period of use of the products [1,2].

Conditions in Iraqi steel production and distribution require a protection strategy compatible with plant practice rather than a coating concept confined to laboratory conditions. A coating applied to reinforcing bars, sections, pipes, or oil-field products must withstand abrasion, edge damage, variable storage conditions, and handling-induced microcracks. Conventional epoxy systems provide an effective barrier while intact, however, once a scratch or pore creates an electrolyte pathway to the steel surface, underfilm corrosion can propagate. Accordingly, a product-upgrading strategy should protect both intact surfaces and mechanically damaged regions [3].

22*Corresponding author: Kldons81@gmail.com

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Self-healing anticorrosion coatings meet this need by incorporating microcapsules, nanocores, or functional fillers into the polymer matrix. While pH-sensitive nanocontainers may release inhibitors close to anodic or cathodic corrosion sites, mechanical rupture can release a healing agent into a fracture. Recent studies have advanced the discipline toward multi-component compositions whereby barrier improvement, inhibitor release, polymeric sealing, and data-assisted formulation selection all function in concert [4-7]. Still, a recurring flaw in applied publications on this subject is the mix of proposed, projected, and experimentally determined results free of a definite validation line.

This study develops a reproducible framework for designing and validating a hybrid self-healing nanoencapsulated epoxy coating for Iraqi steel products. It makes three contributions:

- (1) it establishes consistent B0-E4 surface-state codes and a traceable validation package, (2) it separates model-calibrated design targets from experimental observations and acceptance criteria, and (3) it links electrochemical durability to plant-scale green-cost assessment through transparent equations and sensitivity analysis. The study is deliberately prospective: (5) it specifies the experimental and accounting evidence required for validation but does not report completed laboratory trials.

2. Literature review and research gap

2.1 Passive barrier protection and its defect sensitivity

Organic epoxy coating is often employed as a corrosion protection material due to its ability to prevent electrolytic diffusion, oxygen and chlorides from accessing the steel/epoxy interface layer. Testing of organic coating performance usually entails electrochemical impedance spectroscopy (EIS), salt-spray test, adhesion maintenance and defect progression. Particularly useful is the EIS method due to low-frequency impedance being sensitive to barrier damage, moisture uptake and corrosion reactions occurring at the interface layer [8,9].

The susceptibility of barrier layers to attack via defects is one major problem with barrier coating protection. Reactive species could get to the metal substrate through defects created during manufacturing, handling, transportation scratches, heat expansion, handling of reinforcing steel bar, edges damage and abrasive actions at construction sites. At that point, corrosion reactions could occur and accumulate within the interface, causing adhesion loss and accelerating under-film creep reaction. This explains why the present structure takes into account scraping and repair conditions in its testing criteria.

2.2 Microcapsules, nanocontainers and hybrid self-healing mechanisms

Microcapsule-based self-healing systems store polymerizable or moisture-reactive healing agents inside a shell that ruptures when the coating is damaged. Nanocontainer systems store corrosion inhibitors inside porous silica, layered double hydroxides, halloysite nanotubes, metal-organic frameworks or polyelectrolyte-gated reservoirs. The release trigger may be pH variation, chloride attack, mechanical rupture or interfacial corrosion chemistry [10-12].

Hybrid systems are theoretically stronger than single-mechanism coatings because each component addresses a different failure path. Graphene oxide or related lamellar fillers increase diffusion tortuosity, polymeric microcapsules can physically seal cracks, pH-responsive nanocontainers deliver inhibitors to electrochemically active zones, hydrogen-bonding or dynamic polymer segments improve local repair and stress relaxation. The present coating architecture is therefore designed as a multi-mechanism system rather than as an additive-only epoxy modification.

2.3 Machine-learning-assisted formulation design

Machine-learning-assisted materials design is useful when formulation variables interact nonlinearly. In self-healing epoxy coatings, variables such as dry-film thickness, capsule loading, inhibitor loading, nanocontainer fraction, curing ratio, filler dispersion and surface preparation can interact in ways that are not efficiently explored by one-factor-at-a-time experiments. Bayesian optimization is suitable for small experimental budgets because it balances exploration of uncertain formulations and exploitation of promising candidates [13,14].

