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Analytical Approach to Mathematical Modeling of Corrosion Parameters of Mild Steel in a Microbial Environment

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Abstract: *This research presents a comprehensive analytical approach to the development of mathematical model to analyze and predict corrosion parameters of mild steel in a microbial environment. Understanding the interactions between microorganisms and mild steel is crucial for preventing and mitigating corrosion in various industries.. The methodology involves considering the electrochemical reactions, microbial growth, biofilm formation, and the interactions between microorganisms and the metal surface. The approach is to use a modified form of the Nernst-Plank equation as a fundamental principle. By analyzing the collected data, key corrosion parameters affecting mild steel are identified, such as pH, temperature, humidity, oxygen concentration, chloride ion concentration, and surface roughness. A comprehensive mathematical model is developed to incorporate these parameters and accurately predict the corrosion rate of mild steel under various conditions. The term (1+gP) accounts for the influence of environmental parameters on corrosion. The term (1+fM) represents the influence of microbial activity on corrosion. The developed model is meant to be validated using experimental data not used during the model development phase. This validation process ensures the accuracy and reliability of the model. Additionally, sensitivity analysis is performed to determine the relative importance of each corrosion parameter on the overall corrosion behavior of mild steel. This analysis provides insights into critical factors influencing corrosion and guides the formulation of effective corrosion control strategies.*

Keywords: *modeling, corrosion, mild steel, microbial environment, biofilms.*

1. Introduction

Corrosion of mild steel in a microbial environment is a challenging issue faced by industries such as oil and gas, marine, and water treatment[1]. Microorganisms, including bacteria, fungi, and algae, can colonize the metal surface and create favorable conditions for corrosion to occur. This microbial-induced corrosion (MIC) can lead to severe damage, financial losses, and compromised structural integrity [2]. Therefore, it is essential to comprehensively analyze the corrosion parameters influenced by microorganisms and develop mathematical models to predict the corrosion behavior of mild steel in a microbial environment. [3].

Mild steel is widely used in construction, infrastructure, automotive, and other industries due to its desirable mechanical properties and cost-effectiveness [4]. However, mild steel is susceptible to corrosion, which can lead to structural degradation, reduced durability, and potential failures[5]. To combat these challenges, it is crucial to comprehensively analyze the corrosion parameters that affect mild steel and develop mathematical models that accurately predict corrosion rates and behavior [6]. Corrosion is a pervasive problem that affects various materials, including metals, and it poses significant challenges in terms of economic losses and safety risks. In particular, mild steel, which is widely used in construction, infrastructure, and industrial applications is highly susceptible to corrosion[7]. Corrosion in mild steel can lead to structural degradation, reduced durability, and potential failures, making it crucial to understand the underlying mechanisms and factors influencing the corrosion process[8]. This research project aims to address this issue by developing a comprehensive mathematical model to analyze and predict corrosion parameters in mild steel.

Mild steel, also known as low carbon steel, is favored for its desirable mechanical properties, cost-effectiveness, and versatility. However, its vulnerability to corrosion poses a significant limitation on its applications [9]. Corrosion in mild steel occurs when the metal reacts with its environment, leading to the formation of oxides, hydroxides, or other compounds on its surface. This process can be influenced by various factors, including environmental conditions, chemical composition, surface characteristics, and electrochemical reactions.[10]To effectively combat corrosion and develop appropriate mitigation strategies, a thorough understanding of the corrosion parameters influencing mild steel is crucial. These parameters include pH, temperature, humidity, oxygen concentration, chloride ion concentration, surface roughness, and exposure time. Each of these factors can significantly impact the corrosion rate and behavior of mild steel[11]

The development of a mathematical model specifically designed for analyzing and predicting corrosion parameters in mild steel offers several advantages. Firstly, such a model provides a quantitative and systematic approach to studying corrosion, enabling engineers and researchers to gain insights into the complex corrosion processes. By incorporating the various corrosion parameters into the model, it becomes possible to estimate and predict the corrosion rate under different environmental conditions accurately[12].The main objective of this study is to create an analytical mathematical approach to develop a model that accurately predicts the corrosion rate and behavior of mild steel in a microbial environment while incorporating corrosion characteristics influenced by microorganisms. By reaching this goal, the project hopes to improve knowledge of MIC and offer a useful tool for evaluating, avoiding, and reducing MIC-related problems in mild steel buildings.

