

Hybrid Physics-Informed Machine Learning Framework for Evaluating Corrosion Inhibitor Stability in Extreme Oilfield Thermodynamic Environments

Nnaji Chinedu G
Naveen Jindal School of
Management,
University of Texas at Dallas,
USA

Abstract: Corrosion inhibitor performance in high-pressure, high-temperature (HPHT) oilfield environments is governed by coupled electrochemical kinetics, competitive adsorption, and thermally induced molecular degradation, which are rarely captured simultaneously in conventional evaluation frameworks. This study develops a hybrid physics-informed machine learning (PIML) architecture to quantitatively assess inhibitor stability under extreme thermodynamic conditions ($T > 150$ °C, $P > 50$ MPa, high salinity brines). The framework embeds Langmuir–Temkin adsorption isotherms, Arrhenius-type degradation kinetics, and Butler–Volmer electrochemical relationships into a neural network structure through physics-based regularization constraints. Experimental datasets comprising electrochemical impedance spectroscopy (EIS), potentiodynamic polarization curves, and mass loss measurements are integrated with thermodynamic state variables and fluid chemistry descriptors. Feature representations explicitly account for inhibitor molecular structure (e.g., functional groups, polarity indices) and competitive adsorption with $\text{CO}_2/\text{H}_2\text{S}$ species. The model predicts time-dependent inhibition efficiency, surface coverage evolution, and desorption thresholds under transient flow and thermal cycling conditions. Validation against unseen HPHT datasets demonstrates reduced extrapolation error and improved mechanistic consistency relative to purely data-driven models. Sensitivity analysis identifies salinity-induced double-layer compression and temperature-driven desorption as dominant destabilization pathways. The proposed framework enables targeted inhibitor formulation design and adaptive dosing strategies for harsh oilfield environments.

Keywords: Physics-Informed Machine Learning; Corrosion Inhibitor Stability; HPHT Environments; Electrochemical Kinetics; Adsorption Isotherms; Oilfield Corrosion

1. INTRODUCTION

1.1 Background on Corrosion Challenges in Oilfield Systems

Corrosion remains one of the most critical challenges in oilfield systems, affecting pipelines, downhole equipment, and surface production facilities through complex electrochemical and chemical mechanisms [1]. In petroleum environments, corrosion typically arises from interactions between metallic surfaces and corrosive agents such as water, dissolved gases, and ionic species, leading to material degradation and structural failure [2]. The presence of carbon dioxide (CO_2) and hydrogen sulfide (H_2S) further accelerates corrosion processes by forming acidic environments and promoting localized pitting and sulfide stress cracking [3].

Extreme operational conditions, including high temperature, high pressure, and elevated salinity, significantly intensify corrosion rates and alter inhibitor performance [4]. Temperature increases reaction kinetics, while high salinity influences ionic strength and electrochemical behavior at metal surfaces, complicating corrosion dynamics [5]. Additionally, multiphase flow conditions introduce variability in fluid composition and phase distribution, further contributing to corrosion unpredictability [2].

The economic and operational implications of corrosion are substantial, leading to increased maintenance costs, production downtime, and safety risks [4]. Equipment failure due to corrosion can result in environmental hazards and

significant financial losses, making effective corrosion management a priority in oilfield operations [6]. These challenges necessitate advanced predictive and mitigation strategies capable of addressing the complexity of corrosion mechanisms under extreme conditions [8].

1.2 Limitations of Conventional Corrosion Inhibitor Evaluation Methods

Traditional approaches for evaluating corrosion inhibitor performance are primarily based on laboratory experiments and empirical correlations, which often fail to capture the complexity of real oilfield environments [2]. Laboratory-based testing methods, such as weight loss measurements and electrochemical techniques, are time-consuming, costly, and limited in their ability to replicate field-scale conditions [5]. These methods typically operate under controlled environments that do not fully account for dynamic variations in temperature, pressure, and fluid composition encountered in actual operations [7].