For coating research to remain reproducible, the machine-learning layer must specify the decision variables, numerical bounds, response variables, surrogate model, acquisition function and stopping rule. The revised framework therefore treats machine learning as a transparent formulation-selection tool rather than as an unexplained claim of optimization.

2.4 Product-level and green-cost relevance

Corrosion imposes direct repair and replacement costs and also carries an environmental burden because degraded steel often requires replacement by newly produced steel. In terms of carbon footprint, corrosion protection turns out to be an issue of durability and sustainability, rather than just a case of surface defects [15]. For Iraqi steel products, the relevant outcome from the factory will not just be high impedance values, it will also entail lower amounts of rework, rejection, better marketability in storage through installation, and material savings due to reduced corrosion.

The absence of a process that integrates intelligent coating formulation, realistic factory tests, statistically based acceptance, and environmentally sensitive cost accounting for Iraqi steel products forms the research question addressed here. The paper does not replace metallurgical quality control, it adds a surface-engineering layer that preserves the mechanical quality already achieved by steel production.

2.5 Synthesis of recent evidence and unresolved gap

Recent studies demonstrate substantial progress in the individual components used by the proposed architecture. Machine-learning-assisted discovery has been applied to self-healing epoxy formulation selection [5], while MCM-41-based nanocontainers and multifunctional nanocomposites have shown promising inhibitor-release and long-term corrosion-control mechanisms [16,17]. Related work on graphene-oxide-modified microcapsules, pH-responsive graphene-oxide systems, mesoporous silica nanocontainers, and PANI/graphene-oxide epoxy coatings further supports the technical plausibility of the barrier, release, and repair mechanisms represented in E4 [18,19]. These studies, however, primarily evaluate materials performance and do not integrate model calibration, mandatory experimental evidence, plant accounting, and avoided-emission consequences within one auditable decision protocol.

A second unresolved issue concerns product-specific acceptance. For coated reinforcing steel, corrosion resistance cannot be considered in isolation from steel-concrete bond performance. Recent bond studies and durability reviews indicate that coating chemistry and thickness may alter bond behavior and therefore require a dedicated acceptance gate [20,21]. The resulting research gap is not merely the absence of another coating formulation, it is the absence of a reproducible framework that links formulation selection, replicated laboratory verification, rebar bond compatibility, plant-scale green-cost accounting, and explicit commercial decision thresholds for the Iraqi steel context.

3. Proposed materials, formulation design, and reproducible validation methods

3.1 Plant context and steel-substrate definition

The industrial environment is a Basra/Khor Al-Zubair steel-product region, where electric-arc-furnace and rolling technologies can produce reinforcing bars, sections, and oil-field related products. The plant-level calculations are based on a nominal annual capacity of 580,000 t y⁻¹, and a selective protection share of 30%, which implies 174,000 t y⁻¹ of high-durability coated product. This combination corresponds to the central economic scenario, and is subject to verification through sensitivity analysis (see. Table 1).

The test coupons must be made from representative low-carbon or reinforcing steel. The grade, chemical composition, surface roughness, mill scale condition, and coupon dimensions must be reported. The surfaces should be prepared using the abrasive-blasting or mechanical cleaning method specified in the following section, if applicable, but with a visual cleanliness of Sa 2 ½, with a surface profile of 40-70 micrometres. The dry film thickness must be 90 +/- 5 micrometres for all coated coupons, so that differences in performance can be seen to be due to formulation and not film thickness [22].

Dry-film thickness (DFT) has two distinct roles in the framework. During Bayesian screening, DFT is a decision variable bounded between 70 and 120 micrometres. After a candidate formulation is selected, the confirmatory comparison among E1-E4 fixes DFT at 90 +/- 5 micrometres for all coated groups. This two-stage rule prevents thickness from confounding formulation effects while still allowing DFT optimization during the screening stage [23].