Furthermore, a comprehensive mathematical model allows for the identification of the key corrosion parameters that have the most significant influence on mild steel corrosion[13]. This knowledge is crucial for prioritizing mitigation efforts and designing corrosion control strategies. Sensitivity analysis, conducted as part of this research project, will provide insights into the relative importance of each corrosion parameter and help engineers understand which factors should be addressed to effectively prevent or minimize corrosion in mild steel structures. The significance of this research project extends beyond theoretical considerations. The outcomes of this study will provide engineers, researchers, and industries with a valuable tool for assessing and mitigating corrosion-related issues in mild steel structures in a microbial environment.. By accurately predicting corrosion rates and understanding the critical parameters influencing corrosion, it will be possible to develop tailored corrosion prevention and control strategies, leading to improved structural integrity, extended service life, and cost savings.

2 Reviews of Relevant Literatures

Developing equations for the mathematical modeling of corrosion parameters of mild steel in a microbial environment involves considering the various factors and interactions that influence microbial-induced corrosion (MIC). The equations aim to capture the relationship between these parameters and the corrosion behavior of mild steel. While the specific equations may vary based on the chosen modeling approach. Incorporating biofilm growth into the model allows for the consideration of the changing biofilm characteristics and the influence of biofilm on corrosion parameters, such as localized corrosion and mass transport processes[14]. Numerous factors affect the development of biofilms, but some of the most important ones are surface topography and roughness, surface wettability, and the presence of nutrients. For microbiological cells to settle, surface roughness is crucial. [15] stated that rough surfaces typically give more surface area for microbiological cell attachment since there is generally more cell adherence to rough surfaces. In order to determine how surface roughness affects cell attachment. [16] evaluated the attachment of cells to welded and unwelded surfaces of 304L stainless steel. In comparison to the unwelded surface, a substantial microbiological cell attachment was seen on the welded surface due to its roughness. The presence of a biofilm does not indicate that MIC is always present.

2.1. Microbial Growth and Metabolic Activity:

Microbial growth in a microbial environment plays a crucial role in microbial-induced corrosion (MIC). The logistic growth model, utilized in the mathematical model, captures the population dynamics of microorganisms over time[17]. The model considers the microbial growth rate (r) and the carrying capacity (K), representing the maximum population size that the environment can sustain. By incorporating this growth model, the mathematical model accounts for the influence of microbial population density on corrosion parameters. The growth and metabolic activity of microorganisms can have a significant impact on MIC. The following equation represents a commonly used model for microbial growth, such as the logistic growth model:

$$\frac{dN}{dt} = rN\left(1-\frac{N}{K}\right) \quad (1)$$

Where dN/dt represents the rate of microbial population growth over time, r is the microbial growth rate, N is the microbial population size, K is the carrying capacity representing the maximum population size that the environment can sustain.

2.2 pH Changes and Electrochemical Reactions:

Microbial activity can alter the pH of the environment, leading to significant effects on corrosion processes[18]. The Nernst equation, integrated into the model, relates changes in pH to electrochemical reactions occurring at the mild steel surface. The equation considers the potential difference (E) between the oxidized and reduced forms of mild steel, the standard potential difference (E°), temperature (T), the number of electrons involved in the redox reaction (n), and the concentration of hydrogen ions ([H+]). By accounting for pH changes, the model captures the electrochemical interactions between microorganisms and mild steel, contributing to the overall corrosion behavior. Microbial activity can lead to changes in the pH of the environment, affecting the corrosion behavior of mild steel. The Nernst equation can be used to relate the pH changes to the electrochemical reactions[19]:

$$E = E^o - \left(\frac{RT}{nF}\right) ln\left(\frac{oxidized}{nFreduced}\right) \quad (2)$$

Where E is the potential difference between the oxidized and reduced forms of the mild steel, E° is the standard potential difference, R is the gas constant., T is the temperature, n is the number of electrons involved in the redox reaction, F is Faraday's constant, [oxidized] and [reduced] represent the concentrations of the oxidized and reduced species, respectively.