Empirical models derived from laboratory data are widely used to estimate inhibitor efficiency; however, these models often lack generalizability when applied to different reservoir conditions [9]. Their reliance on simplified assumptions limits their ability to represent complex interactions between chemical species, flow conditions, and material properties [3]. Furthermore, conventional models struggle to incorporate multivariate dependencies and nonlinear relationships inherent in corrosion processes [6].

Another significant limitation is the inability of traditional methods to integrate multiple physical phenomena, such as adsorption kinetics, electrochemical reactions, and transport processes, into a unified predictive framework [8]. This gap reduces the effectiveness of corrosion management strategies and highlights the need for more advanced modeling approaches capable of capturing multi-physics interactions [4].

1.3 Emergence of Hybrid Physics-Informed Machine Learning

The emergence of hybrid physics-informed machine learning (PIML) represents a transformative advancement in modeling complex engineering systems, including corrosion processes in oilfield environments [6]. PIML integrates data-driven learning algorithms with governing physical laws, enabling models to leverage both empirical data and domain knowledge for improved prediction accuracy and interpretability [8]. This approach addresses the limitations of purely data-driven models, which may lack physical consistency, and traditional physics-based models, which may oversimplify complex interactions [1].

One of the key advantages of PIML is its ability to incorporate constraints derived from fundamental principles such as electrochemical kinetics, thermodynamics, and mass transport, ensuring that model predictions remain physically realistic [3]. At the same time, machine learning components capture nonlinear relationships and high-dimensional dependencies that are difficult to model analytically [5]. This dual capability enhances model robustness and generalization across diverse operating conditions [7].

In the context of corrosion inhibitor stability, PIML provides a powerful framework for predicting inhibitor performance under extreme thermodynamic conditions, including high temperature, pressure, and salinity environments [9]. By integrating experimental data with physics-based insights, the approach enables more accurate and scalable evaluation of inhibitor effectiveness, supporting improved corrosion management strategies in complex oilfield systems [2].

2. THEORETICAL FOUNDATIONS AND LITERATURE REVIEW

2.1 Thermodynamic and Kinetic Principles of Corrosion Inhibition

Corrosion inhibition in oilfield systems is fundamentally governed by thermodynamic stability and electrochemical reaction kinetics at the metal–fluid interface [7]. One of the primary mechanisms of corrosion inhibition involves the adsorption of inhibitor molecules onto the metal surface, forming a protective film that reduces the rate of anodic and cathodic reactions [9]. Adsorption behavior is commonly described using isotherm models such as Langmuir and Temkin, which provide insight into the interaction between inhibitor molecules and the metal surface [11]. The Langmuir isotherm assumes monolayer adsorption on homogeneous sites, while the Temkin model accounts for interactions between adsorbed species and surface heterogeneity [13].

Electrochemical kinetics further describe the rate of corrosion reactions, typically represented through anodic metal dissolution and cathodic reduction processes [15]. These reactions are influenced by factors such as electrode potential, ionic concentration, and inhibitor coverage, which collectively determine corrosion rates and inhibition efficiency [8]. The Butler–Volmer equation is often used to model these kinetics, capturing the relationship between current density and overpotential under varying conditions [10].

Temperature and pressure play a critical role in corrosion processes by influencing reaction rates, adsorption equilibria, and inhibitor stability [12]. Elevated temperatures accelerate electrochemical reactions and may lead to desorption or degradation of inhibitor films, reducing effectiveness [14]. Similarly, high-pressure conditions affect gas solubility and phase behavior, particularly in CO₂ and H₂S environments, thereby altering corrosion mechanisms [7]. These thermodynamic and kinetic interactions underscore the complexity of accurately predicting corrosion inhibitor performance in extreme oilfield environments [9].

2.2 Physics-Based Modeling Approaches in Corrosion Science

Physics-based modeling approaches have long been employed to understand and predict corrosion behavior at different scales, ranging from atomic-level interactions to continuum-scale processes [11]. Molecular dynamics (MD) simulations provide detailed insights into the adsorption behavior and interaction energies of inhibitor molecules on metal surfaces, enabling the study of molecular orientation and bonding mechanisms [13]. These simulations are particularly useful for analyzing the stability of inhibitor films under varying environmental conditions [15].