Table 1 Fixed coding of evaluated surface-engineering states

Code	Surface state	Functional role	Use in analysis
B0	Uncoated carbon steel	No engineered barrier or active healing	Baseline for storage deterioration and product-quality model
E1	Conventional epoxy, 90 ± 5 µm	Passive barrier against water, oxygen and chloride ingress	Industrial reference coating
E2	Epoxy + 0.05 wt% graphene oxide	Increases diffusion tortuosity and reduces permeation paths	Barrier-enhanced reference
E3	Epoxy + 10 wt% IPDI-type microcapsules	Crack-triggered local polymeric sealing	Handling-damage protection reference
E4	Hybrid self-healing nanoencapsulated epoxy	GO barrier + IPDI microcapsules + pH-responsive inhibitor nanocontainers +	Target high-durability Iraqi steel product

		dynamic bonding component	
Code	Surface state	Functional role	Use in analysis
B0	Uncoated carbon steel	No engineered barrier or active healing	Baseline for storage deterioration and product-quality model
E1	Conventional epoxy, $90 \pm 5 \mu\text{m}$	Passive barrier against water, oxygen and chloride ingress	Industrial reference coating
E2	Epoxy + 0.05 wt% graphene oxide	Increases diffusion tortuosity and reduces permeation paths	Barrier-enhanced reference

3.2 Coating architecture

The target E4 formulation contains an epoxy matrix, 0.05 wt% graphene oxide, IPDI-type polymeric microcapsules, ZIF-8@Ca pH-responsive microfillers, MCM-41/PEI/PSS inhibitor-loaded nanocontainers and a hydrogen-bonding self-healing component. The design principle is not maximum loading, but balanced dispersion (in figure 1). Excessive nanocontainer or capsule loading may create percolation defects, increase porosity, reduce adhesion and lower coating integrity [24].

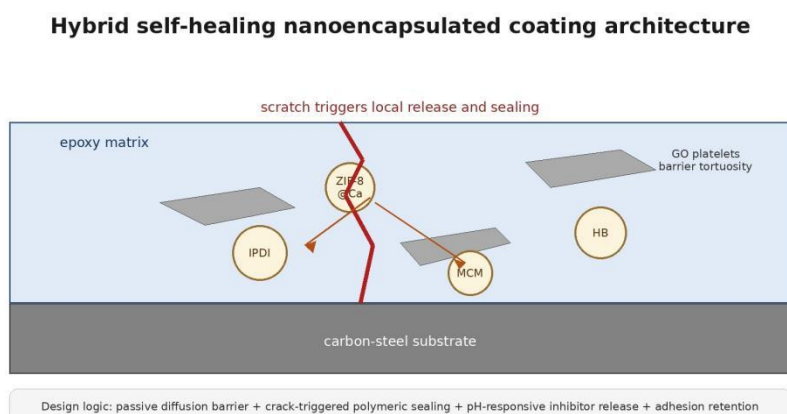


FIGURE 1 Schematic architecture of the hybrid self-healing nanoencapsulated coating.Sections

3.3 Machine-learning formulation selection

The formulation-selection stage uses a Latin-hypercube initialization followed by Bayesian optimization. The recommended minimum design begins with 20 initial formulations and continues with up to 30 sequential Bayesian candidates, subject to laboratory budget. A Gaussian-process surrogate with a Matérn kernel is recommended because it performs well in small-data continuous optimization. Expected improvement is used as the acquisition function, and the search stops when the improvement in the durability-quality index is below 1% for five consecutive candidates or when the experimental budget is exhausted [25].

The dependent variable is the durability-quality index (DQI), and every component is normalized to the range [0, 1] using prespecified technical thresholds. The baseline weights are 0.25 for low-frequency impedance (Z), 0.20 for the inverse corrosion rate (C), 0.15 each for adhesion retention (A), inverse underfilm corrosion width (S), and mechanical-quality retention (Y), and 0.10 for net value per tonne (V). This allocation gives 45% of the index to electrochemical corrosion control, 45% to physical integrity and product-quality retention, and 10% to economic feasibility (see- Table 2).

