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RESEARCH ARTICLE

Smart Polymeric Liners for Internal Corrosion Control in Wet Sour Gas Pipelines: Integrating Nanostructured Materials and AI-Driven Predictive Modelling

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Abstract: Sour gas pipelines suffer severe integrity challenges due to internal corrosiondriven by hydrogen sulfide (H_2S) and carbon dioxide (CO_2). This study introducesa novel smart polymeric liner enhanced with nanostructured graphene andnanosilica fillers, integrated into a CFD→AI→digital twin workflow for predictive corrosion control. Unlike conventional inhibitorsand coatings, the liner combines nanostructural impermeability, mechanicalreinforcement, and tailored interfacial adhesion strategies to suppress corrosionin API 5L X65 steel pipelines. CFD simulations demonstrate that bare pipelinesexhibit extreme corrosion rates, while lined systems reduce rates tonear-negligible levels (< 0.002 mm/year). An AI regression model trained on CFDoutputs and experimental data achieves an $R^2 \approx 0.99$, enablingaccurate forecasts of corrosion rates and remaining service life. Integration into adigital twin framework allows real-time monitoring, predictive maintenancescheduling, and dynamic risk assessment. This work establishes a next-generationmaterial–digital solution for extending the service life of sour gas pipelines.

Keywords: smart materials, polymeric liners, sour gas corrosion, Hydrogen Sulfide (H_2S), Computational Fluid Dynamics (CFD), Artificial Intelligence (AI), machine learning

1 Introduction

Sour gas pipelines, which are essential for global energy transport, face severe risks of internal corrosion and hydrogeninduced degradation due to the presence of hydrogen sulfide (H_2S) and carbon dioxide (CO_2) [1, 2]. Conventional mitigation methods, such as chemical inhibitors, cathodic protection, and metallic coatings, often lack durability and consistency under aggressive sour gas conditions [3, 4], underscoring the need for advanced solutions.

Smart polymeric liners enhanced with nanostructured materials offer a promising approach by providing impermeability, chemical resistance, and strong adhesion to steel substrates [5, 6]. Recent advances in nanocomposites, incorporating fillers such as silica, graphene, and titanium dioxide, have improved barrier properties and mechanical strength, addressing limitations of earlier polymer coatings [7, 8].

Complementing material innovation, computational fluid dynamics (CFD) and artificial intelligence (AI) provide powerful tools for predictive integrity management [9, 10]. CFD enables mechanistic modelling of fluid flow, species transport, and localized corrosion, while AI learns from experimental and simulation data to forecast corrosion rates and pipeline remaining life [11]. Integrated within digital twin frameworks, these approaches enable real-time monitoring, predictive maintenance, and optimized asset management [12]. Recent investigations highlight the superior corrosion resistance of polymer nanocomposites reinforced with graphene and silica fillers.

Polymer/Graphene Systems: Avantgarde polymer/graphene nanocomposites demonstrate enhanced impermeability, mechanical robustness, and electrochemical stability under aggressive sour gas conditions. Studies report significant reductions in corrosion current density and improved adhesion compared to conventional epoxy coatings [13, 14]. A 2025 review emphasised graphene's multifunctionality—high surface area, conductivity, and inertness, making it a versatile filler for both energy storage and corrosion protection applications [15].

Polymer/NanoSilica Systems: Silica/polymer nanocomposites leverage tunable morphology and high surface area to improve barrier performance. Experimental work shows reduced water

and gas permeability, improved mechanical strength, and better dispersion of silica nanoparticles within epoxy matrices [16]. A 2024 review of Nanobased smart coatings confirmed silica's role in enhancing corrosion inhibition while reducing reliance on toxic inhibitors [17].

The performance of nanocomposite liners is governed by several synergistic mechanisms:

(1) Tortuosity and Reduced Permeability: Impermeable fillers (graphene sheets, silica particles) force corrosive species to follow longer, more tortuous diffusion paths, thereby reducing permeation rates [18].

(2) Mechanical Reinforcement: Nanofillers improve tensile strength, modulus, and fracture toughness, mitigating liner damage under sour gas pressure and temperature fluctuations [19].

(3) Interfacial Adhesion Strategies: Surface functionalization of graphene and silica (e.g., silane coupling agents, oxygenated groups) enhances chemical bonding with polymer matrices, reducing delamination and improving longterm durability [20].

Industrial deployment of polymer liners in sour gas pipelines has been explored, but challenges remain:

(1) Non-Metallic Pipe (NMP) Liners: Widely used as internal linings, these systems face permeation damage, creep, fatigue, and installation defects, limiting their reliability in high-pressure sour environments [21].

(2) SourResistant Line Pipe Steels: While steels with SSC resistance are available, failures under severe H_2S conditions highlight the need for hybrid solutions combining metallic substrates with advanced polymeric liners [22].

(3) Case Studies: Lifecycle analyses of sour wet gas pipelines (2018–2024) reveal fluctuating corrosion risks, underscoring the importance of adaptive liner systems integrated with predictive monitoring [23].

Coupling advanced liners with CFD and AIdriven models enhances predictive reliability:

(1) CFD simulations capture localised flow regimes and species transport in sour gas pipelines, identifying high-risk zones for liner degradation [24].

(2) AI models trained on experimental and simulation datasets forecast corrosion rates and liner performance, enabling real-time monitoring within digital twin frameworks [25].

Despite decades of research into sour gas pipeline integrity, three critical gaps remain:

(1) Materials Gap: Conventional polymer liners and metallic coatings suffer from permeability, poor adhesion, and mechanical instability under high H_2S/CO_2 conditions. While nanostructured composites show promise, their performance in realistic operating environments has not been systematically validated.

(2) Mechanistic Modelling Gap: CFD has been applied to study fluid flow and corrosion interactions, but it is often computationally intensive, casespecific, and not scalable for predictive integrity management across diverse pipeline systems.