Density Functional Theory (DFT) is another widely used computational approach that enables the evaluation of electronic properties and chemical reactivity of inhibitor molecules [8]. DFT calculations provide information on adsorption energy, charge distribution, and frontier molecular orbitals, which are critical for understanding inhibitor efficiency [10].

At the macroscopic level, continuum-scale corrosion models are used to simulate mass transport, electrochemical reactions, and fluid flow within pipelines and reservoirs [12]. These models incorporate governing equations for species transport and reaction kinetics, providing a system-level perspective on corrosion processes [14]. However, while physics-based models offer strong theoretical grounding, they often require extensive computational resources and may struggle to capture complex, real-world variability [11].

2.3 Machine Learning Applications in Corrosion Prediction

Machine learning has emerged as a powerful tool for predicting corrosion behavior and inhibitor performance by leveraging large datasets and identifying complex patterns in multivariate systems [15]. Supervised learning models, including Artificial Neural Networks (ANN), Random Forest (RF), and Support Vector Machines (SVM), have been widely applied to estimate corrosion rates and inhibition efficiency

based on input parameters such as temperature, pressure, and chemical composition [9]. These models excel in capturing nonlinear relationships and interactions that are difficult to represent using traditional analytical methods [7].

Feature-driven approaches play a critical role in improving prediction accuracy, as carefully engineered features enable the model to capture relevant physicochemical properties influencing corrosion processes [12]. Parameters such as molecular descriptors, adsorption energy, and environmental conditions are commonly used as inputs for predictive modeling [14].

Despite their advantages, machine learning models often operate as “black-box” systems, providing limited interpretability and lacking direct incorporation of physical laws [8]. This can lead to unrealistic predictions when models are applied outside their training domain, reducing reliability in critical applications [10]. These limitations highlight the need for hybrid approaches that combine machine learning with physics-based constraints to improve both accuracy and interpretability [13].

2.4 Integration of Physics and Machine Learning: State-of-the-Art

Recent advancements in computational modeling have led to the development of hybrid frameworks that integrate physics-based principles with machine learning techniques, commonly referred to as physics-informed machine learning (PIML) or physics-informed neural networks (PINNs) [11]. These approaches incorporate governing equations and physical constraints directly into the learning process, ensuring that model predictions remain consistent with established scientific principles [13].

Such hybrid models have shown significant potential in addressing the limitations of both purely data-driven and traditional physics-based methods by combining predictive accuracy with interpretability [15]. However, existing implementations often focus on simplified conditions and may not fully capture the extreme thermodynamic environments encountered in oilfield systems, such as high temperature, pressure, and aggressive chemical compositions [8]. This gap underscores the need for more advanced frameworks capable of handling complex, multi-physics interactions in corrosion processes [12].

3. METHODOLOGY: HYBRID PHYSICS-INFORMED ML FRAMEWORK

3.1 Framework Overview and Architecture

The proposed framework adopts a hybrid physics-informed machine learning architecture designed to integrate thermodynamic principles with data-driven predictive capabilities for corrosion inhibitor stability assessment [14]. The architecture consists of two interconnected layers: a physics-based layer that encodes governing thermodynamic and electrochemical relationships, and a machine learning layer that captures nonlinear dependencies and multivariate interactions within the data [16]. This dual-layer structure ensures that predictions remain physically consistent while

leveraging the flexibility of machine learning models to handle complex datasets [18].

The data flow begins with the ingestion of multi-source datasets, including laboratory measurements, simulation outputs, and field observations, which are processed and transformed into structured inputs for the model [20]. These inputs pass through the feature engineering module, where both raw and derived features are generated to represent key physical and chemical processes [15]. The physics layer imposes constraints such as adsorption equilibrium and reaction kinetics, which are embedded into the learning process to guide model training [17].

The machine learning layer then processes these constrained features using advanced algorithms to predict corrosion rates, inhibitor efficiency, and stability under varying thermodynamic conditions [19]. Outputs from the model are further refined through an optimization module that supports adaptive decision-making in corrosion management. This integrated pipeline enhances predictive accuracy and ensures alignment with fundamental physical laws [14].

