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The Challenges of Corrosion Control on Metallic Surfaces

Edited by Zeinab Abdel Hamid and Mona Hasan Gomaa

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Aims and Scope of the Series

Materials science has always occupied an extremely high position in the human development process. As we explore the oceans of stars, various industries have put forward more stringent requirements for the performance of materials, forcing us to pay more and more attention to the development of new materials. At the same time, the formation of a data-driven scientific paradigm is dramatically shortening the development cycle of new materials. The huge data generated by synergistically combining theories, high-throughput experiments, high-throughput computation, and artificial intelligence is greatly contributing to our ability to utilize materials science to solve real-world problems. The three topics of this book series - Metals and Nonmetals; Composite Materials; and Surface Science - will address important areas of advancement in materials science. There will be a range of interesting works published under these topics.

Meet the Series Editor

Prof. Chonghe Li received his Ph.D. from the Chinese Academy of Sciences in 1995. From 1995 to 2000, he worked as a researcher at the Shanghai Institute of Metallurgy, Chinese Academy of Sciences, where he also served as director of the research laboratory. In 2000, he was appointed Professor at the Institute of High-Performance Computing in Singapore, where he worked on computation and simulation in materials science until 2004. Since then, he has been a professor at the School of Materials Science and Engineering, Shanghai University, China, as well as the director of the Shanghai Specialty Casting Engineering and Technology Research Center. Prof. Li's research focuses on titanium alloys, titanium-aluminum single crystals, intermetallic compounds, theoretical calculations, alloy design, and special refractory materials. His broad scientific expertise is well recognized by the scientific community around the world. He is a member of the editorial board of the journal Metals. As an author, he has published more than 200 peer-reviewed papers, 2 books, and over 40 patents.

Meet the Volume Editors

Prof. Zeinab Abdel Hamid is the Emeritus Professor at the Central Metallurgical Research and Development Institute (CMRDI). She has published more than 140 papers in international journals and has presented her research at numerous international conferences. Her research interests include nanomaterials and surface treatments. She serves as a reviewer for numerous international journals. She has a State Incentive prize in chemistry in 2003 (Egypt), an Award of Scientific Excellence in Advanced Technological Sciences, and an Award of Scientific Excellence in Basic Science (2014), Egypt, a Medal of Science and Arts of the first class, awarded by the President of the Arab Republic of Egypt (2017), and an Award of the Central Metallurgical Research and Development Institute for outstanding scientific publications, Egypt (2019). Finally, she was ranked among the top 2% of world scientists, according to the American Stanford University classification from 2020 to 2024.

Mona Hasan is currently a Researcher at the Corrosion Control and Surface Protection Department at the Central Metallurgical Research and Development Institute (CMRDI). She earned her Bachelor of Chemistry at Helwan University in Cairo, Egypt, in 2009. In 2014, she obtained her Master's degree from Helwan University in Cairo, Egypt. Additionally, she holds a Ph.D. in Physical Chemistry from Ain Shams University in Cairo, Egypt, which she earned in 2021. She pioneered the development of a superhydrophobic coating from a polyaniline-based polymer nanocomposite in her thesis work, which has implications for various fields, including glass buildings, self-cleaning surfaces, anti-corrosion protection, anti-biofouling properties, and anti-fogging mirrors. Additionally, she has contributed to numerous scientific studies, which have been published in prestigious international peer-reviewed journals. Surface coating and corrosion protection, as well as metal electroplating and electroless plating, and nanocomposite coating for various purposes, are among her areas of interest. She developed expertise in creating and assessing antibacterial and superhydrophobic coatings.

Contents

Preface

In almost every area of human endeavor, corrosion is a persistent problem that compromises the performance, reliability, and integrity of metallic structures. In our technologically advanced civilization, metals are essential for everything from bridges, pipelines, and planes to household appliances and medical implants. However, despite their durability and practicality, metallic materials are still susceptible to environmental deterioration, which costs the world economy billions of dollars per year in replacement, maintenance, and damage.

The goal of this book, *The Challenges of Corrosion Control on Metallic Surfaces*, is to examine this intricate and multidimensional phenomenon from a scientific and applied standpoint. It investigates the fundamental causes of corrosion, the variables that accelerate its development, and the cutting-edge techniques being developed and used to mitigate its consequences. Even as our understanding of corrosion at the microstructural and electrochemical levels has advanced significantly, new materials, harsher conditions, and more stringent sustainability criteria continue to push the limits of conventional protective techniques. The primary objective of this book is to bridge the gap between theory and practice. It is intended for professionals, researchers, engineers, and students who want to apply efficient, long-lasting control methods in addition to comprehending corrosion processes. A thorough discussion of subjects such as corrosion-resistant alloys, surface coatings, cathodic protection, and newly developed nanostructured and intelligent materials is provided. The book also examines the more general issues of corrosion control, including long-term performance monitoring, environmental compatibility, and cost-effectiveness.

Due to its complexity, corrosion necessitates multidisciplinary thinking and teamwork in problem-solving. As such, this work draws upon insights from materials science, chemistry, electrochemistry, mechanical engineering, and environmental studies. It also highlights real-world case studies where corrosion control has succeeded or failed, offering valuable lessons for future advancements.

In compiling this book, we aim to contribute to the ongoing effort to preserve our metallic infrastructure, mitigate economic losses, and foster innovation in protective technologies. We can contribute to extending the service life of vital systems and constructing a more robust and sustainable built environment by expanding our knowledge of corrosion and strengthening our control over it.

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Chapter 1

Introductory Chapter: The Challenges of Corrosion Control for Metallic Surfaces

Zeinab Abdel Hamid and Mona Hasan Gomaa

1. Introduction

The multidisciplinary area of corrosion science studies the chemical and electrochemical processes that cause materials, especially metals, to deteriorate as a result of their interactions with the environment. Materials gradually deteriorate as a result of this natural phenomenon, endangering their functioning, safety, and mechanical strength. In a variety of industries, such as construction, transportation, oil and gas, maritime, and energy, where material failure can result in substantial financial losses, environmental harm, and safety risks, an understanding of corrosion is essential.

Fundamentally, corrosion is the process by which refined metals undergo redox reactions to change into more chemically stable forms like oxides, hydroxides, or sulfides. Iron rusting in the presence of oxygen and moisture is the most well-known example. In order to determine the causes of corrosion, forecast how it will behave in different scenarios, and create practical preventative and control strategies, corrosion science integrates concepts from chemistry, materials science, electrochemistry, and engineering [1].

Because corrosion science research reduces waste, increases resource efficiency, and lessens the need for frequent replacements, it not only helps materials and infrastructure last longer but also promotes sustainability. In order to guarantee dependability and endurance in both conventional and cutting-edge applications, corrosion science plays an ever-more-important role as new materials and technologies are created.

Metals gradually deteriorate as a result of chemical or electrochemical reactions with their surroundings in a process known as corrosion. Although this phenomenon is unavoidable in some circumstances, its management and prevention are essential to guaranteeing the durability, security, and dependability of metallic structures in a variety of sectors, including industry, energy, transportation, and infrastructure [2].

There are several different types of corrosion, including intergranular, uniform, galvanic, crevice, pitting, stress corrosion cracking (SCC), and microbiologically induced corrosion (MIC). The kind of material, oxygen, temperature, environmental pH, moisture and water (electrolyte), aggressive chemicals, microorganisms (microbiologically influenced corrosion, or MIC), and other variables all have an impact on the rate and severity of corrosion [3].

To prevent or decrease the corrosion of materials, there are many techniques that can be used such as protective coatings, cathodic protection, and corrosion inhibitors.

2. Mechanism of corrosion

Metals mostly corrode when they come into contact with oxygen, moisture, acids, salts, or other substances. Electrons are transferred from the metal (anode) to an oxidizing agent (cathode) *via* an electrolyte in the most prevalent type, known as electrochemical corrosion (**Figure 1**) [4, 5].

2.1 Electrochemical reaction and formation of corrosion products

2.1.1 Reactions at the electrodes

At the Anode (oxidation): The metal disintegrates into ions after losing electrons.

$$M \rightarrow M^{2+} + 2e^{-} \tag{1}$$

At the Cathode (reduction): In the electrolyte, a species is reduced by anode electrons.