These initial weights were assigned a priori through an engineering-accounting rationale, they were not derived from an expert panel, the Analytical Hierarchy Process (AHP), or statistical estimation in the present study. They must therefore be treated as provisional decision weights rather than empirically validated coefficients. A future plant implementation should recalibrate them through a documented AHP or Delphi process involving corrosion, production, quality-control, commercial, and accounting specialists [26].

Table 2 Bayesian formulation-selection variables and recommended bounds

Variable	Symbol	Recommended range	Reason for inclusion
Dry-film thickness	DFT	70-120 μm	Optimization-stage variable, fixed at 90 +/- 5 micrometres during confirmatory comparison
GO fraction	G	0-0.15 wt%	Improves tortuosity, aggregation risk at high loading
IPDI microcapsules	M	0-12 wt%	Controls crack sealing capacity
ZIF-8@Ca microfillers	Z	0-8 wt%	pH-responsive inhibitor-release reservoir
MCM-41/PEI/PSS nanocontainers	N	0-3 wt%	Controlled release of corrosion inhibitor
Dynamic-bonding component	H	0-10 mol%	Local self-repair and stress relaxation
Curing ratio	R	0.9-1.1 stoichiometric ratio	Controls crosslink density and adhesion

$$DQI = 0.25Z^* + 0.20C^* + 0.15A^* + 0.15S^* + 0.15Y^* + 0.10V^* \quad (1)$$

Where,

Z = Logarithmic normalized low frequency impedance,

C = Normalized inverse of corrosion rate,

A = Adhesion retention factor,

S = Inverse of under film corrosion width,

Y = Mechanical quality ratio retention,

V = Net normalized value per tonne.

The weights should then be determined using sensitivity analysis on each coefficient by varying it by $\pm 20\%$.

Because the baseline weights are normative rather than empirically estimated, robustness must be tested by varying each coefficient by $\pm 20\%$, renormalizing the weights to sum to 1.00, and reporting whether the rank ordering of E1-E4 changes. The sensitivity analysis must also identify any weight combination that changes the preferred formulation.

3.4 Electrochemical and corrosion-rate testing

EIS is measured on intact, scratched and healed states after open-circuit stabilization in 3.5 wt% NaCl. The recommended frequency range is 10^5 to 10^{-2} Hz with a perturbation amplitude small enough to maintain approximate linearity. The main reporting value is $|Z|$ at 0.01 Hz, accompanied by equivalent-circuit fitting where justified and by confidence intervals across replicates.

The corrosion rate is calculated from corrosion current density using the standard expression below. To avoid the inconsistency present in many coating manuscripts, all reported corrosion-rate values are recomputed from the same equivalent weight and density assumptions.

$$CR = (0.00327 \times i_{corr} \times EW) / \rho \quad (2)$$

where CR is the corrosion rate in mm y^{-1} , i_{corr} is the corrosion current density in $\text{microampere cm}^{-2}$, EW is the equivalent weight of iron ($27.92 \text{ g equivalent}^{-1}$) and ρ is the steel density (7.87 g cm^{-3}). With these constants, $CR = 0.01160 i_{corr}$.

3.5 Salt-spray, adhesion, microscopy and thermal confirmation

Scribed coated panels will be exposed to neutral salt fog for 720 h under ASTM B117-type conditions. Underfilm corrosion width, rusting, blistering, delamination, and edge degradation will be recorded at the end of exposure. Pull-off adhesion will be measured before and after exposure using an ASTM D4541-type method, and the failure mode will be classified as cohesive, adhesive, or mixed. SEM will be used to verify capsule morphology, dispersion, and coating cross-section quality, while TGA will verify capsule loading, core fraction, and thermal stability before incorporation into the epoxy (see- Table 3) .

When the coated steel product is intended for reinforced concrete, the protocol adds a bond-performance test. A coating that improves corrosion resistance but causes unacceptable loss of steel-concrete bond should not be recommended for reinforcing bars without a design adjustment. Therefore, pull-out or beam-end testing is included as a product-specific acceptance gate [27].