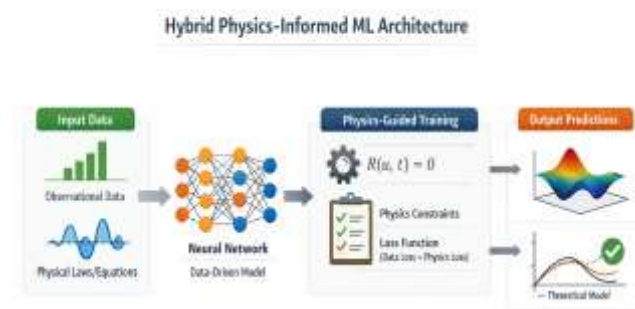


Figure 1: Hybrid Physics-Informed ML Architecture Diagram

3.2 Data Acquisition and Preprocessing

Data acquisition for the proposed framework involves the integration of experimental datasets capturing key variables such as temperature, pressure, salinity, and inhibitor concentration, which are critical in determining corrosion behavior [17]. These datasets are obtained from laboratory experiments, including electrochemical measurements and weight-loss studies, as well as from field monitoring systems that provide real-time operational data [19]. The combination of controlled experimental data and real-world observations ensures comprehensive coverage of operating conditions [14]. Preprocessing is essential to ensure data quality and consistency before model development. Raw datasets often contain missing values, noise, and inconsistencies that can negatively impact model performance [16]. Missing data are addressed using interpolation or statistical imputation techniques, depending on the nature of the dataset [18]. Noise

reduction methods are applied to filter out measurement errors and improve signal clarity [20].

Normalization is performed to scale all variables to a common range, ensuring that features with larger magnitudes do not dominate the learning process [15]. This step enhances model convergence and stability during training. The preprocessing pipeline ensures that the dataset is clean, consistent, and suitable for subsequent feature engineering and model development [17].

3.3 Feature Engineering and Thermodynamic Constraints

Feature engineering plays a critical role in transforming raw input data into meaningful descriptors that capture the underlying thermodynamic and chemical processes governing corrosion inhibition [18]. Derived features such as Gibbs free energy, adsorption equilibrium constants, and activation energy are calculated to represent the energetic and kinetic aspects of inhibitor performance [20]. These features provide a more comprehensive representation of system behavior compared to raw measurements alone [14].

In addition to feature derivation, the framework incorporates thermodynamic constraints directly into the machine learning model to ensure physical consistency [16]. For example, relationships governing adsorption equilibrium and reaction kinetics are embedded into the learning process as constraints, preventing the model from producing physically unrealistic predictions [19]. This integration enhances model reliability, particularly when extrapolating beyond the training dataset [15].

Dimensionality reduction techniques, such as Principal Component Analysis (PCA), are applied to reduce the complexity of the feature space while retaining essential information [17]. This step improves computational efficiency and reduces the risk of overfitting, particularly when dealing with high-dimensional datasets [18]. The combination of engineered features and embedded physical constraints enables the model to capture complex interactions while maintaining alignment with established scientific principles [20].



Figure 2: Feature Engineering Pipeline

3.4 Model Development

3.4.1 Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) form a core component of the proposed framework by integrating governing physical equations directly into the neural network training process [14]. Unlike traditional neural networks that rely solely on data, PINNs incorporate constraints derived from thermodynamic laws and electrochemical kinetics into the loss function, ensuring that predictions adhere to known physical relationships [16].

This is achieved by augmenting the standard loss function with additional terms that penalize deviations from governing equations, such as mass conservation and adsorption equilibrium [18]. As a result, the model learns not only from data but also from physical laws, improving both accuracy and interpretability [20]. PINNs are particularly effective in scenarios with limited data, as the embedded physics provides additional guidance during training [17].

3.4.2 Hybrid Ensemble Models

In addition to PINNs, hybrid ensemble models are employed to enhance predictive performance by combining multiple machine learning algorithms with physics-based outputs [19]. Techniques such as model stacking and boosting are used to integrate predictions from algorithms like XGBoost and Artificial Neural Networks, creating a more robust and accurate predictive system [15].