In acidic environments (presence of H^{+}):

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

In neutral or basic environments (presence of O_2 and water):

$$O_2 + 2H_2O + 4e- \rightarrow 4OH^{-} \tag{3}$$

The metal ions (e.g., Fe^{2+}) react with $OH^{-}$to form metal hydroxides:

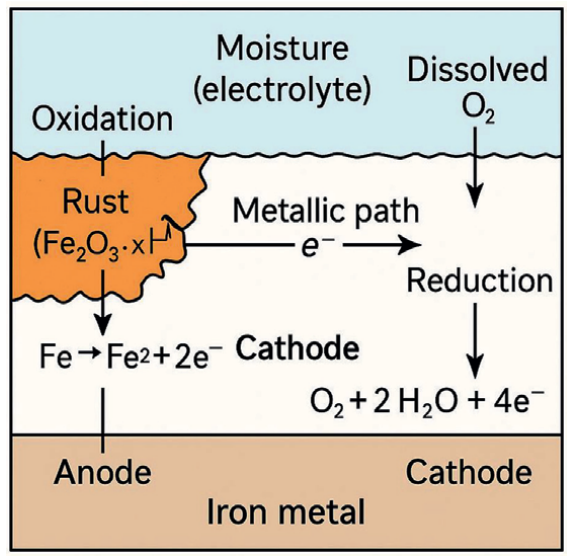

Figure 1.
Corrosion mechanism.

$$Fe^{2+} + 2OH^{-} \rightarrow Fe(OH)_2 \quad (4)$$

This can further oxidize to form iron (III) hydroxide, which dehydrates to form *rust* ($Fe_2O_3 \cdot xH_2O$) (Corrosion Products) [6].

3. Corrosion control methods

For metal buildings, equipment, pipelines, and infrastructure to remain intact, safe, and functional, corrosion management is crucial. Material deterioration results from corrosion, which happens when metals interact with their surroundings, particularly oxygen, moisture, and other corrosive substances. Several primary strategies can be used to classify effective corrosion control methods:

3.1 Selection of materials

One of the most important steps in preventing corrosion is selecting the appropriate material for the climate. Stainless steel, titanium, or nickel alloys that create stable passive oxide layers are examples of corrosion-resistant alloys. Materials that are not metals include ceramics, composites, and plastics in situations where metals are extremely reactive. Moreover, to minimize galvanic corrosion and lower the potential difference, choose metals that are next to one another in the galvanic series [7, 8].

3.2 Coatings for protection

The metal surface and the corrosive environment are separated by protective coatings such as:

a. *Organic coatings and paints:* Epoxy, polyurethane, and acrylic paints are frequently applied on equipment and structures. For increased longevity, multilayer coating systems consist of a primer, an intermediate layer, and a topcoat.

b. *The use of metal coatings*: Applying a zinc coating on steel, which serves as a sacrificial anode, is known as galvanizing. Moreover, a class of industrial procedures known as thermal spray coatings involves heating a feedstock material (in wire or powder form) and then spraying it onto a surface. These coatings improve surface qualities like electrical conductivity, heat resistance, corrosion resistance, and wear resistance. Fast deposition rates, thick coatings (50 μm to several mm), and versatility in handling a variety of materials are some of this process's benefits [9].

3.3 Cathodic protection (CP)

It is a method of lowering the rate of corrosion by using the metal surface as an electrochemical cell's cathode. More reactive metals, such as magnesium, aluminum, or zinc, are used in sacrificial anode CP (SACP) [10, 11] .While Current Impressed CP (ICCP) is used to stop the corrosion process, a direct current is applied from an external power source. It is better suited for massive structures such as offshore platforms, storage tanks, and ship hulls.

3.4 Anodic protection

It is utilized for passive metals (like titanium and stainless steel) in harsh settings (like sulfuric acid tanks). The metal is kept in its passive state by applying a little anodic current [12].

3.5 Inhibitors of corrosion

The two main types of corrosion inhibitors, anodic and cathodic, work to prevent electrochemical corrosion of metals by interfering with the respective processes that occur during corrosion. These are chemicals added to the environment to slow down the corrosion rate. Anodic inhibitors form a protective oxide layer on the metal, reducing metal dissolution by preventing metal ions from dissolving. However, they can cause localized corrosion, such as pitting, if the passive layer breaks down. Conversely, cathodic inhibitors slow the cathodic reaction, including oxygen reduction. The drawbacks of cathodic inhibitors include reduced effectiveness in highly acidic conditions and the potential to interfere with other water treatment processes. Mixed inhibitors impact both anodic and cathodic reactions [13].

4. Challenges in corrosion control using super-hydrophobic coatings (SHCs)

Specialized surface treatments known as super-hydrophobic coatings make a substance incredibly water-repellent. They draw inspiration from natural surfaces such as lotus leaves, which, because of their low surface energy and micro/nanoscale surface roughness, have both strong water repellency and self-cleaning qualities. A high contact angle >150° (water droplets bead up and roll off the surface readily) and a low sliding angle (< 10°, droplets slide off with minimal tilt) are characteristics of super-hydrophobic coatings [14]. Additionally, it is self-cleaning (rolling water droplets remove dirt and particles), anti-icing, and anti-corrosion (less water adhesion helps avoid frost and rust formation). Surface roughness is usually used to achieve super-hydrophobicity because texture at the micro and nanoscales increases surface area and traps air pockets. Additionally, low surface energy materials that reject water molecules include silicones and fluorinated chemicals [15].

Super-hydrophobic coatings can be deposited using a variety of coating techniques, each with unique benefits, drawbacks, and applicability based on the substrate and application. These techniques seek to provide a surface made of low surface energy materials that is also rough at the micro/nano scale. Here is the description of different techniques:

Diping process: The alternative method for creating super-hydrophobic coating is the dip procedure. This procedure involves dipping the substrate into a solution that contains the hydrophobic substances, then carefully pulling it out [16]. This process's merits include homogeneity coating, even on intricate geometries, and easy scalability for industrial application; its drawbacks include slowness in big quantities and coating material waste in the solution.

Spray coating: It is one of the popular ways for creating super-hydrophobic surfaces. Using an airbrush or spray gun, a material with micro/nanostructures and low surface energy is deposited onto a substrate. By spraying a mixture of hydrophobic polymers and nanoparticles onto the substrate, the spray technique can produce

super-hydrophobic coatings. This approach is characterized by low equipment costs, simplicity and scalability, and suitability for big or uneven surfaces. Without post-treatment, this method may not be very durable and has little control over thickness and homogeneity [17].

Spin coating: In this coating, a tiny drop of coating liquid is applied to the center of a substrate, which is then quickly spun to use centrifugal force to distribute the liquid. Thin films produced by this method are homogeneous, and it fits flat substrates like silicon wafers well. However, it has drawbacks, such as not working with huge or three-dimensional objects [18].

The chemical vapor deposition: In chemical vapor deposition, a desirable thin film or coating is created by the reaction or breakdown of gaseous precursors on the heated substrate surface. There are various forms of CVD. Heat (usually between 250 and 1200°C) is used in thermal CVD to start chemical reactions. Deposition on heat-sensitive substrates is made possible by plasma-enhanced CVD (PECVD), which uses plasma to reduce the deposition temperature. Compound semiconductors like GaAs or InP are deposited using metal-organic precursors in a process known as metal-organic CVD (MOCVD). Finally, to increase film uniformity, low-pressure CVD (LPCVD) uses subatmospheric pressure. The advantages of the different CVD processes are strong adhesion, high purity and conformity, and long-lasting coatings, while the disadvantages are expensive and complex equipment [19].

Electrospinning: This method creates a web-like structure on the surface by drawing thin threads from a polymer solution using a high-voltage electric field. The creation of highly rough nanostructured coatings and customization of fiber diameter and porosity are the primary benefits of this method. However, the primary drawbacks are the need for meticulous parameter control and the restricted scalability [20].

Electrodeposition: Electrochemical deposition technique has been widely used to fabricate SHC. This technique is independent of the shape and size of the substrate. It is a method of forming a coating by the migration of positive and negative ions from an electrolyte solution and the redox reaction of gaining and losing electrons at the electrode under an applied electric field. SHC has been created using a variety of electrochemical techniques, including electrochemical polymerization and electrochemical deposition. Because the polymerization rate can be readily adjusted by changing the oxidation potential, the polymerization media can be reused, doping can occur concurrently, the film thickness and morphology can be better controlled, and cleaner polymers can be formed; electrochemical polymerization offers some benefits. Step current, step potential, galvanostatic, and potentiodynamic (cyclic voltammetry) approaches are the three primary groups into which electrochemical techniques fall. All of these techniques use a three-electrode setup, which includes a reference electrode, a counter electrode, and a working electrode [21].

The most applicable material in fabrication of super-hydrophobic coating is reduced graphene oxide (rGO), based on their chemical durability and water resistance. Super-hydrophobic surfaces have been created using a variety of polymers and oxide nanoparticles. Because of their many applications, the conducting polymers that are most researched are polyaniline (PANI), polyacetylene (PAC), polypyrene (PPY), and polythiophene (PT). PANI is the most promising conducting polymer because of its unique properties, which include relatively high electrical conductivity, ease of production, and environmental resilience. All of these characteristics are connected to its distinct chemical structure, which has three redox forms, each with a distinctive base and salt form [22].