Table 3 Experimental validation package and acceptance evidence

Component	Minimum requirement	Acceptance evidence
Replicates	At least five coated coupons per group for E1-E4, B0 used as uncoated deterioration reference	Mean, standard deviation, 95% confidence interval and full specimen log
EIS	Intact, scratched and healed states in 3.5 wt% NaCl	Bode/Nyquist plots, $ Z _{0.01\text{Hz}}$, healing efficiency, equivalent-circuit fit if statistically defensible
Salt spray	720 h scribed neutral salt-fog exposure	Underfilm creep width, rust grade, blistering and photographic record
SEM	Capsules and coating cross-sections	Capsule diameter distribution, shell continuity and dispersion quality
TGA	Capsules before mixing	Core loading percentage, onset temperature and residue fraction
Pull-off adhesion	Before and after ageing	MPa values, retention percentage and failure mode
Concrete bond gate	Required for coated rebar applications	Pull-out or bond-strength data relative to uncoated control

3.6 Statistical treatment

All quantitative outputs will be reported as mean $\pm$ standard deviation with 95% confidence intervals. Normality will be assessed using the Shapiro-Wilk test and residual diagnostics, and homogeneity of variance will be evaluated before one-way ANOVA. If parametric assumptions are violated, groups will be compared using the Kruskal-Wallis test. Holm correction will be applied to multiple comparisons. Effect sizes will be reported alongside p-values because practical coating improvement is more informative than statistical significance alone.

Logarithmic impedance recovery will be used to calculate self-healing efficiency without overstating performance. The healed condition will be compared with both the scratched and intact conditions. Values above 100% will be reported in raw form and explained before any truncation, because such values may arise from measurement scatter or inhibitor-release overcompensation.

$$\eta_{\text{H}} = [\log_{10}|Z|_{\text{healed}} - \log_{10}|Z|_{\text{scratched}}] / [\log_{10}|Z|_{\text{intact}} - \log_{10}|Z|_{\text{scratched}}] \times 100 \quad (3)$$

3.7 Plant-scale green cost model

The green-cost model converts coating performance into plant-scale value. Conservative, central, and high-adoption scenarios are reported separately to avoid conclusions based on a single assumption set. The model includes incremental coating cost, avoided rework and rejection, avoided claims and storage loss, a market premium for high-durability classification, and avoided corrosion-related material replacement. Every monetary input must be replaced with factory-verified accounting data before commercial adoption.

$$AR = (C_{RW, \text{baseline}} - C_{RW, \text{coated}}) / Qp \quad (4)$$

$$AC = (C_{CL, \text{baseline}} - C_{CL, \text{coated}}) / Qp \quad (5)$$

$$PM = P_{\text{coated}} - P_{\text{baseline}} \quad (6)$$

$$IC = (C_{\text{material}} + C_{\text{application}} + C_{\text{curing}} + C_{\text{inspection}}) / Qp \quad (7)$$

$$NV = (AR + AC + PM) - IC \quad (8)$$

$$ANG = Qp \times NV \quad (9)$$

$$CO2e_{\text{avoided}} = M_{\text{avoided}} \times EF_{\text{steel}} \quad (10)$$

where AR is avoided rework and rejection per tonne, AC is avoided claims and storage loss per tonne, PM is the price premium per tonne, IC is incremental coating cost per tonne, C_{RW} and C_{CL} are total rework/rejection and claims/storage-loss costs in the baseline and coated scenarios, P is selling price, Qp is protected product volume, NV is net value added per tonne, ANG is annual net gain, M_{avoided} is avoided material replacement or rework, and EF_{steel} is the emission factor per tonne of avoided steel replacement [28].

4. Model-calibrated outputs and experimental acceptance thresholds

No physical coating synthesis or experimental testing was conducted for this manuscript. The numerical values in this section are model-calibrated design targets and proposed acceptance thresholds; they are not laboratory observations and must not be interpreted as evidence of coating performance. Before publication as an experimentally validated study, Tables 4-7 must be supplemented or replaced with measured means, standard deviations, confidence intervals,

Bode/Nyquist and polarization curves, SEM micrographs, TGA curves, salt-spray photographs, and adhesion and bond-test records.