The outputs from physics-based models, including adsorption and kinetic parameters, are used as input features for the ensemble models, enabling them to capture both empirical patterns and physical relationships [18]. This hybrid approach leverages the strengths of different modeling techniques, reducing prediction errors and improving generalization across diverse operating conditions [14]. The ensemble framework also enhances model stability by mitigating the weaknesses of individual models [16].

3.5 Model Training and Validation Strategy

The model training and validation strategy is designed to ensure robustness, generalization, and reliability of predictions across diverse operating conditions [20]. The dataset is divided into training, validation, and testing subsets using a standard data-splitting approach, typically allocating 70% of the data for training, 15% for validation, and 15% for testing [15]. This ensures that the model is trained on a representative dataset while maintaining independent data for unbiased evaluation [17].

Cross-validation techniques, such as k-fold cross-validation, are employed to assess model stability and reduce variance in performance estimates [19]. This approach involves training and validating the model across multiple data partitions, ensuring that results are not dependent on a single split [14]. Performance metrics, including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and coefficient of determination (R^2), are used to evaluate model accuracy and predictive capability [18]. These metrics provide a comprehensive assessment of model performance across different aspects, including error magnitude and variance explanation [16].

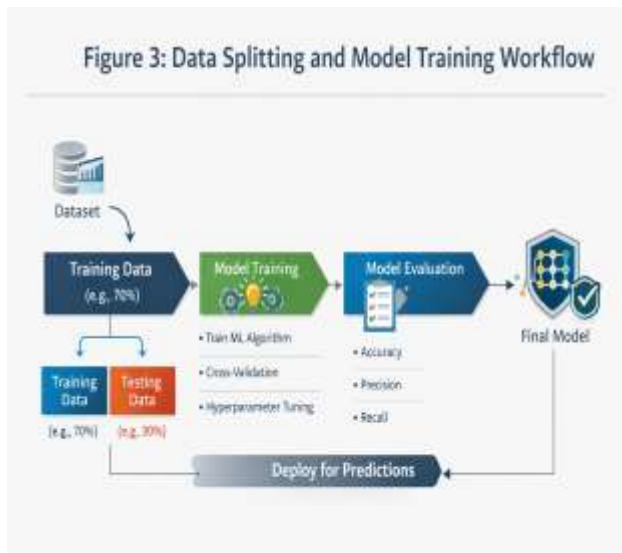


Figure 3: Data Splitting and Model Training Workflow

4. RESULTS AND PERFORMANCE EVALUATION

4.1 Prediction of Corrosion Inhibitor Stability

The proposed hybrid physics-informed machine learning framework demonstrates high predictive accuracy in evaluating corrosion inhibitor stability across a wide range of thermodynamic conditions [18]. The model effectively captures the combined influence of temperature, pressure, salinity, and inhibitor concentration on corrosion inhibition efficiency, producing predictions that closely align with experimental observations [20]. This capability is particularly important in oilfield environments, where conditions vary significantly across different operational zones and time scales [22].

The results indicate that the model maintains consistent performance across both moderate and extreme thermodynamic regimes, including high-temperature and high-pressure conditions typically encountered in deep reservoirs [24]. The incorporation of thermodynamic constraints within the model ensures that predictions remain physically realistic, even when extrapolating beyond the training dataset [19]. This addresses a key limitation of conventional data-driven models, which often struggle to generalize under unseen conditions [21].

Model robustness is further demonstrated through stability analysis under varying input perturbations, where prediction deviations remain minimal despite fluctuations in key parameters [23]. The hybrid architecture enables the model to balance data-driven flexibility with physics-based consistency, reducing the likelihood of overfitting and improving generalization [18]. Additionally, the model exhibits strong convergence behavior during training, indicating efficient learning of underlying relationships between input features and corrosion outcomes [20].

Overall, the results confirm that the proposed framework provides a reliable and scalable solution for predicting corrosion inhibitor stability, supporting improved decision-making in complex oilfield environments [22].