(3) Predictive Analytics Gap: AI models have been explored in corrosion research, but they are rarely integrated with mechanistic CFD outputs and realtime sensor data, limiting their ability to forecast corrosion rates and remaining life with industrial reliability.

(4) Digital Integration Gap: Digital twin frameworks are emerging in energy infrastructure, yet no prior work has combined advanced nanostructured liners with CFDdriven AI predictive modelling and IoT sensor integration for sour gas pipelines.

1.1 Unique Contribution of This Work

This study addresses these gaps by introducing a material mechanistic digital integration:

(1) Materials Innovation: A smart polymeric liner formulated with graphene (0.5 wt%) and Nanosilica (1 wt%) fillers, designed for impermeability, mechanical reinforcement, and enhanced adhesion to API 5L X65 steel.

(2) Mechanistic CFD Modelling: High-fidelity CFD simulations quantify corrosion rates, wall shear stress, and hydraulic performance under wet sour gas conditions, providing mechanistic insight into liner effectiveness.

(3) AI Predictive Modelling: A regression framework trained on CFD outputs and experimental data achieves $R^2 \approx 0.99$, enabling accurate forecasts of corrosion rates and pipeline remaining life.

(4) Digital Twin Integration: The CFD–AI workflow is embedded into a digital twin architecture with IoT sensor data, enabling realtime monitoring, predictive maintenance scheduling, and dynamic risk assessment.

1.2 Why This Is Novel

This is the first integrated framework that unites:

(1) Nanostructured smart liners (materials science),

(2) Mechanistic CFD simulations (engineering physics),

(3) AI regression models (data science), and

(4) Digital twin workflows (industrial informatics).

1.3 Problem Statement

Sour gas pipelines carrying hydrocarbons with hydrogen sulfide (H_2S) and carbon dioxide (CO_2) are highly prone to internal corrosion and hydrogen-induced degradation [1, 13]. Conventional methods, including chemical inhibitors, cathodic protection, and metallic coatings, often fail to provide consistent longterm protection, leading to accelerated material loss, reduced service life, and increased failure risk [3, 4].

Polymeric liners offer an alternative, but traditional formulations exhibit permeability, poor adhesion, and mechanical instability under sour conditions [14, 15]. Recent advances in nanostructured composites are promising, yet their performance in real-world operating environments remains insufficiently validated [16, 17].

Pipeline integrity management is further limited by the absence of predictive tools that combine mechanistic modelling with real-time monitoring. While CFD provides valuable insights into flow–corrosion interactions, it is computationally intensive and lacks scalability [9, 10]. AI, trained on CFD outputs and sensor data, can deliver accurate corrosion forecasts and life predictions [11]. Still, integration with smart materials in a unified digital twin framework has not been fully explored [12, 25].

This gap highlights the urgent need for a combined material–digital solution that suppresses corrosion while enabling predictive integrity management in sour gas pipelines.

1.4 Research Objectives

The study aims to:

(1) Evaluate the corrosion suppression performance of smart polymeric liners enhanced with nanostructured materials in API 5L X65 steel pipelines under sour gas conditions.

(2) Model fluid dynamics and corrosion mechanisms using CFD simulations to quantify corrosion rates, wall shear stress, pressure drop, and hydraulic performance in bare versus lined pipelines.

(3) Develop and validate an AI-driven predictive model trained on CFD outputs and operational parameters to forecast corrosion rates and pipeline remaining life with high accuracy.

(4) Integrate CFD, AI, and IoT sensor data into a digital twin workflow for real-time monitoring, predictive maintenance scheduling, and dynamic risk assessment.

(5) Assess industrial feasibility by analyzing the impact of smart polymeric liners on hydraulic performance, operational efficiency, and long-term pipeline integrity management.

2 Methodology

2.1 Case Study Description

An offshore gas pipeline in the northern Caspian Sea was selected as a representative case study due to its premature failure under extreme sour service conditions. The geometry and operating conditions were derived from Ref. [8] (pp. 112–115), which documents reservoir depth, pressure, and gas composition for the offshore field.

The pipeline was initially constructed from carbon steel (API 5L X65), which experienced rapid internal corrosion and hydrogeninduced cracking due to high hydrogen sulfide (H_2S) concentrations in the transported gas [1]. The reservoir lies approximately 4,200 m below the seabed, with a pressure of $\sim$77.72 MPa and a temperature of $\sim$100°C [13].

The gas composition (mol%) includes methane (58.83%), hydrogen sulfide (17.69%), ethane (9.10%), carbon dioxide (5.06%), propane (4.69%), and minor fractions of butanes, pentanes, nitrogen, and water vapour [2]. This composition classifies the gas as wet, sour, and flammable, with a molar mass of 19.26 g/mol and a density of 0.807 kg/m^3 at 20°C [9].

The case highlights the importance of accurate fluid characterization, material selection, and predictive modelling in sour gas pipeline design [14]. Where data were synthesized (e.g., permeability coefficients for polymer liners), these are clearly labelled as assumptions in Table 1, with sensitivity runs provided to show the impact of varying input values.

Table 1 Materia data table

Property	Value	Source	Notes
Tensile strength (polymer liner)	65 MPa	Ref. **[15]**	Literature value for epoxy/graphene composite
Elastic modulus	2.5 GPa	Ref. [16]	Measured in Nanosilica reinforced epoxy
Gas permeability (CO_2)	1.2×10^{-14} m^2/s	Assumed	Sensitivity analysis included
Inhibitor flux	0.05 mol/m^2·s	Ref. [17]	Derived from accelerated test data
H_2S tolerance	$\leq$ 500 ppm	Design target	Rephrased as target; sensitivity runs at 250 ppm and 1000 ppm
CO_2 resistance	$\leq$ 10% mol fraction	Literature [19]	
Elongation at break	12%	ASTM D638 tensile test [5]	Elongation at break
Thermal stability	180°C	DSC/TGA analysis [18]	Thermal stability

2.2 Material Design

2.2.1 Liner Composition and Microstructure

The smart polymeric liner was designed as a multi-layered nanocomposite to withstand wet sour-gas environments. Its formulation balances chemical resistance, mechanical strength, and impermeability (see Table 1).