4.1 Challenges of super-hydrophobic coatings (SHCs)

SHCs have a lot of potential for anti-corrosion, self-cleaning, anti-icing, and drag reduction, but their long-term performance and widespread industrial application are limited by a number of issues such as:

Mechanical durability: Because this surface is sensitive and frequently degraded under stress, the majority of SHCs are mechanically fragile and rapidly damaged by abrasion, impact, or even moderate touch. Additionally, the result is the loss of functioning and water-repellent qualities in practical settings.

Thermal stability: Because organic materials employed for low surface energy can dissolve and cause nanostructures to collapse, SHCs may lose structure or degrade when exposed to high temperatures.

Environmental stability: SHC's performance can be deteriorated by exposure to contaminants, moisture, acids, and UV light. Additionally, erosion corrosion was caused by oil and dust contamination, while chemical corrosion was caused by acid rain. Contact angle and surface integrity gradually diminish as a result of the impact.

Adhesion to substrates: Because the coating material and the underlying surface are incompatible, SHCs frequently have poor adherence to the substrate, which results in peeling or flaking and necessitates surface pre-treatment or intermediary adhesive layers.

Complex fabrication methods: A large number of SHC deposition methods are costly, time-consuming, or non-scalable. Applying to big or uneven surfaces might be challenging.

Scalability and reproducibility: It is challenging to replicate reliable super-hydrophobic performance over sizable regions or batches. Reason: Sensitivity to material qualities, ambient factors, and deposition parameters.

Challenge	Impact	Strategies to Improve
Mechanical fragility	Loss of function after abrasion	Through the incorporating hard nanoparticles like SiO_2, Al_2O_3, or TiO_2 into polymer matrices.
Thermal instability	Degradation at high temperatures	Through using ceramic-based or carbon-based materials (like graphene oxide) for higher thermal resistance.
Environmental degradation	Loss of hydrophobicity over time	Through using strong covalent bonding of hydrophobic molecules (e.g., silanes) to the surface resists erosion. Transparent protective films can shield the SHC without affecting its function.
Poor substrate adhesion	Peeling or delamination	Through the surface pretreatment methods, like plasma treatment or acid etching.
Complex fabrication	High cost and low scalability	Through the application of simple method like spray and immersion
Anti-icing limitations	Reduced performance in real-world	A newer approach where a lubricant is infused into a porous layer, offering better anti-icing.

Table 1.
Summary of the challenges of superhydrophobic coatings (SHCs).

Health and environmental risks: A lot of SHCs use harmful, long-lasting, and nonbiodegradable fluorinated chemicals.

Limited anti-icing performance over time: Despite SHC's ability to postpone icing, ice eventually forms and sticks in real-world scenarios (humidity, wind, and supercooling). Issue: The surface microstructure may sustain damage from ice formation, decreasing its long-term efficacy [23–25]. These challenges can be summarized in **Table 1**.

5. New developments and studies to increase materials' resistance to corrosion

Use of smart and self-healing coatings: Materials that are responsive and self-healing can fix little damage or spot corrosion early.

Nanotechnology application: Using nano-engineered devices to improve inhibitor delivery and barrier qualities.

Real-time data analytics: Using for predictive maintenance is possible with digital twins and artificial intelligence (AI) modeling.

Use of Green Inhibitors: Green corrosion inhibitors are eco-friendly compounds that lessen or stop corrosion on metal surfaces. They are frequently made from natural sources. In place of conventional synthetic (and frequently dangerous) corrosion inhibitors, they are sustainable, non-toxic, and biodegradable [26].

6. Conclusion

- Corrosion of metallic surfaces is a multifaceted problem with significant technical and economic implications. While numerous methods exist for its mitigation, the selection of an appropriate strategy requires a holistic understanding of the environment, material properties, and operational demands. Ongoing research and innovation are key to developing more effective, sustainable, and economical corrosion control solutions.

- Infrastructure can deteriorate and natural resources can be wasted when metals like steel, copper, magnesium, and aluminum corrode. One remarkable use of super-hydrophobic surfaces is boosting these metals' durability against corrosion. Research on super-hydrophobic surfaces that are resistant to corrosion shows that the metal surfaces' interaction with liquid is reduced by the creation of air barriers and a decrease in the area of water contact. This results in exceptional resistance to corrosion and a reduced rate of corrosion. These surfaces' corrosion resistance and long-lasting super-hydrophobicity also promise well for practical applications in both everyday life and business.

- SHCs have a lot of potential for anti-corrosion, self-cleaning, anti-icing, and drag reduction, but their long-term performance and widespread industrial application are limited by several issues. Additional consideration must therefore be given to the study of super-hydrophobic surfaces as barriers against metal corrosion.

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Chapter 2

Recent Advances and Challenges of the Thermo-Reactive Deposition-Diffusion (TRD) Process for Corrosion Control in Steels

Fabio Enrique Castillejo Nieto
and Diana Maritza Marulanda Cardona

Abstract

In this chapter, the thermo-reactive deposition-diffusion (TRD) technique is examined as a surface treatment method to enhance the corrosion resistance of machine components. The chapter begins by discussing the fundamentals of the process, including an analysis of the variables that influence the TRD technique. This is followed by an explanation of the mechanisms involved in the formation of carbide layers and their electrochemical behavior. Finally, the chapter addresses the challenges associated with using this technique for corrosion control in metals, providing a review of the most significant and recent publications in the field. These insights allow for the formulation of conclusions regarding the current limitations and future prospects of the TRD technique.

Keywords: thermo-reactive deposition-diffusion, TRD, corrosion, electrochemical properties, carbides, steels

1. Introduction

In the industrial and metal-mechanical sectors, it is crucial to obtain materials with high core toughness and excellent surface resistance to corrosion and wear. These materials are essential for manufacturing various cutting tools and machine components that operate under friction conditions, such as forming dies, gears, brakes, and wire drawing dies, among others.

For this reason, various studies have been conducted to implement techniques and procedures that enable the formation of surface layers enriched with carbon or nitrogen, enhancing the mechanical properties of metals in service. Additionally, severe plastic deformation (SPD) processes have been explored to modify the microstructure of metals, including high-pressure torsion (HPT) and simple shear extrusion (SSE),

among others. SPD techniques allow processed materials to acquire ultrafine, nanometric-sized grains, significantly improving the mechanical and electrochemical properties of metals [1, 2].

In recent years, another alternative has been considered: the production of coatings or thin films on the surfaces of metallic materials to provide protection. These coatings have been manufactured using industrial techniques such as physical vapor deposition (PVD), chemical vapor deposition (CVD), and certain thermochemical treatments, including carburizing and nitriding. However, these processes require specialized equipment to achieve extremely low pressures, making industrial scaling highly costly.

As an alternative for achieving such coatings on metallic surfaces, the thermo-reactive deposition-diffusion (TRD) process has emerged. This method generates carbide, nitride, or silicide layers through thermal diffusion processes, ensuring excellent adhesion of the coatings to the treated metal surfaces.

2. Thermo-reactive deposition-diffusion (TRD) process

The thermo-reactive deposition-diffusion (TRD) technique is a thermal treatment process that enables the formation of compact, pore-free carbide coatings. These coatings are deposited on steels with a carbon content greater than 3%. The steels are immersed in a molten borax bath at temperatures exceeding 1346.15 K.

The carbide coatings typically deposited—such as Vanadium Carbide (VC), Niobium Carbide (NbC), and Chromium Carbide (Cr_7C_3), among others—are formed through a reaction between the carbon atoms in the steel and the atoms of carbide-forming elements (CFEs), which are introduced into the molten borax in powder form. These CFEs include ferro-vanadium, ferro-niobium, ferro-tungsten, ferro-titanium, and ferro-chromium.

The carbide layers formed on steel exhibit excellent adhesion, corrosion, and oxidation resistance, as well as wear resistance. As a result, this process effectively enhances the performance of dies, cutting tools, machine components, and other industrial elements.

In the TRD process, the carbon from the steel reaches the surface via thermal diffusion to chemically react with the CFEs, forming the corresponding carbide layer. This differs from traditional thermochemical hardening treatments, where specific elements (carbon and nitrogen) diffuse into the substrate to harden it. Another key difference is that, in the TRD process, a carbide layer grows outward from the substrate surface.

2.1 Process characteristics

Through the TRD process, it is possible to deposit carbide, nitride, or carbonitride coatings on tool steels. This thermochemical treatment can be performed using three different methods: the first involves a salt bath using borax and CFEs [3–8]; the second method uses a fluidized bed, where a gas is blown upward through a layer of fine aluminum oxide particles. This particle layer inside the furnace chamber behaves like a fluid, and the gas flow maintains continuous motion, causing particle collisions that ensure a uniform temperature throughout the furnace's effective volume [9]. The third method is the powder-pack process, which uses a sealed steel container with refractory cement, where the parts to be treated are immersed in CFEs and alumina.