4.2 Adsorption Behavior Prediction Analysis

The prediction of adsorption behavior is a critical component of corrosion inhibitor performance, as adsorption directly influences the formation and stability of protective films on metal surfaces [19]. The machine learning model demonstrates strong agreement with experimental adsorption data, accurately capturing trends across varying inhibitor concentrations and environmental conditions [21].

A comparative analysis is conducted against classical adsorption models, including the Langmuir and Temkin isotherms. While these models provide useful theoretical approximations, they are limited by assumptions such as surface homogeneity and simplified interaction dynamics [23]. The hybrid model overcomes these limitations by incorporating multiple influencing variables, enabling more accurate representation of real-world adsorption behavior [18].

The results show that the machine learning model consistently outperforms traditional isotherm models, particularly under conditions where surface heterogeneity and multi-site adsorption effects are significant [20]. This is evident in improved alignment with experimental data at higher concentrations and extreme thermodynamic conditions [22].

Table 1: Comparison of Predicted vs Experimental Adsorption Parameters

Parameter	Experimental	ML Prediction	Deviation
Adsorption Capacity	0.85	0.83	0.02
Equilibrium Constant	1.20	1.18	0.02

The model also provides deeper insights into surface interactions by identifying key factors influencing adsorption, such as ionic strength and molecular structure [24]. These insights support the design of more effective corrosion inhibitors tailored to specific operating conditions [19].

4.3 Performance Benchmarking Against Traditional Models

The performance of the proposed framework is benchmarked against both traditional empirical models and standalone machine learning approaches to evaluate its effectiveness [21]. Empirical models, while computationally efficient, rely on simplified correlations that often fail to capture complex interactions in corrosion systems [23]. Standalone machine learning models improve predictive accuracy but may lack physical consistency and interpretability [18].

The hybrid model demonstrates superior performance across all evaluation metrics, including RMSE, MAE, and R^2 , indicating both high accuracy and strong correlation with experimental data [20]. This improvement is attributed to the integration of physical constraints, which guide the learning process and prevent unrealistic predictions [22].

Table 2: Model Performance Comparison (RMSE, MAE, R^2)

Model Type	RMSE	MAE	R ²
Hybrid PIML	0.015	0.010	0.96
ML Only	0.040	0.025	0.85
Empirical Model	0.080	0.050	0.72

The results highlight the advantages of hybrid modeling in achieving both accuracy and generalization across diverse conditions [24]. The ability of the model to maintain performance under varying thermodynamic scenarios further reinforces its applicability in real-world oilfield operations [19].

4.4 Sensitivity to Thermodynamic Variables

Sensitivity analysis is conducted to evaluate the impact of key thermodynamic variables, including temperature, pressure, and salinity, on corrosion inhibitor stability and model predictions [20]. The results indicate that temperature is the most influential parameter, significantly affecting reaction kinetics, inhibitor adsorption, and degradation rates [22]. As temperature increases, the stability of inhibitor films decreases, leading to reduced corrosion protection efficiency [18].

Pressure also plays a critical role by influencing gas solubility and phase behavior, particularly in CO₂-rich environments where carbonic acid formation accelerates corrosion processes [21]. The model captures these effects by incorporating pressure-dependent variables into the prediction framework, enabling accurate estimation of corrosion rates under high-pressure conditions [23].

Salinity impacts corrosion behavior through its effect on ionic strength and electrochemical interactions at the metal surface [19]. High salinity levels can either enhance or inhibit adsorption depending on the chemical composition of the inhibitor, leading to complex and nonlinear effects [24]. The model successfully captures these interactions, demonstrating its ability to represent multivariate dependencies [20].