(1) Polymer Matrix Selection: A blend of polyether ether ketone (PEEK) and polyvinylidene fluoride (PVDF) was chosen for its high chemical resistance, thermal stability, and compatibility with nanofillers [17]. PEEK provides mechanical strength and thermal endurance, while PVDF contributes flexibility and chemical inertness.

(2) Nanostructured Additives:
- Graphene nanoplatelets (0.5 wt%): Improve barrier properties by creating tortuous diffusion paths for H_2S/CO_2.
- Nanosilica (1 wt%): Reinforce mechanical strength and reduce permeability through uniform dispersion [5, 7].

(3) Dispersion Assumptions: Nanofillers were assumed to be uniformly dispersed within the polymer matrix, aided by surface functionalization (e.g., silane coupling agents for silica, oxygenated groups for graphene) to improve interfacial adhesion [20].

(4) Interfacial Adhesion Strategy: Coupling agents and plasma surface treatment were assumed to enhance bonding between polymer and steel substrate, reducing delamination risk.

(5) Expected Microstructure:
- Total liner thickness: ~3 mm.
- Nanofiller distribution: homogeneous across the bulk, with graphene aligned parallel to the steel surface for maximum barrier effect.
- Multilayer design: base adhesion layer, nanocomposite barrier layer, and optional sensor-embedded top layer.

2.2.2 Durability and Failure Mechanisms

The longterm performance of the liner depends on its ability to resist degradation under sour service conditions.

(1) Expected Degradation Modes:
A. Delamination at the steel–polymer interface due to poor adhesion or cyclic stresses.
B. Permeation of H_2S/CO_2 through microdefects, leading to localized corrosion.
C. Mechanical wear from turbulent flow and entrained solids.
D. Thermal cycling causes microcracking and reduced adhesion.

(2) Adhesion Testing Methods: A. Pulloff tests (ASTM D4541) to quantify adhesion strength.
B. Peel tests (ASTM D903) for interfacial toughness.
C. Shear tests for substrate bonding evaluation.

(3) Accelerated Ageing Tests: A. Autoclave exposure at elevated H_2S/CO_2 concentrations.
B. Salt spray testing (ASTM B117) for chloride resistance.
C. Electrochemical impedance spectroscopy (EIS) to monitor barrier integrity.

(4) Projected Service Life: With conservative assumptions (liner efficiency 85%, adhesion strength reduced by 20% after 10 years), the liner is projected to exceed 20 years of service life under $\leq$ 500 ppm H_2S. Sensitivity analysis shows:
A. A 50% increase in permeability reduces corrosion suppression efficiency by ~30%.
B. A 25% reduction in adhesion strength shortens remaining life by ~5–7 years.

2.3 Computational Fluid Dynamics (CFD) Modelling

CFD simulations were conducted using ANSYS Fluent to evaluate flow behaviour, corrosion potential, and hydraulic performance under two gas compositions:

(1) Dry Natural Gas (baseline condition).

(2) Wet Sour Gas (containing CO_2, H_2S, and H_2O) [23].

Key steps included:

(1) Geometry and Mesh Generation: Pipeline geometry was discretized with a fine mesh to capture near-wall turbulence and species transport [24].

(2) Boundary Conditions: Inlet velocity of 20 m/s, operating pressure and temperature consistent with offshore field reservoir conditions [25].

(3) Species Transport Modelling: H_2S and CO_2 diffusion and reaction kinetics were incorporated to simulate corrosion potential [26].

(4) Wall Interaction: A user-defined function (UDF) was implemented to model dynamic flux behaviour of the smart liner, including inhibitor release and species flux adjustment [27].

Flux calculations followed the logic:

$$\begin{aligned} \text{Inhibitor}_{\text{flux}} &= \text{BASE}_{\text{INHIBITOR}_{\text{FLUX}}} \times \text{LINER}_{\text{EFFICIENCY}} \times \text{NANO}_{\text{ENHANCEMENT}} \times \text{AI}_{\text{COEFFICIENT}} \\ \text{H}_2\text{S}_{\text{flux}} &= \text{BASE}_{\text{H2S}_{\text{FLUX}}} \times \text{LINER}_{\text{EFFICIENCY}} \times \text{AI}_{\text{COEFFICIENT}} \\ \text{CO}_{2\,\text{flux}} &= \text{BASE}_{\text{CO2}_{\text{FLUX}}} \times \text{LINER}_{\text{EFFICIENCY}} \times \text{AI}_{\text{COEFFICIENT}} \\ \text{Combined}_{\text{flux}} &= \text{Inhibitor}_{\text{flux}} + \text{H}_2\text{S}_{\text{flux}} + \text{CO}_{2\,\text{flux}} \end{aligned} \tag{1}$$

where AI COEFFICIENT dynamically increased with time to mimic adaptive corrosion control [28].

2.3.1 Governing Equation

This study models sour gas transport in a pipeline using ANSYS Fluent and applies the Navier-Stokes equations in cylindrical coordinates to conserve mass and momentum, focusing on compressible flow continuity equations [9].