Carbide layers obtained through salt bath immersion were first developed in Japan and have been used industrially since approximately 1971 under the name Toyota Diffusion (TD) Coating Process. The TD method uses molten borax with the addition of carbide-forming elements such as vanadium, niobium, titanium, and chromium, which combine with carbon from the steel substrate to produce carbide layer deposition.

The process performed with the salt bath requires temperatures ranging from 1073.15 K to achieve layers between 4 and 12 μm, with processing times between 1 and 8 hours. Coated steels are typically cooled and subsequently reheated for hardening, or the salt bath temperature during the process can be set to match the austenitizing temperature of the steel, making it possible to harden the steel after the coating process. **Figure 1** shows a basic schematic of the steps followed when treating a part using the TRD process [10].

Steels with a carbon content greater than 0.3% are suitable for this treatment. Typical steels include tool steels, high-speed steels, and other steels with austenitizing temperatures above 1323.15 K, which can be reheated after the TRD process and subsequently hardened.

Figure 2 shows the typical cycle diagram. High-speed steels and other steels with austenitizing temperatures above 1323.15 K can be reheated after the TRD process and treated in a vacuum, gas, or protective bath to achieve full substrate hardening.

2.2 Influence of TRD process variables

Various parameters of the TRD process affect the quality of the obtained coating layer. This section presents these parameters and their relevance to the properties achieved in the coating.

2.2.1 Bath temperature and immersion time

At first glance, one might assume that the process temperature is directly proportional to the thickness of the obtained layer. However, **Figure 3** clearly illustrates the influence of temperature on the coating thickness for a niobium-vanadium carbide

Figure 1.
General scheme for the thermo-reactive deposition-diffusion (TRD) process [10].

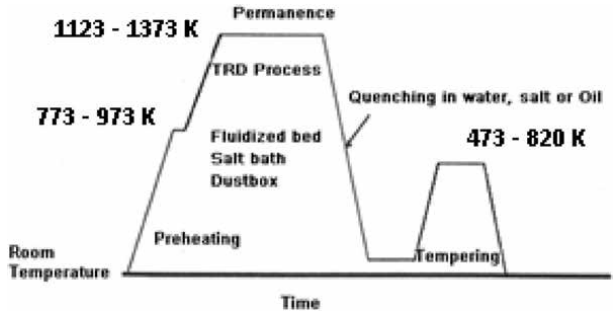

Figure 2.
Schematic representation of the typical TRD process cycle.

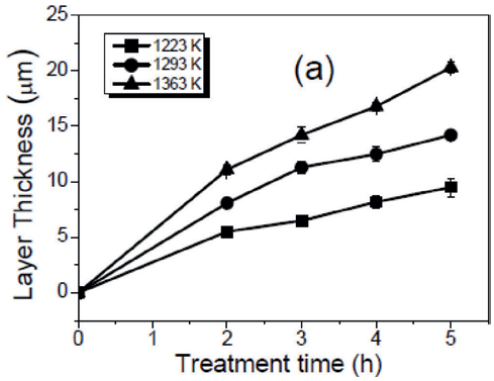

Figure 3.
Effect of temperature and treatment time on the layer thickness of Nb-V carbide formed on AISI D2 [11].

deposited on AISI D2 steel at four different temperatures and times. An Arrhenius-type exponential trend can be observed as follows:

$$\frac{d^2}{t} = K_0 e^{-\frac{Q}{RT}} \quad (1)$$

Where d is the coating thickness (cm), t is the time (s), Q is the activation energy (experimentally determined for each coating in KJ/mol), T is the absolute temperature (K), R is the universal gas constant (8.314 J/mol·K), K is the growth rate constant (cm^2/s), and K_0 is a constant (cm^2/s).

Figure 4 shows the optical microscopy images obtained for the Nb-V system deposited on AISI D2 steel samples at temperatures of 1223 K and 1363 K, respectively, for a treatment time of 5 hours. The figure clearly demonstrates that as the treatment time increases, the obtained layer thickness also increases, eventually reaching an asymptotic behavior after approximately 4 to 5 hours.

2.2.2 Substrate type

This relationship is not yet fully defined; however, some trends can be inferred from reported results. **Figure 5** shows the vanadium carbide layer thickness at

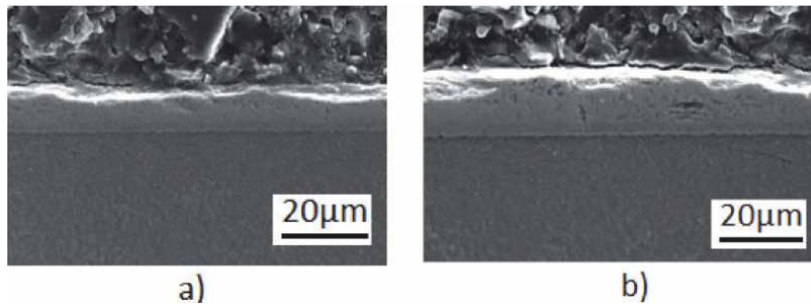

Figure 4.
Optical microscopy images of the Nb-V system on AISI D2 steel after 5 hours at (a) 1223 K, and (b) 1363 K [11].

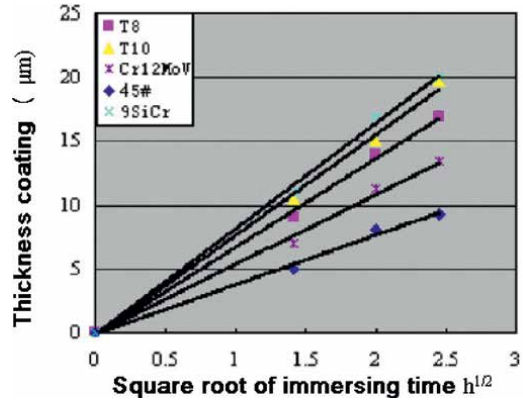

Figure 5.
Effect of immersing time on thickness of vanadium carbide layers at bath temperature 1223 K [12].

1223.15 K as a function of the square root of time for different steels, whose chemical composition is presented in **Table 1**. This information indicates that the obtained layer thickness tends to be greater as the carbon content of the substrate material increases [12].

Additionally, **Figure 6** shows the optical microscopy images of niobium carbide coatings on AISI H13 steel (0.39 wt% C) and AISI M2 steel (0.9 wt% C). It is clearly observed that the higher the carbon content in the substrate, the greater the achieved layer thickness. In this study, a layer thickness of 6.2 ± 0.2 µm was reported for AISI H13 steel (a) and 9.0 ± 0.3 µm for AISI M2 steel (b). Both coatings were deposited under the same conditions [13].

Steel	C	Cr	V	Si	Mn	Mo
45	0.43			0.24	0.28	
T8	0.79			0.25	0.3	
T10	1.02			0.31	0.28	
9SiCr	0.85	0.99		1.34	0.42	
$Cr_{12}MoV$	1.4	12.58	0.35	0.22	0.48	1.00

Table 1.
Chemical composition of the steels used in **Figure 5**.

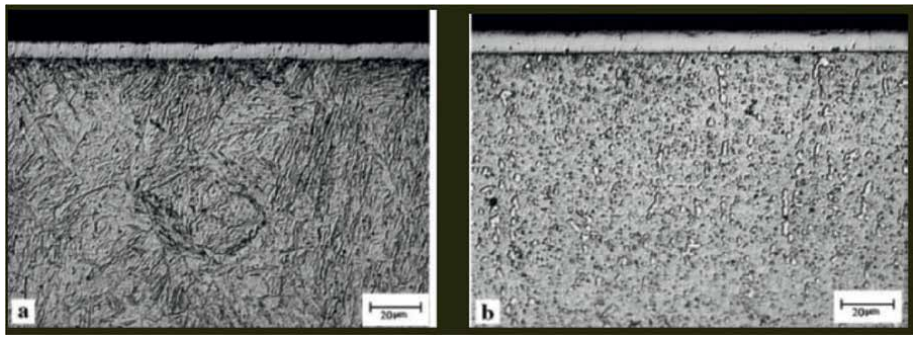

Figure 6.
NbC coating deposited on (a) AISI H13, and (b) AISI M2 [13].

2.2.3 Carbide type

The key parameter for the formation of any type of coating on steel is determined by the free energies of formation. In general, chemical reactions with negative Gibbs free energy will occur spontaneously, according to the second law of thermodynamics. On the other hand, if the Gibbs free energy is zero, the reaction is in equilibrium, and finally, if the Gibbs free energy is positive, there is no possibility for the reaction to occur spontaneously or naturally. **Table 2** presents the Gibbs free energy of formation for selected oxides and carbides [14].