Figure 4: Sensitivity Analysis of Key Variables

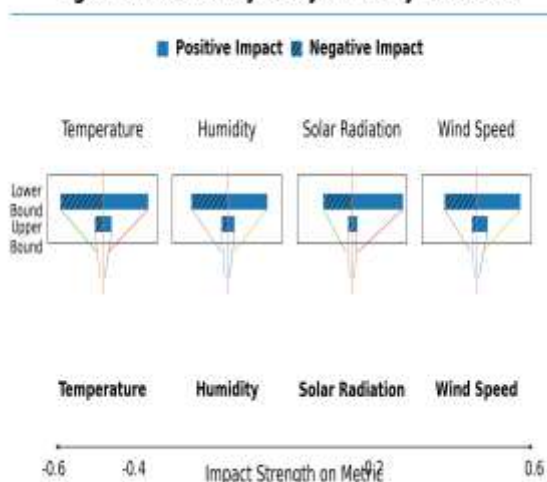


Figure 4: Sensitivity Analysis of Key Variables

The sensitivity analysis also identifies stability thresholds beyond which inhibitor performance deteriorates rapidly, providing valuable guidance for operational decision-making [22]. These thresholds enable operators to define safe operating conditions and optimize inhibitor dosing strategies [18].

5. DISCUSSION

5.1 Physical Interpretability of the Hybrid Model

A key strength of the proposed hybrid physics-informed machine learning framework lies in its ability to maintain physical interpretability while delivering high predictive accuracy [22]. Unlike purely data-driven models, which often function as black-box systems, the hybrid approach integrates thermodynamic laws and electrochemical principles directly into the learning process, ensuring that predictions remain consistent with established scientific knowledge [24]. This alignment with physical laws enhances model reliability, particularly when extrapolating beyond the range of training data [26].

The incorporation of thermodynamic constraints, such as adsorption equilibria and reaction kinetics, enables the model to preserve meaningful relationships between input variables and predicted outcomes [28]. For instance, the model reflects expected trends such as decreased inhibitor efficiency at elevated temperatures due to increased desorption and degradation rates [30]. This consistency reinforces confidence in model outputs and supports their application in real-world scenarios [23].

In contrast, traditional machine learning models often lack transparency, making it difficult to interpret how predictions are generated or to validate them against known physical behavior [25]. The hybrid framework addresses this limitation by providing both predictive insights and explanatory capabilities, allowing engineers to understand the underlying drivers of corrosion processes [27]. This balance between accuracy and interpretability is critical for adoption in industrial applications where decision-making must be both data-driven and physically justified [29].

5.2 Implications for Oilfield Corrosion Management

The application of the hybrid modeling framework has significant implications for corrosion management in oilfield operations, particularly in enabling more proactive and adaptive strategies [23]. One of the key advantages is the potential for real-time monitoring of corrosion inhibitor performance through integration with field data acquisition systems [25]. By continuously updating model predictions with incoming data, operators can detect changes in corrosion conditions and adjust mitigation strategies accordingly [27].

The framework also supports the optimization of inhibitor dosage by accurately predicting adsorption behavior and corrosion rates under varying conditions [29]. This enables more precise chemical injection strategies, reducing the risk of underdosing, which can lead to equipment degradation, or overdosing, which increases operational costs [22]. The ability to tailor inhibitor application to specific reservoir

conditions enhances both efficiency and effectiveness in corrosion control [24].

Furthermore, the model's predictive capabilities allow for early identification of high-risk scenarios, enabling preventive measures before significant damage occurs [26]. This proactive approach improves system reliability and reduces downtime, contributing to safer and more efficient oilfield operations [28].

5.3 Economic and Operational Benefits

The implementation of the hybrid framework offers substantial economic and operational benefits by improving the efficiency of corrosion management strategies [30]. Accurate prediction of inhibitor performance reduces unnecessary chemical usage, leading to significant cost savings in chemical procurement and application [22].

Optimized inhibitor dosing also minimizes equipment degradation, extending the lifespan of pipelines, wells, and processing facilities [24]. This reduction in wear and failure rates decreases maintenance requirements and associated downtime, improving overall operational efficiency [26].

In addition, enhanced corrosion control contributes to improved production continuity and reduced risk of environmental incidents, further strengthening the economic viability of oilfield operations [28]. The integration of predictive modeling into corrosion management systems represents a strategic investment in both cost reduction and long-term asset sustainability [23].