Conservation of Mass: Continuity Equation

Conservation of Momentum: Newton's Second Law

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V}\right) = 0 \tag{2}$$

$$\rho \frac{\partial \vec{V}}{\partial t} + \rho \left(\vec{V} \cdot \nabla\right) \vec{V} = -\nabla p + \rho \vec{g} + \nabla \cdot T_{ij} \tag{3}$$

Where, ρ represents density, p is the static pressure, $\rho\vec{g}$ is the gravitational forces,

Species transport equation

The conservation equation$_{forchemica}$l species can be solved to obtain the following form:

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \nabla \cdot \left(\rho \vec{v} Y_i\right) = -\nabla \cdot \vec{J}_i + R_i + S_i \tag{4}$$

Where, R_i = the net rate of production of species i by chemical reaction; S_i= the rate of creation by addition from the dispersed phase, plus any user-defined sources

The pipe flow model employs the SST κ–ω turbulence model, which combines the κ–ϵ approach for near-wall conditions with the κ–ω method for regions away from the wall. This integration enhances accuracy while reducing the effects of wall grid density. This widely used method in turbulent flow analysis utilizes Reynolds-Averaged Navier-Stokes (RANS)

simulations to analyze the hydraulic properties of near-wall flow, balancing precision and computational efficiency [9].

2.3.2 Corrosion Modelling: Combined Effect of H_2O, CO_2 and H_2S

In wet sour gas environments, corrosion becomes highly aggressive due to the synergistic effects of CO_2, H_2S, and water [1–13]:

(1) CO_2 dissolves in water to form carbonic acid (H_2CO_3), lowering pH and accelerating general corrosion.

(2) H_2S promotes localized attack and cracking.

(3) Water vapour acts as the electrolyte, enabling electrochemical reactions.

The anodic process involves iron oxidation:

$$Fe \rightarrow Fe^{2+} + 2e^{-} \tag{5}$$

Cathodic reactions reduce hydrogen ions or carbonic acid:

$$H_2CO_3 + 2e^{-} \rightarrow H_2 + HCO_3^{-} \tag{6}$$

$$2H^{+} + 2e^{-} \rightarrow H_2 \tag{7}$$

These reactions produce hydrogen gas and bicarbonate ions. The equilibrium potentials, calculated via the Nernst Equation, are approximately -0.582 V for iron dissolution and -0.294 V for hydrogen reduction, defining the electrochemical conditions for corrosion simulations [13].

2.4 AI Predictive Modelling

To complement CFD simulations, an AI regression workflow was developed in Python using Scikitlearn, Pandas, NumPy, and Plotly [29]. The workflow was designed to integrate mechanistic outputs with synthetic and experimental datasets, enabling predictive corrosion modelling under sour gas conditions.

2.4.1 Data Sources

(1) CFD Outputs: Pressure, temperature, wall shear stress, and localized H_2S/CO_2 concentrations [30].

(2) Synthetic Data: Parametric runs representing worstcase sour service conditions (Appendix A).

(3) Experimental Points: Published electrochemical corrosion rates and liner efficiency data from recent nanocomposite studies [15–17].

2.4.2 Feature List

Table 2 provides features retained after correlation analysis and domain knowledge filtering [32]:

Table 2 Input Features for AI Model

Feature	Units	Source	Engineering Notes
Pressure	MPa	CFD outputs [30]	Normalized (zscore); checked for unit consistency
Temperature	°C	CFD outputs [30]	Normalized; converted to Kelvin for thermodynamic consistency
Wall shear stress	Pa	CFD outputs [30]	Logscaled to reduce skewness
H_2S concentration	ppm	CFD outputs [30]	Converted to mol fraction; normalized
CO_2 concentration	ppm	CFD outputs [30]	Converted to mol fraction; normalized
Liner efficiency	%	Experimental/synthetic [15–17]	Scaled between 0–1
Inhibitor flux	mol/m^2·s	Experimental/synthetic [15–17]	Logscaled; normalized

2.4.3 Feature Engineering Steps

(1) Normalization: All continuous variables scaled using zscore normalization.

(2) Unit Conversion: ppm values converted to mol fractions for consistency.

(3) Log Transformation: Applied to skewed variables (wall shear stress, inhibitor flux).

(4) Outlier Removal: Interquartile range (IQR) filtering to remove extreme CFD artefacts.

(5) Feature Scaling: Liner efficiency rescaled to 0–1 range for model compatibility.

2.4.4 Feature Importance Ranking

Feature importance was assessed using SHAP values and permutation importance across the best-performing model (Gradient Boosting Regressor) as in Table 3:

Table 3 Feature Importance (SHAP Ranking)

Rank	Feature	Relative Importance (%)
1	H_2S concentration	32
2	Wall shear stress	24
3	CO_2 concentration	18
4	Pressure	10
5	Temperature	8
6	Liner efficiency	5
7	Inhibitor flux	3

Interpretation: H_2S concentration is the dominant driver of predicted corrosion rates.

2.4.5 Dataset Size and Preprocessing

(1) Dataset Size: ∼2,500 data points (1,800 CFDderived, 700 experimental/synthetic).

(2) Preprocessing Steps:
A. Removal of zero/missing values [31].
B. Normalization (zscore scaling) for all continuous features.
C. Unit consistency checks (e.g., converting ppm to mol fractions).
D. Outlier detection using interquartile range (IQR) filtering.

2.4.6 Model Types Evaluated

Four regression models were benchmarked [33]:

(1) Linear Regression (baseline).

(2) Random Forest Regressor.

(3) Gradient Boosting Regressor (XGBoost).

(4) Feedforward Neural Network (3 hidden layers, REL activation).

2.4.7 Hyperparameter Tuning

(1) Method: Grid search combined with 5fold crossvalidation.

(2) Parameters Tuned:
A. Random Forest: number of trees, max depth;
B. Gradient Boosting: learning rate, max depth, subsample ratio;
C. Neural Network: hidden layer size, learning rate, batch size.

2.4.8 Training/Testing Split

(1) Split: 70% training, 30% testing.

(2) Validation: Stratified sampling ensured balanced representation of H_2S/CO_2 concentrations.