2.2.4 Workpiece geometry

When performing the TRD process, it is essential to consider the cross-section of the surface to be coated. The larger the area to be coated, the greater the likelihood

Oxide	***ΔG(Kcal/mol de O_2***	**Carbide**	***ΔG(Kcal/mol de C***
CaO	−242	ZrC	−62
La_2O_3	−234	UC	−42
MgO	−220	TiC	−53
ZrO_2	−204	ThC_2	−33
Al_2O_3	−203	ThC_3	−28
TiO	−190	U_2C	−25
B_2O_3	−154	VC	−25
SiO_2	−154	Mn_3C	−22
V_2O_3	−146	$Cr_{23}C_6$	−18
NbO	−144	Cr_7C_6	−16
MnO	−140	CaC_2	−14
CoO	−63	Na_2C_2	−11
		NbC	−32

Table 2.
Gibbs free energy of formation of oxides and carbides [14].

of layer delamination, lower thermal shock resistance, and a higher probability of distortion of the treated piece [14, 15].

2.3 Mechanism of carbide layer formation through the TRD process

Starting with steel containing dissolved carbon in the matrix at concentrations above 0.3 wt.%, it is known that when subjected to high temperatures, thermal diffusion drives carbon atoms toward the substrate surface. Once at the surface, these carbon atoms chemically react with the carbide-forming elements (CFEs) present in the salt bath. At the appropriate temperature, this reaction leads to the formation of surface carbide layers.

This occurs when the Gibbs free energy of the respective carbide is negative. However, if this energy is only slightly negative, the reaction quickly reaches equilibrium, preventing the formation of a stable layer. In this sense, the growth of the coating is subject to certain limitations. At typical process temperatures (1073.15–1373.15 K), three critical conditions apply:

- The activation energy required for the formation of transition metal carbides is significantly lower than the activation energy for carbon diffusion.
- The diffusion coefficient of carbon in the deposited layer is lower than in the austenite phase of the substrate.
- The diffusion coefficient of carbon in the deposited layer is lower than that of CFEs in the molten borax salt.

These conditions are of vital importance because they allow for predicting that the growth rate of the carbide layer is entirely controlled by the diffusion of carbon atoms within the carbide layer and the diffusion of metal atoms in the carbide [16]. **Figure 7** shows the mechanism by which carbide layers are formed on the substrates.

3. Electrochemical properties of carbide layers obtained by TRD

The corrosion rate of a coating-substrate system can be measured using potential vs. current curves, known as potentiodynamic polarization curves or Tafel polarization curves, as well as electrochemical impedance spectroscopy (EIS) tests.

3.1 Potentiodynamic polarization curves

To perform the measurements required to obtain polarization curves, the setup shown in **Figure 8** is used. When the sample is immersed in the electrolyte, it acquires potential that can be measured against a reference electrode. This potential is known as the corrosion potential or equilibrium potential. If the equilibrium of the system is disturbed by increasing or decreasing the applied potential, a net current will begin to flow in a certain direction, causing a shift in the electrode potential. This new potential will differ from the equilibrium potential, with its magnitude and sign depending on the flowing current. The deviation of the electrode potential from its equilibrium value is referred to as polarization, and this value is known as the overpotential (η):

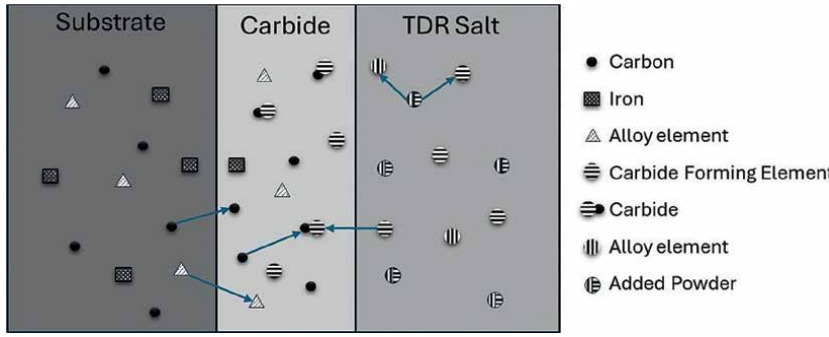

Figure 7.
Mechanism of carbide layer formation.

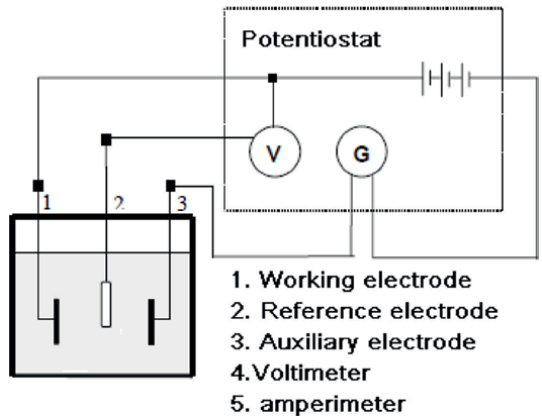

Figure 8.
Instrumental methods for polarization resistance.

$$\eta = \boldsymbol{E} - \boldsymbol{E}_{\boldsymbol{equilibrium}} \tag{2}$$

Where is the applied potential? If the voltage source is polarized to values lower than the corrosion potential, only metal reduction will occur. Conversely, when applying potentials above the corrosion potential, the metal will lose electrons, leading to an oxidation reaction.

The phenomenon of electrochemical kinetics that describes the corrosion process and relates the current to the applied overpotential is predicted by the Butler-Volmer equation:

$$\mathrm{i} = \mathrm{i}_{\mathrm{corr}} \left[\mathrm{e}^{\frac{\alpha n F}{RT}\eta} - \mathrm{e}^{\frac{-(1-\alpha)nF}{RT}\eta} \right] \tag{3}$$

Where α is the charge transfer coefficient, n is the number of electrons transferred, F is the Faraday constant, R is the universal gas constant, η is the applied overpotential, and i_{corr} is the corrosion current. If the applied overpotentials are between −120 and 120 mV, eq. (3) can be rewritten as follows:

$$\mathrm{i} = \mathrm{i}_{\mathrm{corr}} \frac{nF}{RT}\eta \tag{4}$$

Through this linear equation, it is possible to calculate the corrosion current, which can then be used in the Stern-Geary equation to determine the polarization resistance R_p:

$$\left[\frac{d\eta}{di}\right]_{\eta=0} = R_p = \frac{\beta_a \beta_b}{2.303(\beta_a + \beta_b) i_{corr}} \quad (5)$$

Where β_a and β_c are the anodic and cathodic slopes, respectively. **Figure 9** shows the typical polarization curve obtained in the experiment. It can be observed that the point where the cathodic and anodic lines intersect corresponds to the coordinates that determine the corrosion current on the horizontal axis and the corrosion potential on the vertical axis. A metal will have better electrochemical properties if it exhibits higher corrosion potentials E_{corr}, as the system requires more energy to initiate the process, and lower corrosion currents i_{corr}, since the corrosion rate is directly proportional to the current.

Figure 10 presents the potentiodynamic polarization curves for AISI D2 and H13 steels, as well as for each of the binary systems NbC, VC, and CrxCy deposited on these steels using the TRD process. The coatings on both steels show an increase

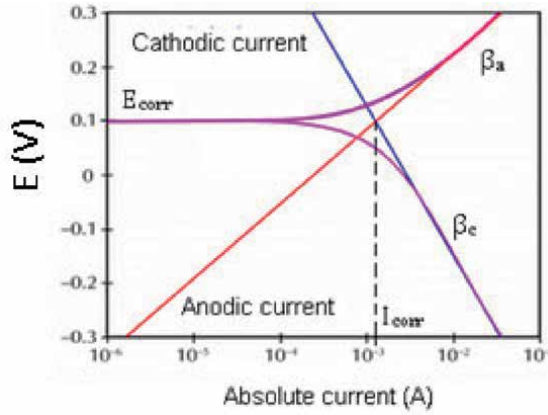

Figure 9.
Typical experimental polarization curve.