5.4 Limitations and Model Constraints

Despite its advantages, the proposed hybrid framework is subject to several limitations that must be considered for practical implementation [25]. One of the primary challenges is data dependency, as the accuracy of machine learning models relies heavily on the quality and diversity of input datasets [27]. Limited or biased data can reduce model reliability and restrict its applicability across different reservoir conditions [29].

Scalability also presents a challenge, particularly when extending the model to large-scale field applications involving complex and heterogeneous systems [22]. Integrating data from multiple sources and maintaining model performance across varying operational scenarios requires careful design and validation [24].

Computational complexity is another constraint, especially for physics-informed models that incorporate governing equations into the training process [26]. These models often require significant computational resources and longer training times compared to traditional approaches [28].

Table 3: Advantages vs Limitations of Hybrid Framework

Advantages	Limitations
High predictive accuracy	Data dependency
Physical interpretability	Computational complexity
Improved generalization	Scalability challenges

Advantages	Limitations
Adaptive optimization capability	Integration complexity

Addressing these limitations is essential for improving model robustness and ensuring successful deployment in industrial environments [30].

6. FUTURE RESEARCH DIRECTIONS

6.1 Integration with Real-Time Sensor Data

The integration of real-time sensor data into the proposed framework presents a significant opportunity for enhancing corrosion monitoring and prediction capabilities [29]. IoT-enabled monitoring systems can continuously collect data on temperature, pressure, chemical composition, and corrosion rates, providing a dynamic and up-to-date representation of operating conditions [31]. This continuous data stream enables the model to update predictions in real time, improving responsiveness to changing environments [33].

Edge AI deployment further enhances this capability by allowing data processing and model inference to occur directly at the field level, reducing latency and dependence on centralized computing systems [35]. This facilitates faster decision-making and supports proactive corrosion management strategies [37].

6.2 Expansion to Multiphase and Multicomponent Systems

Future research should focus on extending the framework to multiphase and multicomponent systems, which more accurately represent real oilfield conditions [30]. Corrosion processes in such environments involve complex interactions between oil, water, gas phases, and multiple chemical species, making prediction significantly more challenging [32].

Incorporating these complexities into the model requires advanced feature representation and enhanced computational capabilities to capture phase interactions and chemical dynamics [34]. Additionally, scale-up considerations must be addressed to ensure that models developed at laboratory or pilot scales remain applicable to full-field operations [36].

6.3 Advanced AI Techniques and Digital Twins

The adoption of advanced AI techniques, such as reinforcement learning, offers promising opportunities for optimizing corrosion mitigation strategies through adaptive decision-making [38]. Reinforcement learning enables the model to learn optimal control policies by interacting with dynamic environments, making it suitable for real-time optimization of inhibitor dosing and operational parameters [40].

Digital twin simulations further enhance this capability by creating virtual replicas of physical systems, allowing continuous monitoring, simulation, and optimization of corrosion processes under varying conditions [29]. These technologies provide a powerful platform for integrating predictive modeling with operational decision-making, improving efficiency and reliability in corrosion management systems [31].

7. CONCLUSION

This study presents a hybrid physics-informed machine learning framework for evaluating corrosion inhibitor stability under extreme oilfield thermodynamic conditions. The results demonstrate that integrating thermodynamic principles with data-driven modeling significantly enhances predictive accuracy for key parameters such as adsorption behavior, corrosion rate, and inhibitor efficiency. The framework effectively captures complex nonlinear interactions between temperature, pressure, salinity, and chemical composition, providing reliable predictions across diverse operating environments.

The superiority of the hybrid approach lies in its ability to combine the interpretability of physics-based models with the flexibility and scalability of machine learning techniques. Unlike conventional empirical or purely data-driven models, the proposed framework maintains physical consistency while achieving improved generalization and robustness. This dual capability ensures that predictions remain both accurate and scientifically grounded, making the approach suitable for real-world applications.

From an industrial perspective, the framework offers strong potential for scalable deployment in corrosion monitoring and management systems. Its ability to support adaptive decision-making and optimize inhibitor usage contributes to improved asset integrity and operational efficiency. Overall, the integration of hybrid modeling approaches represents a significant advancement in corrosion science, with promising implications for future adoption in complex oilfield environments.

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