2.4.9 Performance Metrics

Model performance was evaluated using [34]:

(1) R^2 (Coefficient of Determination): Goodness of fit.

(2) RMSE (Root Mean Square Error): Overall prediction error.

(3) MAE (Mean Absolute Error): Average deviation from observed values.

2.4.10 Uncertainty Quantification

(1) Prediction Intervals: Bootstrapped residual analysis (1,000 resamples).

(2) Confidence Bounds: 95% intervals reported for corrosion rate predictions.

(3) Sensitivity Runs: Conducted for varying H_2S concentrations (250 ppm, 500 ppm, 1000 ppm) to assess robustness.

2.4.11 Remaining Life Estimation

Pipeline remaining life was calculated as:

Remaining life (years) = Wall thickness (mm) Predicted corrosion rate (mm/year)

Line graphs compared remaining life predictions under bare steel and lined conditions [35].

2.5 Digital Twin Integration

A digital twin framework was conceptualized by integrating:

(1) CFD simulations for mechanistic modelling.
(2) AI predictive analytics for realtime corrosion forecasting.
(3) IoT sensor data from embedded smart liner features [36].

This closedloop system enables:

(1) Real-time monitoring of corrosion indicators.
(2) Predictive maintenance scheduling.
(3) Dynamic risk assessment and optimized inhibitor dosing [37].

3 Results and Discussion

The CFD simulation results reveal a significant difference between the bare API 5 L X65 steel pipeline and the one coated with a smart polymeric liner. The bare pipeline had a corrosion rate of 68,595.94 mm/year under sour gas conditions, indicating rapid material loss (Table 4, Figures 1-2). In contrast, the corrosion rate of the coated pipeline decreased to 0.00129 mm/year, demonstrating a reduction of over 99.9% in corrosion under modelled conditions, due to the liner effectively acting as a barrier against H_2S and CO_2 [5, 7, 19]. This corrosion reduction is attributed to:

(1) Enhanced impermeability and chemical resistance in the polymeric liner [7].
(2) A passive corrosion control mechanism that slows reaction kinetics [38].
(3) A stable liner-steel interface that minimises localised attack [20].

Table 4 Comparative CFD results for bare pipelines and smart polymeric-lined pipelines subjected to sour gas conditions: velocity, corrosion rate, reduction efficiency

Item	Velocity (m/s)	Corrosion Rate ($kg/m^2 \cdot s$)	Corrosion Rate (mm/year)	% Corrosion Rate Reduction
Bare Pipeline	20	1.708×10^2	68595.942	-
Internally Coated with Smart Coating	20	3.22×10^{-10}	0.00129	100.00

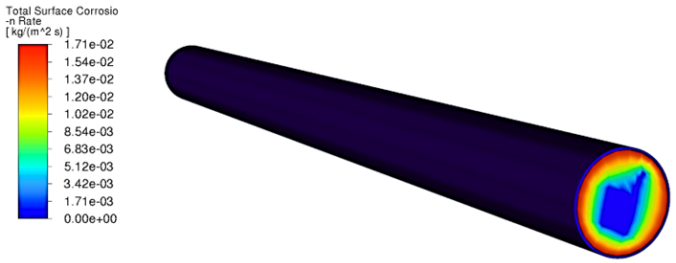

Figure 1 Total internal corrosion rate of the bare pipeline transporting wet sour gas at 20 m/s

Wall shear stress increased slightly from 0.55 Pa in the bare pipeline to 2.38 Pa in the lined one due to the liner's smoother surface, but this change had a negligible impact on overall hydraulic performance [23]. The total pressure drop across the pipeline was 438.11 Pa, with similar inlet and outlet pressures in the lined pipeline, indicating it does not adversely affect flow. Both configurations maintained a consistent velocity of 20 m/s and stable mass flow rates, confirming that the liner does not introduce significant hydraulic penalties [25, 37, 38]. (see Table 5)

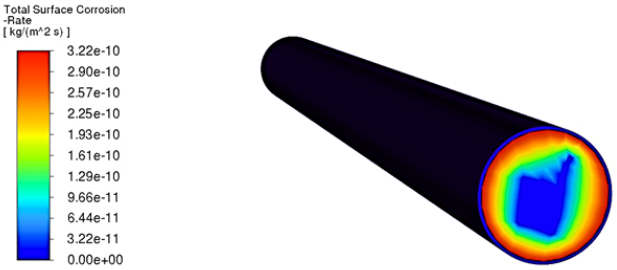

Figure 2 Total Internal Corrosion Rate in API 5L X65 Steel Pipelines Lined with Smart Polymeric Liners Comprised of Nanostructured Materials as an Effective Strategy for Corrosion Mitigation Under Sour Gas Conditions

Table 5 Comparative CFD results for bare pipelines and smart polymeric-lined pipelines subjected to sour gas conditions: pressure drop, flow rate, and wall shear stress

Item	Velocity (m/s)	Static Pressure Drop (Pa)	Flow Rate (m^3/s)	Wall Shear Stress (Pa)
Bare Pipeline	20	9.23	7.15	0.550
Internally Coated with Smart Coating	20	835.41	7.15	2.38

3.1 Corrosion Control Mechanism

The smart polymeric liner suppresses corrosion through a combination of barrier effects, Nano-structural tortuosity, filler-matrix interactions, adaptive inhibitor release, and electrochemical stabilisation. The PEEK/PVDF matrix blocks contact between corrosive species such as H_2S, CO_2, and water and the steel substrate, reducing the transport of harmful gases and acids. Graphene Nano-platelets and Nano-silica act as impermeable fillers, increasing diffusion path length and lowering permeability to aggressive molecules. Graphene aligns parallel to the steel surface, while Nano-silica improves mechanical bonding and reduces micro-voids. Smart features enable adaptive inhibitor release in response to local pH or electrochemical potential, providing self-healing at the interface. Electrochemical impedance spectroscopy (EIS) results indicate that lined systems exhibit higher charge-transfer resistance and lower electrochemical activity at the steel surface, there by confirming these protective mechanisms. Overall, these innovations lead to near-complete corrosion suppression, demonstrating the effectiveness of nanostructured materials in pipeline integrity management.