2.3. Biofilm Formation and Surface Roughness

Microorganisms have the ability to form biofilms on the surface of mild steel, which can profoundly impact corrosion processes. The mathematical model incorporates a simplified biofilm growth model, assuming a linear relationship between biofilm thickness (B) and time (t). This representation acknowledges the gradual increase in biofilm thickness over time. Additionally, the model considers surface roughness, quantified by the root mean square roughness. The empirical coefficient (β) determines the influence of biofilm thickness (B) on surface roughness. By including these parameters, the model accounts for the physical effects of biofilm formation on mild steel surfaces. Microorganisms often form biofilms on the surface of mild steel, influencing its corrosion behavior. The formation of biofilms can be described using a growth model such as the Monod equation:[20]

$$\frac{dB}{dt} = \mu B\left(1 - \frac{B}{K}\right) \quad (3)$$

Where dB/dt represents the rate of biofilm growth over time,μ is the specific growth rate of the biofilm, B is the biofilm thickness, K is the maximum biofilm thickness.

Surface roughness, affected by the biofilm, can be quantified using parameters such as the root mean square roughness, The relationship between biofilm thickness and surface roughness can be represented by an empirical equation, such as:

$$B = \alpha\, Rq^{\beta} \quad (4)$$

Where B is the biofilm thickness, Rq is the root mean square roughness, α and β are empirical coefficients

2.4. Corrosion Rate:

The corrosion rate of mild steel in a microbial environment is a critical parameter to quantify and predict. The mathematical model incorporates an empirical equation to estimate the corrosion rate. It considers factors such as the potential difference between open-circuit potential and corrosion potential (ΔE), the corrosion potential (E_p), a constant (K) accounting for environmental conditions, the biofilm thickness (B), and an empirical coefficient (γ) that characterizes the influence of biofilms on corrosion rate. By incorporating these parameters, the model provides an estimation of the corrosion rate of mild steel in a microbial environment, considering both the electrochemical and physical effects. The corrosion rate of mild steel in a microbial environment can be estimated using an empirical equation that incorporates the various corrosion parameters:

$$CR = K\,(\Delta E - E_p)\,(1 + \gamma B) \quad (5)$$

Overall, the mathematical model developed for the corrosion parameters of mild steel in a microbial environment provides a comprehensive framework for understanding and predicting MIC. By incorporating microbial growth, pH changes, biofilm formation, surface roughness, and corrosion rate, the model captures the intricate interactions between microorganisms and mild steel[21]. However, it is important to note that the model's accuracy and reliability can be further enhanced through calibration and validation using experimental data from specific microbial systems and environmental conditions. These equations provide the foundation for a mathematical model of mild steel corrosion caused by microorganisms. Additional equations and parameters can be included to account for additional aspects including ambient conditions, particular microbial species, nutrient availability, and the influence of other corrosion characteristics, depending on the details of the study's requirements and the data that is available. It is crucial to keep in mind that the model's accuracy and dependability can be increased by calibration and validation utilizing experimental data from pertinent studies on microbial corrosion.

2.6 Mechanistic Approach to Model Development

2.6.1. Corrosion Indices:

To develop the mathematical model, it is essential to have a thorough understanding of the corrosion process of mild steel in a microbial environment. This includes considering the electrochemical reactions, microbial growth, biofilm formation, and the interactions between microorganisms and the metal surface.

2.6.2. Electrochemical Reactions:

The corrosion of mild steel in a microbial environment involves electrochemical reactions at the metal surface. From a first principles perspective, the fundamental principles of electrochemistry, such as Faraday's laws and the Nernst equation, can be applied to describe the corrosion process. Faraday's Laws relates the amount of substance undergoing a redox reaction to the electric charge transferred during the reaction. They can be used to determine the relationship between the corrosion current and the corrosion rate.

The Nernst equation relates the potential difference between the oxidized and reduced forms of the metal to the activities or concentrations of the species involved in the redox reaction. By considering the pH changes resulting from microbial activity, the Nernst equation can be applied to account for the influence of pH on the corrosion process.

2.6.3. Microbial Growth and Biofilm Formation:

Microbial growth and biofilm formation significantly affect the corrosion behavior of mild steel. From first principles, principles of microbial ecology and population dynamics can be applied to develop equations for microbial growth and biofilm formation [22]. The logistic growth model, derived from the principles of population dynamics, can be used to describe the growth of microorganisms in a microbial environment. This model takes into account factors such as the growth rate, carrying capacity, and the interaction between microorganisms and their environment.