4.1 Formulation-selection output

The E4 configuration is identified as the preferred model-calibrated candidate because it balances barrier effectiveness, inhibitor release, local crack healing, adhesion, and economic feasibility. The model penalizes high-load formulations that may increase porosity or weaken film integrity and also penalizes low-load formulations that may provide insufficient active-healing capacity. This selection is a design hypothesis to be tested experimentally, not a measured ranking (in table 4).

Table 4 Model-calibrated durability-quality index by fixed surface code

Code	Predicted DQI	Probability of meeting high-durability target	Dominant limiting factor
B0	0.08	0.00	No engineered barrier or active-healing function
E1	0.41	0.18	Scratch sensitivity and underfilm corrosion
E2	0.58	0.46	Barrier improves, but active repair remains limited
E3	0.73	0.71	Crack sealing occurs, but inhibitor release is limited
E4	0.91	0.96	Balanced barrier, pH-responsive inhibitor release, crack sealing and adhesion retention

4.2 Electrochemical design targets

As per the unified equation for the corrosion rate, the target E4 conditions yield an approximate increase in the magnitude of low frequency impedance by about 5.91 when compared with scratched conventional epoxy coating and a reduction in corrosion rate by 97.6 percent when compared with E1 conditions (in table 5). The value of corrosion rate is calculated using i_{corr} as shown by the formula $CR = 0.01160 i_{corr}$.

Table 5 Model-calibrated electrochemical design targets for the evaluated surface states

Code	$\log_{10} Z $ at 0.01 Hz after damage/healing	$ Z $ at 0.01 Hz (ohm cm^2)	i_{corr} (microampere cm^{-2})	Calculated CR (mm y^{-1})	Reduction vs E1 (%)
B0	3.25	1.78×10^3	12.40	0.1440	Not applicable
E1	5.68	4.79×10^5	2.70	0.0313	Reference
E2	7.32	2.09×10^7	0.68	0.0079	74.8
E3	9.82	6.61×10^9	0.21	0.0024	92.2
E4	11.59	3.89×10^{11}	0.065	0.00075	97.6

4.3 Scratch, salt-spray and adhesion acceptance targets

For the planned validation, E4 will be accepted only if it demonstrates limited scribe creep, high adhesion retention after ageing, and reproducible microcrack closure relative to E1-E3. The final experimental manuscript must include dated photographs of the scribed panels and adhesion dollies, together with specimen identifiers and replicate statistics (in table 6).

Table 6 Model-calibrated scratch, salt-spray, and adhesion acceptance targets

Code	Underfilm corrosion after 720 h (mm)	Adhesion retention after exposure (%)	Microcrack closure after 24 h (%)	Interpretation
B0	General rusting	Not applicable	0	Unacceptable for high-value stored product
E1	7.80	22	0	Severe scribe corrosion and edge degradation
E2	3.60	61	8	Moderate degradation, barrier effect dominant

E3	1.20	82	68	Localized healing along scratches
E4	0.35	95	93	Minor local staining, product remains marketable

4.4 Product-quality preservation model

The model does not assume that a coating increases the intrinsic metallurgical yield strength of steel. Instead, it estimates preservation of the effective load-bearing area through reduced pitting and mass loss. The values in Table 7 are scenario outputs and must not be reported as measured mechanical properties.

Table 7 Model-calibrated product-quality preservation under a 90-day aggressive-storage scenario

Indicator	B0	E1	E2	E3	E4	Improvement of E4 vs B0
Mass loss (%)	5.80	2.10	1.10	0.72	0.35	94.0% lower mass loss
Maximum pit depth (μm)	410	165	95	58	24	94.1% lower pit severity
Effective cross-section retained (%)	91.5	95.8	97.2	98.6	99.2	7.7 percentage-point gain
Retained yield-strength ratio (%)	90.9	95.4	96.8	98.4	99.1	8.2 percentage-point gain
Predicted rejection risk after outdoor storage (%)	12.5	7.4	5.0	3.6	2.1	83.2% lower rejection risk
Estimated storage-to-installation marketability (%)	84	91	94	96	98	14 percentage-point gain