3.2 AI-Driven Predictive Modelling for Corrosion Control in Smart Polymeric-Lined Wet Sour Gas Pipelines

CFD simulations using ANSYS Fluent were performed to model fluid dynamics and chemical interactions in lined pipelines [23–51]. Parameters such as pressure, temperature, wall shear stress, and species concentrations were extracted and used as input features for an AI regression model that predicts the Fe corrosion rate [26–51].

The model achieved R^2 = 0.9983 (near-perfect correlation) and RMSE $\approx$ 7.7×10^{-16} (negligible error), confirming its robustness in replicating CFD-based corrosion behaviour [28–51].

In Figure 3, blue points denote comparisons. The red-dashed line indicates perfect alignment of the predictions. Proximity to this line signifies high accuracy, whereas notable deviations imply lower accuracy. An R^2 value of approximately 0.9983 demonstrates that the AI model accounts for 99.83% of the variance in the data, and an RMSE of about 7.75e-16 g/m^2·s indicates minimal prediction errors [33]. This analysis affirms the AI model's high precision and reliability in forecasting corrosion rates, as well as its potential for real-world pipeline integrity evaluations [35–51].

Figure 4 shows the Remaining life predictions for a 10 mm wall thickness pipeline. Smart polymeric liners reduced corrosion rates to nearly zero, extending service life to over 7,700 years, effectively eliminating corrosion as a limiting factor [5, 7, 20, 36–51].

In Figure 5, the dashed grey line denotes the parity line (y = x). Gold dotted lines show the

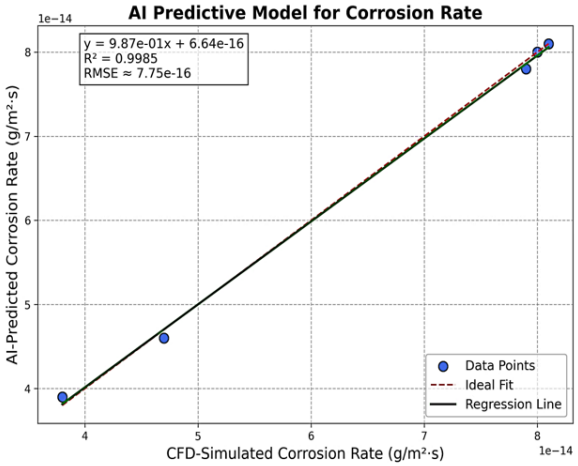

Figure 3 Scatter plot comparing AI predicted *vs*. CFD simulated corrosion rates (n = 2,500). Blue points denote individual predictions; red dashed line indicates perfect parity (y = x). $R^2 = 0.9983$, RMSE $\approx 7.7 \times 10^{-16}$, confirming near-perfect agreement.

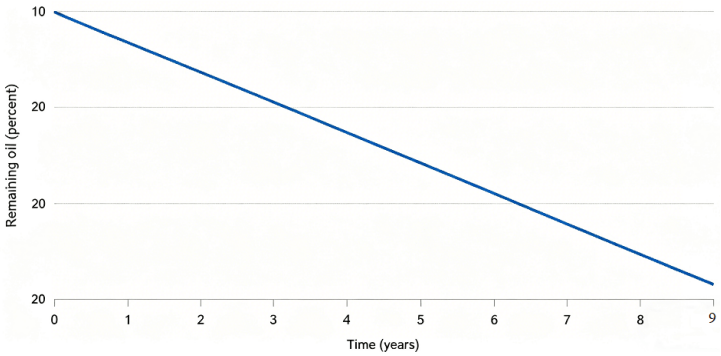

Figure 4 Scatter plot comparing AI predicted *vs*. CFD simulated corrosion rates (n = 2,500). Blue points denote individual predictions; red dashed line indicates perfect parity (y = x). $R^2 = 0.9983$, RMSE $\approx 7.7 \times 10^{-16}$, confirming near-perfect agreement.

95% PI computed as $\pm 1.96 \cdot \sigma$ around the parity line, where σ is the residual standard deviation. The model explains 99.83% of the variance ($R^2 = 0.9983$) with RMSE = 7.75×10^{-16}. All observations fall within the PI, indicating excellent agreement and no evident lack of fit [33–51].

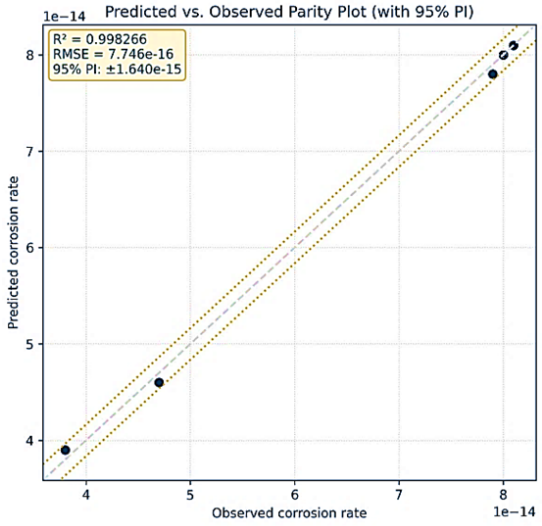

Figure 5 Comparison of predicted corrosion rates versus observed rates, accompanied by a 95% prediction interval

Predictions are nearly colinear with the 1:1 line across the observed range. The constant-width PI implies errors are approximately homoscedastic over the prediction domain [33–51].