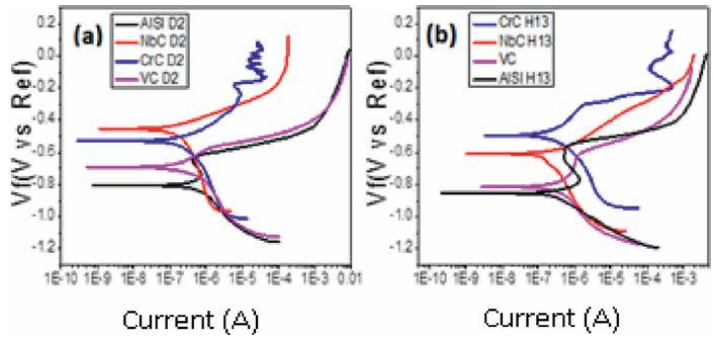

Figure 10.
Potentiodynamic polarization curves for steels and binary carbides. (a) AISI D2 steel, (b) AISI H13 steel, (c) Niobium, vanadium and chromium carbides on D2, and (d) Niobium, vanadium and chromium carbides on H13 [17].

in corrosion resistance, which can be clearly seen due to the increased corrosion potential and decreased corrosion current in the three carbide coatings compared to uncoated steel. In general, a very similar behavior is observed for both uncoated steels. It is evident that chromium carbides exhibit the best performance, followed by niobium carbide and, finally, vanadium carbide. This can be explained by the chemical stability of the oxides formed by each metal (chromium, vanadium, and niobium). Chromium oxide (Cr_2O_3) exhibits high chemical stability and is industrially used as a protective layer against material degradation in the form of coatings or thin films [18, 19]. Niobium oxide (Nb_2O_5) also demonstrates very high chemical stability and excellent corrosion resistance in both acidic and basic environments [20, 21]. In contrast, vanadium oxide (V_2O_5) is highly unstable and incapable of protecting a metal from degradation, especially in basic environments [22–27]. The literature reports numerous studies analyzing potentiodynamic polarization curves, generally presenting results similar to those shown in **Figure 10** for binary carbides on AISI D2, M2, 52,100, and H13 steels [17, 28, 29].

Table 3 shows the summary for the corrosion potential and currents of the uncoated substrate and coated with the three binary carbides (Nb, V and Cr).

3.2 Electrochemical impedance spectroscopy (EIS)

This electrochemical technique is relatively modern, having emerged in the 1970s due to the development of electronic circuits with sufficient resolution to analyze and generate signals with variable frequency and phase.

This technique is highly adaptable and precise for studying metallic materials and biomaterials, as it allows for easy measurement of current and transfer impedance of the analyzed material. Fundamentally, a variable electrical potential is applied to the sample, and the complex current response is recorded. With this information, it is possible to determine the electrochemical transfer impedance of the material as a complex value, which, through appropriate mathematical processing, can be separated into a real and imaginary component, allowing the determination of corrosion resistance.

By analyzing the impedance versus frequency graph, it is possible to model or propose an electrical circuit with resistors and capacitors that replicate the same results. Each circuit element can then be assigned a specific role in terms of the electrochemically studied coating. **Figure 11** illustrates a case where the coating is free of pores

System	Steel	Icorr	Standard deviation	Ecorr	Standard deviation
CrxCy	D2	2,21E-07	1,02E-08	−457,5	1,9
NbC	D2	3,78E-07	5,59E-08	−554,5	2,8
VC	D2	6,66E-07	9,50E-08	−692,7	5,2
AISI D2	D2	1,09E-06	1,07E-07	−807.3	1,2
CrC	H13	5,81E-07	13051E-08	−489.4	2,6
NbC	H13	3,07E-07	10263E-08	−619.3	1,2
VC	H13	6,29E-07	29738E-08	−815.7	1,5
AISI H13	H13	9,13E-07	25697E-08	−866.6	7

Table 3.
Summary for the corrosion potential and currents of the uncoated substrate and coated with the three binary carbides (Nb, V and Cr).

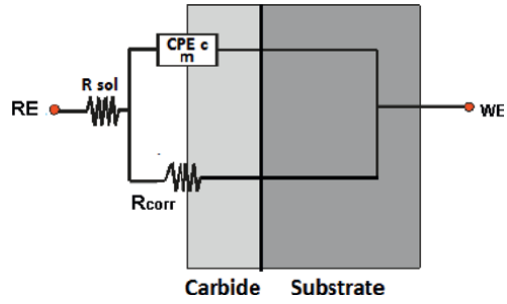

Figure 11.
Equivalent circuit for Electrochemical Impedance Spectroscopy (EIS).

and acts as a passivating film that slows down the corrosion process of the metallic substrate. A first impedance, R_{sol}, appears, corresponding to the electrolyte solution in the setup (typically a 3% saltwater solution). Then, a second resistance, R_{corr}, represents the impedance of the coating, along with the coating capacitance, CPE_m.

This coating, modeled using the proposed electrical circuit, typically generates two types of diagrams: (I) The Bode diagram shown in **Figure 12a**. From a theoretical perspective, it is established that the higher the impedance value at low frequencies, the better the electrochemical performance of the studied material, and consequently, the greater its corrosion resistance, and (II) The Nyquist diagram shown in **Figure 12b**. In which it is shown that corrosion resistance is also observed at low frequencies and it is expected that the larger the diameter of the semicircle, the better the electrochemical behavior of the coating will be.

Figure 13 presents EIS results for two different steels (AISI H13 and AISI D2) coated with niobium carbide (NbC) [29]. **Figure 13a** and **c** show the uncoated steels with their respective Bode diagrams. In both cases, the impedance is in the order of 1000 Ω. For **Figure 13b** and **d**, which correspond to the coated steels, it is evident that the impedance value increased by an order of magnitude, significantly improving the electrochemical properties of both steels.

These impedance curves were made by subjecting the sample to corrosive attack for times of 1, 24, 48, and 168 hours. It can be noted that the AISI D2 steel substrates were not affected by time since the impedance was very similar at low frequencies for the 4 times (**Figure 13a**); however, the AISI H13 steel did decrease the impedance over time (**Figure 13c**). This phenomenon is due to the higher percentage of chromium in

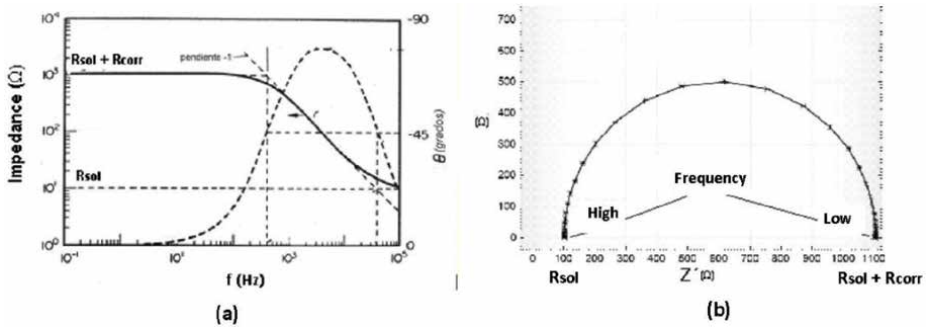

Figure 12.
Bode plot (a) and plot Nyquist, and (b) for non-porous coating [30].

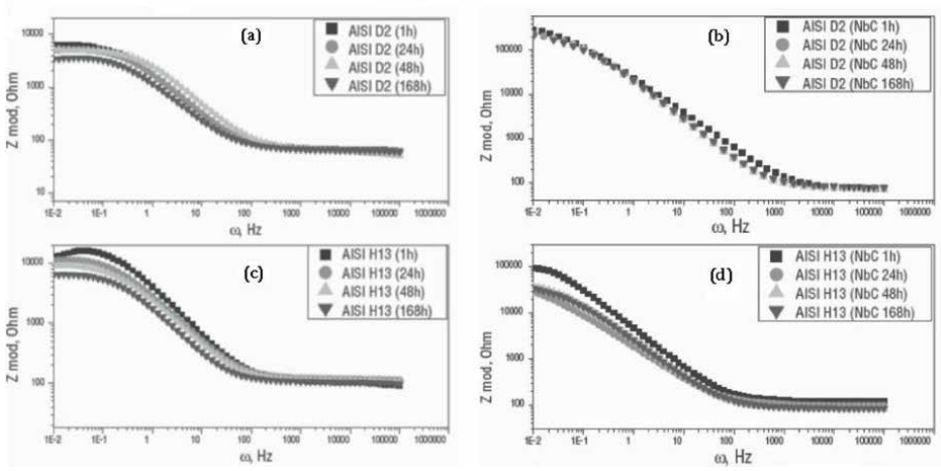

Figure 13.
Bode plots for steel. (a) Uncoated AISI D2, (b) NbC on AISI D2, (c) Uncoated AISI H13, and (d) NbC on AISI H13 steel [29].

D2 steel (11.5%) compared to H13 steel (5.2%) which significantly improves corrosion resistance. It is also observed that the impedance at low frequencies for AISI D2 steel coated with niobium carbide remains practically constant over time (**Figure 13b**), while for the same carbide deposited on AISI H13 steel, the impedance at low frequencies decreases as the exposure time increases (**Figure 13d**). This occurs because the thickness of the niobium carbide coatings deposited using the TRD technique strongly depends on the percentage of carbon in the treated steel; in this case, for D2, it is 1.5%, while for H13, it is only 0.4%. Since the layers on H13 steel are thinner, they present greater porosity. These pores increase in size as the immersion time increases. In this way, a greater penetration of the corrosive solution into the steel occurs, which produces localized corrosion. However, it is important to note that these results indicated that the impedance decreases slowly with time, which shows that very long times are required for the electrolyte to penetrate to the surface of the steel [31].