Biofilm Growth Model: Biofilm formation involves the colonization and growth of microorganisms on the surface of mild steel. From a first principles perspective, biofilm growth can be described by considering factors such as attachment kinetics, detachment rates, nutrient availability, and the influence of environmental conditions.

2.6.4. Integration of Parameters:

To develop a comprehensive mathematical model, the derived equations for electrochemical reactions, microbial growth, and biofilm formation need to be integrated and interconnected. This integration allows for the consideration of the interactions and feedback between these parameters in the microbial corrosion process.

2.6.5. Calibration and Validation:

Once the mathematical model has been developed, it is crucial to calibrate and validate it using experimental data from microbial corrosion studies. This step involves adjusting model parameters and comparing the model predictions with experimental results to ensure accuracy and reliability.

By following these steps and considering the fundamental principles underlying the corrosion process, it is possible to develop a mathematical model for microbial corrosion of mild steel from first principles. The model can provide insights into the mechanisms involved, help predict corrosion rates, and guide the design of corrosion mitigation strategies in microbial environments.

3. Methodology and Discussion

1. Microbial Culture Preparation: Prepare microbial cultures representative of those commonly found in the target environment. This involves isolating and cultivating relevant microorganisms under controlled laboratory conditions.

2. Experimental Corrosion Studies: Conduct corrosion experiments using mild steel samples exposed to the microbial culture. Monitor and measure corrosion parameters such as corrosion rate, pit formation, and surface morphology using appropriate techniques and instruments.

3.. Data Analysis: Analyze the experimental data to identify and quantify the key corrosion parameters influenced by microbial activity. Parameters may include microbial population, metabolic activity, pH changes, biofilm formation, and electrochemical interactions.

4. Mathematical Model Development: Develop a comprehensive mathematical model that incorporates

the identified corrosion parameters influenced by microorganisms. The model should accurately predict the corrosion rate and behavior of mild steel in a microbial environment.

5. Model Validation: Validate the developed model using experimental data not used during the model development phase. Compare the model predictions with the actual corrosion rates and behaviors observed in the experimental studies to assess the accuracy and reliability of the model.

6. Sensitivity Analysis: Perform sensitivity analysis to determine the relative importance of each corrosion parameter influenced by microorganisms. This analysis will provide insights into the critical factors driving microbial-induced corrosion and guide the formulation of effective corrosion control strategies. The chart can be seen in fig 1.

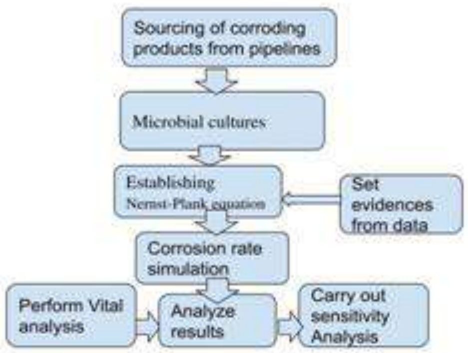

Fig1: Stepwise Approach to Model Formation

3.1 Model Development

When modeling mild steel corrosion in a microbial environment, one common approach is to use a modified form of the Nernst-Plank equation, taking into account the microbial activity and its impact on corrosion.

$$\frac{dC}{dt} = -KC(1+fM+gP+fgMP) \quad (6)$$

Where dC/dt represents the rate of corrosion (change in concentration of the corroding species over time), C represents the concentration of the corroding species in the solution, k is the corrosion rate constant, which depends on environmental factors and the specific mild steel being studied, M represents the microbial activity, which can be quantified using appropriate parameters. P represents the environmental parameters that affect corrosion, such as temperature, pH, and oxygen concentration, f and g are empirical coefficients that reflect the influence of microbial activity and environmental factors, respectively.

Rearranging equation (6) above yields

$$\frac{dC}{dt} = -KC(1+fM+gP) - KC(fgMP) \quad (7)$$

It should be noted that the additional term in the second part of the equation can be considered as an interaction term between the factors M and P. Simplify the equation further by introducing a new constant coefficient β to represent the combined effect of the interaction term..

$$\frac{dC}{dt} = -KC(1+fM+gP) - \beta KC(MP) \quad (8)$$

$$\frac{dC}{dt} = -KC(1+fM)(1+gP-\beta MP) \quad (9)$$

$$\frac{dC}{dt} = -KC(1+fM)(1+gP) \quad (10)$$

Including additional terms h and D, Equation 10 gives

$$\frac{dC}{dt} = -KC(1+fM)(1+gP)(1+hD) \quad (11)$$

Where D represents the deposition or attachment of microbial biofilms on the mild steel surface. Biofilms can accelerate corrosion processes by creating localized micro environments, h is an empirical coefficient that accounts for the influence of biofilm deposition on corrosion.