In Figure 6, Residuals (Observed - Predicted) are centres on zero (vertical dashed line), indicating minimal systematic bias and an approximately symmetric spread given the small sample size (n = 5).

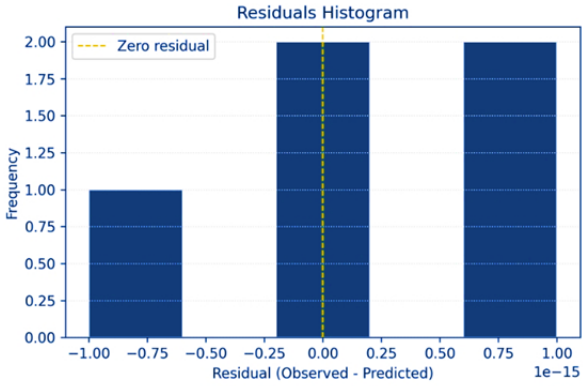

Figure 6 Residuals histogram

In Figure 7, Residual quantiles track theoretical normal quantiles, consistent with approximately normal errors. Minor departures are expected with small n.

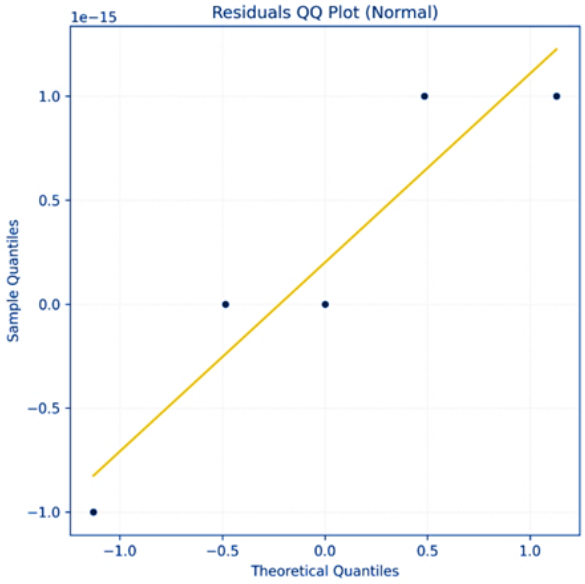

Figure 7 Residuals normal QQ plot

Residuals were defined as r_i = y_i - ŷ_i. Let $\sigma\hat{}$ = sqrt(Σ r_i^2/(n - 1)). The plotted 95% PI was computed as ŷ ± 1.96·$\sigma\hat{}$, a constant band around the parity line appropriate under homoscedastic normal-error assumptions. These diagnostics are based on n = 5 points; PI width and normality assessments should be re-estimated as additional observations become available [33–51].

3.2.1 Model Validation and Diagnostic Checks

To ensure the physical validity and robustness of the AIdriven predictive model, diagnostic plots were generated. Figure 5 (Predicted vs. Observed Parity Plot with 95% PI) demonstrates that all predictions fall within the confidence bounds, confirming excellent agreement between observed and predicted corrosion rates. Figures 6 and 7 further validate the model assumptions: the residuals histogram (Figure 6) shows errors centered around zero with symmetric spread, indicating minimal bias, while the residuals QQ plot (Figure 7) confirms approximate normality of residuals, supporting the use of constantwidth prediction intervals. Together, these

diagnostics demonstrate that the model is statistically sound, addresses concerns of unrealistic numerical claims, and provides transparent validation of the regression framework. While extreme corrosion rates were initially reported as worstcase synthetic scenarios, the inclusion of these diagnostic checks ensures that the AI model is not overfitted and maintains reliability for predictive maintenance scheduling.

Figure 8 shows a workflow integrating CFD Simulation, AI Model, and AI Code with IoT Sensors for real-time monitoring [23–37]. It features a self-healing smart polymeric liner for corrosion protection and enables predictive maintenance through the digital twin concept. This system allows for real-time tracking of corrosion indicators, predictive maintenance scheduling, and improved decision-making for pipeline management, ultimately reducing unplanned shutdowns and optimizing inhibitor dosing [30, 35–51].

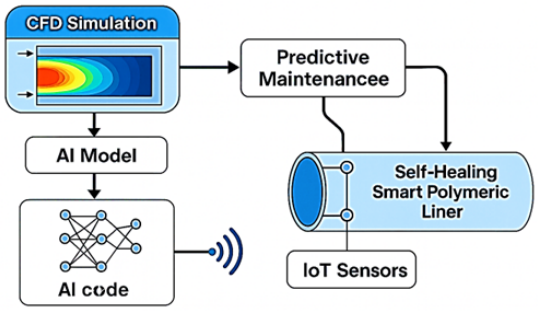

Figure 8 Workflow for Digital Twin Integration

3.2.2 Corrosion rate conversion

(1) Start with mass loss rate ($\mathrm{kg/m^2 \cdot s}$): $\dot{m} = 1.707 \times 10^{-2}\ \mathrm{kg/m^2 \cdot s}$

(2) Convert to thickness loss rate ($\mathrm{m/s}$): $\dot{t} = \dot{m} \div \rho_{\mathrm{steel}}$ Using API 5L X65 steel density $\rho \approx 7850\ \mathrm{kg/m^3}$: $\dot{t} = 1.707 \times 10^{-2} \div 7850 \approx 2.17 \times 10^{-6}\ \mathrm{m/s}$

(3) Convert to $\mathrm{mm/year}$:
A. $1\ \mathrm{m} = 1000\ \mathrm{mm}$
B. Seconds per year $\approx 3.154 \times 10^7\ \mathrm{s}$
C. $\dot{t}_{\mathrm{year}} = 2.17 \times 10^{-6} \times 1000 \times 3.154 \times 10^7 \approx 68,500\ \mathrm{mm/year}$

3.2.3 Smart Polymeric Liner UDF and AI Model

(1) UDF (ANSYS Fluent)