Currently, binary carbides of niobium, vanadium, chromium, and titanium have been extensively studied. Recent advancements in the deposition of carbides on metallic surfaces using the TRD process have aimed to leverage the specific properties of each coating. For example, niobium carbide exhibits high hardness and excellent wear resistance, while chromium carbide provides outstanding corrosion resistance. From this perspective, it is entirely reasonable to consider that the production of a ternary Nb-Cr carbide could result in a new coating capable of combining the electrochemical and mechanical properties of the individual binary carbides.

According to this emerging trend of producing mixed carbides through the TRD process to achieve superior coatings with excellent mechanical and electrochemical properties, several studies have been reported. These studies focus on hardness, wear resistance, coating growth kinetics, adhesion, and electrochemical properties of mixed carbides containing niobium, vanadium, and chromium on various tool steels such as AISI D2, AISI H13, AISI M2, and AISI D6 [32–36].

The effect of niobium carbide formations in FeAl coatings on wear, corrosion, and oxidation performance has also been studied. The reported results predict that the carbon contained in spherical graphite nodules—which leads to lower mechanical

properties and corrosion resistance in ductile cast irons due to its presence in FeAl coatings—will transform into NbC coatings through interaction with niobium. This transformation is expected to result in improved coatings [37].

Other studies report the production of niobium and vanadium layers using the TRD process on vermicular cast irons, generating uniform carbide coatings with thicknesses exceeding 25 μm, as shown in **Figure 14** [38]. These layers exhibited good

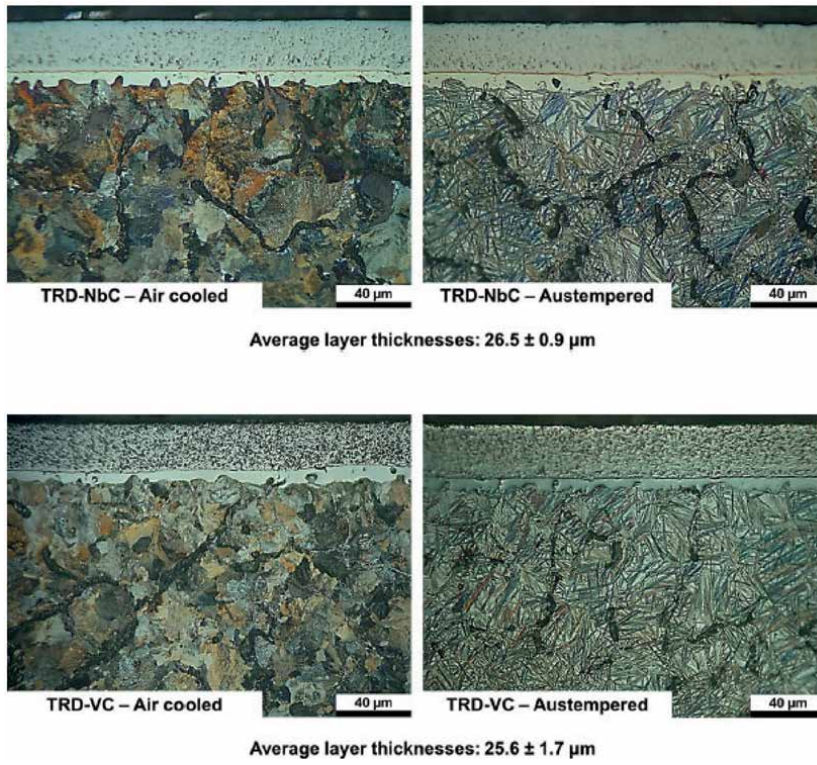

Figure 14.
Optical micrographs of the cross sections of the vermicular cast iron after the TRD-NbC treatment [38].

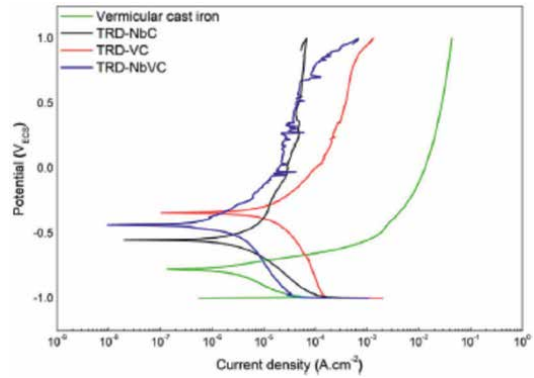

Figure 15.
Potentiodynamic polarization curves in 3.5% de NaCl for vermicular cast iron after TRD treatments [38].

adhesion and hardness values of over 2300, 2500, and 3050 HV for Nb, V, and Nb-V carbides, respectively. The wear resistance of the coated samples increased by a factor of 10 to 30 compared to the austempered substrate. Additionally, the coatings demonstrated significantly higher corrosion resistance than the substrate, as evidenced in **Figure 15** by the potentiodynamic polarization curves, which show a higher corrosion potential and lower corrosion current.

4. Challenges and future directions in using the TRD technique for corrosion control in metals

Despite being extensively studied, the TRD technique still presents challenges and areas for improvement, including:

- Conducting similar studies but incorporating a quaternary coating composed of *NbxVyCrzC* to determine whether it is possible to enhance the electrochemical and mechanical properties of existing coatings.

- Since the TRD technique can only be applied to steels or metallic materials with carbon content above 0.3%, it would be beneficial to perform *preliminary carburizing treatments* before the TRD process. This would allow for the study of potential applications of these carbides on steels with initially lower carbon content, such as *AISI 1010 or AISI 1020*, to assess whether they meet service requirements.

- Expanding electrochemical property studies by conducting *erosion-corrosion tests* on these carbides to better understand their durability in aggressive environments.

- On a *simulation level*, it is crucial to predict *ternary phase diagrams* for systems such as *C-V-Cr, Nb-V-C, and Nb-Cr-C* using computational tools like *CALPHAD*. This would help theoretically estimate the properties of these carbides and optimize their performance.

5. Conclusions

The TRD process is a highly effective technique for producing transition metal carbide coatings (niobium, vanadium, chromium, titanium, among others). These carbides are characterized by being pore-free, having uniform thickness, high hardness, and excellent wear resistance.

All carbide coatings deposited using the TRD process exhibit superior electrochemical performance compared to steel. This improvement is evident through higher corrosion potential values and lower exchange current densities in potentiodynamic polarization curves. Similarly, electrochemical impedance spectroscopy results show higher total impedance values for the coatings at low frequencies. This behavior is primarily attributed to the chemical stability of the oxides and carbides of each transition metal.

Beyond the initial binary carbides developed using the TRD process, current research focuses on combining two carbide-forming elements (CFEs) to create ternary carbides with enhanced hardness and improved electrochemical properties.

It is essential to expand the application of this technique to steels with carbon content below 0.3% by implementing a thermochemical treatment prior to the TRD process.

Furthermore, the development of quaternary carbides could unlock new possibilities for the TRD process, enabling the creation of carbide coatings with superior mechanical and electrochemical properties compared to binary and ternary carbides.

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Chapter 3

Exploring Corrosion Inhibitor Adsorption on Metal Surfaces through Density Functional Theory and Molecular Dynamics Simulations

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Abstract

This chapter explores the ways corrosion inhibitors stick to metal surfaces using cutting-edge computer methods. It shows how density functional theory (DFT) and molecular dynamics (MD) simulations help us grasp the tiny interactions that make corrosion inhibition work. The main points include studying how inhibitors stick, how charges move, and what the inhibitors look like at the electron level. It also looks at how the inhibitor's parts, like functional groups and heteroatoms, play a role. The chapter points out how things like the environment, surface features, and changes over time affect how well inhibitors work and how stable the protective film is. Besides theory, this chapter talks about real-world uses, giving examples of both man-made inhibitors and natural, plant-based ones that are better for the environment. It also touches on new ideas like using machine learning to predict outcomes and mixing computer methods with lab tests. This big-picture look connects basic science to industry use, helping to create lasting and powerful ways to stop corrosion.