4.5 Green-cost sensitivity results

The central scenario estimates net value added of $\text{USD } 32 \text{ t}^{-1}$ and an annual net gain of USD 5.57 million for $174,000 \text{ t y}^{-1}$ of protected product (in table Table 8). The result remains favorable only when avoided rework, avoided claims, and the price premium exceed the incremental coating cost. It is therefore a sensitivity-based business case, not a factory-verified profit statement (in table Table 9).

Table 8 Plant-scale green-cost assumptions and model-calibrated central calculation

Variable	Central value	Calculation basis
Nominal plant capacity	$580,000 \text{ t y}^{-1}$	Industrial scenario assumption for Basra/Khor Al-Zubair context
Protected high-durability share	30%	Selective conversion of rebar, section, pipe and oil-field product lines
Protected product volume	$174,000 \text{ t y}^{-1}$	$580,000 \times 0.30$
Incremental coating cost	$\text{USD } 31 \text{ t}^{-1}$	Materials, application, curing, inspection and quality control
Avoided rework and rejection	$\text{USD } 29 \text{ t}^{-1}$	Lower rust cleaning, reclassification, cutting loss and rejected dispatch
Avoided claims and storage loss	$\text{USD } 11 \text{ t}^{-1}$	Reduced market complaints and outdoor-storage downgrading
Price premium	$\text{USD } 23 \text{ t}^{-1}$	High-durability product classification
Net value added	$\text{USD } 32 \text{ t}^{-1}$	$29 + 11 + 23 - 31$
Annual net gain	$\text{USD } 5.57 \text{ million y}^{-1}$	$174,000 \times 32$
Avoided steel replacement/rework	$2,088 \text{ t y}^{-1}$	1.2% avoided material loss over protected volume
Avoided emissions	$3,132 \text{ t CO}_2\text{e y}^{-1}$	$2,088 \times 1.5 \text{ t CO}_2\text{e t}^{-1} \text{ steel}$

Table 9 Sensitivity scenarios for plant-scale adoption

Scenario	Protected volume ($t\ y^{-1}$)	Incremental cost ($USD\ t^{-1}$)	Gross benefit ($USD\ t^{-1}$)	Net value ($USD\ t^{-1}$)	Annual net gain ($USD\ million\ y^{-1}$)	Avoided CO_2e ($t\ y^{-1}$)
Conservative	87,000	35	48	13	1.13	1,044
Central	174,000	31	63	32	5.57	3,132
High adoption	232,000	29	75	46	10.67	5,568

5. Discussion and implementation pathway

5.1 Technical interpretation

The model assigns E4 the highest DQI because it combines four complementary functions: a graphene-oxide diffusion barrier, crack-triggered polymeric sealing, pH-responsive inhibitor release, and dynamic-bond-assisted local repair. E1 provides only passive protection; E2 improves diffusion tortuosity but lacks an active repair mechanism; and E3 provides crack sealing without the full inhibitor-release architecture. The modeled advantage of E4 therefore arises from functional complementarity rather than from any single additive.

This interpretation is consistent with recent reports on machine-learning-assisted coating design [5], MCM-41 inhibitor nanocontainers [6], multifunctional self-healing nanocomposites [7], and graphene-oxide or pH-responsive coating systems [12-15]. The present framework extends those studies by combining their mechanisms with a fixed validation code, a DQI, a bond-performance gate, and plant-scale green-cost equations. Nevertheless, the predicted E4 ranking cannot establish superiority until replicated electrochemical, microscopy, salt-spray, adhesion, and bond data are available.

The unified corrosion-rate calculation improves internal auditability because every value is derived from the same equivalent weight and steel-density assumptions. This prevents apparent performance differences from being created by inconsistent unit conversion. In the eventual experimental study, the same calculation should be reported together with raw i_{corr} values, fitting uncertainty, and replicate-level data rather than only summary targets.