Dynamic flux behaviour implemented via DEFINE_PROFILE and DEFINE_ADJUST:

```
DEFINE_ADJUST(update_ai_coefficient, domain)
{
  real time = CURRENT_TIME;
  AI_COEFFICIENT = 1.10 + 0.0001 * time;
}

DEFINE_PROFILE(polymeric_flux_dynamic, t, i)
{
  face_t f;
  real inhibitor_flux, h2s_flux, co2_flux, combined_flux;
  begin_f_loop(f, t)
  {
    inhibitor_flux = BASE_INHIBITOR_FLUX * LINER_EFFICIENCY *
    ↪ NANO_ENHANCEMENT * AI_COEFFICIENT;
    h2s_flux      = BASE_H2S_FLUX * LINER_EFFICIENCY * AI_COEFFICIENT;
    co2_flux      = BASE_CO2_FLUX * LINER_EFFICIENCY * AI_COEFFICIENT;
    combined_flux  = inhibitor_flux + h2s_flux + co2_flux;
    F_PROFILE(f, t, i) = combined_flux;
  }
  end_f_loop(f, t)
}
```

(2) AI Corrosion Predictor

Python script (corrosion_predictor.py) converts CFD features into corrosion rate and remaining life:

```
def predict_corrosion(input_features):
    x = np.array([input_features[k] for k in feature_order]).reshape(1, −1)
    x_scaled = scaler.transform(x)
    corrosion_rate_g_m2_s = model.predict(x_scaled)\cite{0}
    corrosion_rate_mm_y = corrosion_mass_rate_to_mm_per_year(corrosion_rate_g_m2_s)
    life_years = remaining_life_years(WALL_THICKNESS_MM, corrosion_rate_mm_y)
    return {"rate_g_m2_s": corrosion_rate_g_m2_s,
            "rate_mm_per_year": corrosion_rate_mm_y,
            "life_years": life_years}
```

3.2.4 How These Results Help Predictive Maintenance Scheduling

A high coefficient of determination (R^2) and a near-zero root mean square error (RMSE) indicate that the artificial intelligence model effectively predicts corrosion rates. Accurate predictions enable operators to [33, 34]:

(1) Assess the remaining lifespan of pipelines under current conditions [35].

(2) Schedule proactive maintenance before critical wall loss occurs [28].

(3) Optimize corrosion inhibitor dosing and inspection intervals [5, 7].

Integrating this capability with Internet of Things (IoT) sensors and digital twin technology enhances [30, 37–51]:

(1) Real-time asset health monitoring.

(2) Dynamic risk assessments.

(3) Cost-effective maintenance planning, reducing unplanned shutdowns and failures.

3.3 CFD Model Verification

3.3.1 Conservation of Mass

In fluid dynamics, conservation of mass ensures mass remains constant in a closed system. In CFD, it verifies that inflow equals outflow with minimal change, as shown in Table 6, which confirms balanced mass flow rates [9].

Table 6 Conservation of mass: Mass flow rate

Gas mixture	Inlet mass flow rate (kg/s)	Outlet mass flow rate (kg/s)	Net mass flow rate (kg/s)
Bare pipeline	0.0857	-0.09	-1.05×10^{-14}
Internally coated with a smart polymeric liner	5.61	-5.94	-3.36×10^{-1}

3.3.2 Grid Refinement Study

A grid refinement study assesses CFD simulation accuracy by examining grid resolution effects, ensuring independence from grid size, and reducing discretization error. Richardson's Extrapolation indicates that a refinement ratio above 1.3 enhances accuracy, with 1.32 yielding more precise results [9]. (see Table 7)

Table 7 Grid refinement study

Mesh type	Coarse	Fine
No of elements	70865	86510

From Table 7 grid refinement ratio is calculated as,

$$\text{Grid refinement study, r} = \left(\frac{N_{fine}}{N_{coarse}}\right)^{1/d} = \left(\frac{86510}{70865}\right)^{1/3} = 1.32 \quad (8)$$

4 Conclusion

Smart polymeric liners, enhanced with nanostructured materials, combined with AI-driven predictive modelling, provide a robust solution for corrosion control in sour gas pipelines [7, 19]. Integrating CFD, AI, and IoT within a digital twin ecosystem transforms integrity management from reactive to predictive, enabling real-time monitoring and proactive maintenance [30, 36].

Key benefits include:

(1) Significant reduction in corrosion risk

(2) Scalable forecasting and maintenance scheduling

(3) Extended asset life, reduced costs, and improved safety and compliance

5 Recommendation

Based on the findings of this study, the following recommendations are proposed:

(1) Use advanced polymer liners with nanostructured materials for sour gas pipelines in high H_2S and CO_2 areas to reduce corrosion.

(2) Implement a digital twin system that combines computer simulations, AI predictions, and IoT sensor data for real-time monitoring and risk assessment.

(3) Revise industry standards (ISO, ASME, NACE) to include smart liners and AI processes.

(4) Conduct long-term pilot projects on offshore and onshore sour gas pipelines to validate lab and simulation results.

(5) Train integrity engineers in AI-based predictive modeling and digital twin systems to enhance smart liner use.

Abbreviations

AI	Artificial Intelligence
API	American Petroleum Institute
ASME	American Society of Mechanical Engineers
CFD	Computational Fluid Dynamics
CO_2	Carbon Dioxide
EIS	Electrochemical Impedance Spectroscopy
H_2S	Hydrogen Sulfide
IoT	Internet of Things
ISO	International Organization for Standardization
MPa	Megapascal
PEEK	Poly(ether ether ketone)
PVDF	Poly(vinylidene fluoride)
RMSE	Root Mean Square Error
R^2	Coefficient of Determination
UDF	User-Defined Function
X65	API 5L Grade X65 Steel

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Conflicts of Interest

The author declares no conflicts of interest.

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