Expanding the equation (11) yields

$$\frac{dC}{dt} = -KC(1+fM+gP+hD+fgMP+fhMD+ghPD+fghMPD) \quad (12)$$

$$\frac{dC}{dt} = -KC(1+fM+gP+hD) - KC(fgMP+fhMD+ghPD+fghMPD) \quad (13)$$

The additional terms in the second part of the equation can be considered as interaction terms between the different factors (M, P, and D).

The combine effect of the interactive term is accounted for by the introduction of a new constant coefficient γ as shown in equation (14).The specific value of γ would need to be determined based on experimental data

$$\frac{dC}{dt} = -KC(1+fM+gP+hD) - \gamma KC(fgMP+fhMD+ghPD+fghMPD) \quad (14)$$

$$\frac{dC}{dt} = -KC(1+fM+gP+hD) - \gamma KC(MP+MD+PD+MPD) \quad (15)$$

4. Results

A comprehensive analytical mathematical model for predicting corrosion rates and behavior of mild steel in a microbial environment as shown in equation (15).it consist of key corrosion parameters influenced by microorganisms which gives insights into the relative importance of each corrosion parameter through sensitivity analysis. The equation as developed will enhanced understanding of microbial-induced corrosion processes in mild steel and will serve as a valuable tool for engineers and researchers to assess, prevent, and mitigate microbial-induced corrosion in mild steel structures. The Equation as derived allows us to model the corrosion rate of mild steel under the influence of microbial activity (M) and environmental parameters (P). The equation captures the corrosion rate (dC/dt) as a function of the concentration of the corroding species (C). The negative sign indicates that the concentration of the corroding species decreases over time due to corrosion. The term (1 + fM) represents the influence of microbial activity on corrosion. The coefficient f captures the impact of microbial activity, such as biofilm formation or microbial metabolites on the corrosion process. Higher values of f indicate a greater effect of microbial activity on corrosion.

The term (1 + gP) accounts for the influence of environmental parameters on corrosion. The coefficient g represents the sensitivity of corrosion to factors such as temperature, pH, oxygen concentration, or salinity. Higher values of g indicate a stronger correlation between environmental conditions and corrosion rate. The multiplication of (1 + fM) and (1 + gP) in the equation captures the combined effects of microbial activity and environmental parameters. This highlights the interaction and potential synergistic or antagonistic effects between these factors. The coefficient k represents the corrosion rate constant, which encompasses various factors affecting corrosion, including material properties, electrolyte composition, and surface conditions. The specific value of k depends on the system under study and should be determined experimentally It's important to note that the derived equation provides a mathematical framework for modeling mild steel corrosion in a microbial environment. However, the values of the coefficients f and g, as well as the corrosion rate constant k, need to be determined based on experimental data.

By utilizing this equation, researchers can gain insights into the relative contributions of microbial activity and environmental parameters on mild steel corrosion. They can also investigate how changes in these factors affect the corrosion rate and develop strategies to mitigate or control microbial-induced corrosion.

Moreover, this equation can be used to simulate corrosion scenarios and predict the corrosion behavior of mild steel in different microbial environments. By varying the values of M and P, researchers can study the sensitivity of corrosion to different microbial activities and environmental conditions, aiding in the design of corrosion-resistant materials or corrosion prevention strategies.

5. Conclusion

In conclusion, this research project on mathematical modeling of corrosion parameters in mild steel aims to address the pervasive issue of corrosion by developing a comprehensive mathematical model. By incorporating various corrosion parameters and analyzing their influence on corrosion rates, this study will contribute to our understanding of corrosion behavior in mild steel. The outcomes of this research will provide valuable insights and practical guidance for engineers and industries to effectively assess, prevent, and mitigate corrosion-related problems in mild steel structures, ultimately enhancing their performance and durability. In summary, the derived equation provides a valuable tool for mathematical modeling and understanding the complex interplay between microbial activity, environmental parameters, and mild steel corrosion. Its application can aid in the prediction, prevention, and management of corrosion in various microbial environments.

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