5.2 Product-quality interpretation

The product-quality model concerns preservation rather than enhancement of the steel produced by melting, casting, rolling, or heat treatment. For reinforcing bars, reduced pitting may preserve effective cross-section and surface acceptability; for sections, pipes, and oil-field products, the principal benefits are reduced storage deterioration, fewer claims, and improved marketability. These outcomes must be verified through mass-loss, pit-depth, and mechanical-retention measurements.

For coated reinforcing bars, corrosion resistance alone is insufficient. Recent bond-performance research and durability reviews [16,17] show why pull-out or beam-end testing is necessary: a coating that performs well in EIS and salt spray but causes an unacceptable reduction in steel-concrete bond cannot pass the product-specific acceptance gate.

5.3 Green-cost interpretation

The economic model is a scenario analysis rather than a verified factory balance sheet. Its outcome depends on coating materials, labor, curing, inspection, rejection rates, storage duration, claims, and the market premium actually obtainable for a high-durability product. From a green-cost management perspective, the relevant benefit is the reduction of hidden failure costs-rework, rejection, replacement, claims, and premature material loss-rather than the coating expenditure viewed in isolation. The conservative, central, and high-adoption scenarios therefore function as decision boundaries for a pilot line, not as forecasts of realized profit.

5.4 Limitations and validation requirements

The principal limitation is the absence of physical synthesis and experimental validation. The DQI, electrochemical values, salt-spray response, adhesion retention, product-quality indicators, and green-cost values are model-calibrated targets or scenarios. They cannot support causal or commercial claims until the proposed tests are completed with adequate replication, uncertainty reporting, and factory-verified cost records.

A second limitation is that the DQI weights are provisional and may reflect the priorities embedded in the present framework. External validation should therefore include expert-based weight calibration, out-of-sample formulation trials, and sensitivity analysis across steel grades, surface preparation conditions, storage environments, and protected-product volumes.

5.5 Practical implementation sequence

Sequence of recommended implementation:

1. Selection of an appropriate steel grade and surface preparation process representative of factory
2. Production of four E1-E4 coating batches under the same dry-film thickness and curing conditions
3. Verification of capsule morphology through SEM and TGA prior to corrosion testing
4. Electrochemical impedance spectroscopy for intact, scratched, and healed states
5. Exposure test for 720 hours in salt spray with photos;
6. Pull-off adhesion tests, and concrete adhesion for rebars;
7. Statistical analysis of differences with effect sizes
8. Green cost analysis update using accounting from factory

Pilot testing cannot start with full-scale factory coating operation but rather with controlled coupon tests and production of a sample batch.

Only after the E4 coating system satisfies electrochemical, adhesion, salt-spray resistance and practical application acceptance gates can a factory consider producing a high-durability product range.

6. Conclusions

This study contributes a reproducible framework for the experimental validation and green-cost assessment of hybrid self-healing nanoencapsulated coatings for Iraqi steel products; it does not claim experimentally verified coating performance.

The fixed B0-E4 coding links formulation, testing, model calibration, and decision criteria without changing the meaning of a surface state across sections. The proposed validation package requires replicated EIS and polarization testing, 720 h salt spray, SEM, TGA, pull-off adhesion, and a steel-concrete bond gate when the product is reinforcing bar.

The DQI and Bayesian-search structure provide a transparent method for balancing electrochemical protection, physical integrity, product-quality retention, and economic feasibility. The baseline weights are provisional and must be recalibrated and stress-tested before plant adoption.

The model-calibrated values in Tables 4-7 are acceptance-oriented hypotheses, not observed results. Accordingly, the manuscript should be upgraded to an experimental article only after measured curves, micrographs, photographs, replicate statistics, and uncertainty estimates are incorporated.

Commercial implementation should proceed through controlled coupon testing, a pilot batch, factory-verified green-cost accounting, and predefined technical and financial acceptance gates. Only when those requirements are satisfied can the E4 architecture be considered for a high-durability Iraqi steel-product line.

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CONFLICTS OF INTEREST

The authors declare no conflict of interest

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