Keywords: adsorption, molecular dynamics, density functional theory, surfaces, metals

1. Introduction

1.1 Importance of corrosion inhibition

Inhibiting corrosion is of great importance to the protection of materials, especially metals, against adverse oxidation and environmental effects that include humidity, temperature, and other chemicals [1]. It is a prerequisite for increasing the life and performance of materials across different sectors, such as construction, manufacturing, and energy [2]. The phenomenon of corrosion can cause huge economic impacts in the form of equipment breakdowns, repairs, maintenance, and the replacement of damaged parts [3]. Corrosion inhibitors are substances that

are used in the application of metal surfaces to create a layer that limits interaction between the metal and the surroundings; thus, the corrosion process is minimized or prevented [4]. Inhibitors can be divided into two categories, anodic inhibitors, which retard anodic reactions of corrosion, and cathodic inhibitors, which affect cathodic reactions [5]. Besides showing their efficiency in preventing corrosion, inhibitors have also been responsible for improving the mechanical properties of the material, like strength and resistance to wear, which is important to keep the integrity of structures and machinery under harsh operation conditions. The use of corrosion inhibitors is environmentally positive when eco-friendly and biodegradable compounds are employed, thereby minimizing the environmental footprint that is typically aligned with conventional corrosion prevention techniques [6]. Due to the burgeoning demand for durable and sustainable materials, the development of more efficient, cost-effective, and environmentally safe corrosion inhibitors has shifted into focus [7]. The importance of corrosion inhibition extends beyond industrial applications, influencing the overall safety and longevity of infrastructure and machinery across diverse sectors.

1.2 Overview of the economic and structural impact of corrosion on industries

It is a common aspect in industries worldwide where costly corrosion devastates both the economy and the structure of any industry [8]. According to Prasad et al. [9], the estimated global loss on corrosion is above $2.5 trillion annually, which amounts to about 3–4% of the global Gross Domestic Product (GDP). Such staggering figures include both direct costs, such as repairing and replacing damaged equipment and corrosion prevention techniques, as well as indirect costs like production downtime, reduced efficiencies, or safety risks. Oil and gas, as well as construction, transportation, and energy production industries, are the most severely affected by corrosion because they rely on their metal bases whose infrastructure is exposed to harsh, extreme environmental and operational conditions [10]. For instance, corrosion in the oil and gas industry affects pipelines, storage tanks, and drilling facilities, leading to failures in supply chains and incurring expensive repairs. In other words, corrosion in transportation breaks that which has integrity in vehicles, bridges, and railways, hence compromising structural integrity, which can lead to catastrophic failures [11]. Among other factors, corrosion damages the economy as it compromises the safety of personnel and the environment from varied issues such as oil spills, gas leaks, and the collapse of structures—all of which may have dire consequences on both communities and ecosystems.

Corrosion incidents will have greater effects according to the kinds of industries that are fabricated today, and not just limited to localized corrosion damage or effects spreading out into the systems as a whole [12]. Preventing corrosion, such as by effective materials selection, protective coatings, cathodic protection, and corrosion inhibitors, will minimize these losses and extend the life cycle of industrial assets [12]. Although investing in corrosion management involves maintenance cost reductions, it also brings increased reliability in operations to keep industries competitive and sustainable over the long term.

1.3 Traditional approaches vs. modern computational techniques for studying corrosion inhibitors

For several decades now, there has been research on corrosion inhibitors with laboratory studies as well as modern computerized techniques, each of which has its

merits and demerits [13]. These are experimental methods based primarily on laboratory investigations such as weight loss measurements, electrochemical techniques such as potentiodynamic polarization and electrochemical impedance spectroscopy, and surface characterization techniques that include scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR) [13]. They reflect potentials rather directly on inhibitor performance for corrosion rates and surface morphology of metals exposed to corrosive environments; however, traditional approaches can be time-consuming, labor-intensive, and costly because they demand exhaustive experimental runs to discover and optimize the most effective inhibitors and their variations with environmental conditions. A modern method, be it quantum chemical calculation, molecular dynamics (MD) simulations, or machine learning algorithms, in fact, has brought the corrosion inhibition research to reality by offering speedy and cheap predictive tools for developing an understanding of the behavior of just about most inhibitors at atomic as well as molecular levels. Quantum chemical methods like density functional theory (DFT) enable the calculation of parameters such as frontier molecular orbitals, adsorption energies, and dipole moments to predict adsorption efficiency when using corrosion inhibitors [14]. Molecular dynamics simulations help one be able to evaluate the interactions between the metal and the inhibitor in these environments that undergo several dynamic changes, as well as provide information about the adsorption mechanisms and the stability of these inhibitors under varying conditions [15]. Machine learning can really use all the huge experimental databases to make predictions regarding corrosion rates and screen possible inhibitors, streamlining the amount of trial-and-error experimentation required [16]. The traditional methods are still relevant in validating theoretical results and truly understanding performance in the field. However, modern computational techniques supplement and speed up the discovery of new, green corrosion inhibitors. The comprehensive understanding of the corrosion-inhibition mechanism development is going to foster innovative solutions to address corrosion in the industries.

1.4 Computational techniques in corrosion studies

1.4.1 Introduction to density functional theory (DFT) and molecular dynamics (MD) simulations

Density functional theory (DFT) and molecular dynamics (MD) simulations, the two powerful computational approaches, have become necessary tools in material science, chemistry, and, specifically, corrosion research [17]. Density functional theory (DFT) is widely employed as a quantum mechanical method for investigating the electronic structure of atoms, molecules, and condensed phases. Hohenberg-Kohn theorems established the basic premise of the method that states ground state properties for a many-electron system can be derived by making use of electron density and not by using an enormous wave function [18]. The practical use of the DFT necessitates the solution of the Kohn-Sham equations as approximations of the document concerning certain energetic properties, like energy levels, electron density distribution, and chemical reactivity descriptors, including HOMO-lowest unoccupied molecular orbital (LUMO) energy gap, dipole moments, and Fukui indices. Energy, density, and chemical reactivity descriptors such as HOMO-LUMO energy gap, dipole moment, Fukui indices, etc., which are very much required for possible prediction and understanding of chemical reactivity and adsorption characteristics of the molecules, make DFT very important for corrosion inhibition studies. On the

other hand, molecular dynamics (MD) simulations complement each other in studying molecular systems' dynamic behavior with time.

Molecular dynamics is that which comprises Newtonian motion equations for a system of associated and self-interacting particles [19]. Such systems can be used for simulated studies regarding the behavior of atomic positions and velocities under given temperature, pressure, and boundary conditions [20]. MD simulations have offered significant information on the nature of molecular interaction and adsorption processes as well as any thermodynamic property on the effect of inhibitors on metallic surfaces [21]. With DFT and MD together, it has become possible to create a multi-scale view of materials: the accurate electronic structure calculational power of DFT is integrated with the dynamic real-world processes that MD bridges from the theoretical prediction gap. This results in revolutionized materials science and computer-based resources since the reduction of experimental costs accompanies the fast track to finding efficient and eco-friendly corrosion inhibitors. This technique provides great potential: managing general forecasting on material behavior, optimization for molecular structures, and image creation for complex molecular systems with unprecedented precision.

1.4.2 Advantages of computational methods in understanding adsorption mechanisms at the molecular level

With highly accurate, detailed, and cost-effective information on molecular interactions, often very difficult to observe with experimental means, computational techniques have completely transformed the understanding of the adsorption mechanism at the molecular level. Such techniques, most notably density functional theory (DFT) and molecular dynamics (MD) simulations, capture the events at the atomic level, providing the electronic picture, interaction energies, and dynamics of molecules adsorbed at surfaces. Among the various facilities computational methods offer, the most advantageous is predicting adsorption behavior under various environmental conditions such as temperature, pressure, or pH, without the labor-intensive in-the-laboratory experiments [22]. DFT allows computation of adsorption energies, electron density distributions, and chemical reactivity descriptors such as the HOMO-LUMO gap and Fukui indices, which can be used to ascertain the strength and the character of a molecule-surface interaction [23].

These are very instrumental properties for understanding how inhibitors, adsorbates, or other molecules bind to the metal surfaces and how they cause differences in corrosion resistance or catalytic processes. Likewise, MD simulations treat the time-dependent behavior of the adsorbed species while accommodating thermal fluctuations and eventful interactions between molecules and surfaces, which contributes essentially to the comprehension of true systems reported in the literature [24]. Thus, indeed, virtual techniques also allow one to screen and design new corrosion-resistant materials and inhibitors when mechanisms of adsorption are analyzed along with predictions for efficiencies by molecular means prior to experimental validation, thus shortening much development time and costs. The combination of machine learning and artificial intelligence methods along with computational methods is further speeding up the discovery process by allowing predictions on adsorption behavior to be made using large databases of molecular descriptors [25]. Most importantly, these allow visualization and measurement of adsorbing mechanisms at the nanoscale, which indeed gives a better understanding of surface chemistry and interaction dynamics required by corrosion inhibition, catalysis, and material science

applications [26]. In a nutshell, computational approaches have shown the best merits over others by developing innovations in material design while maximizing efficiency in molecular processes by elucidating the adsorption mechanisms.

2. Mechanisms of corrosion inhibitor adsorption

2.1 Fundamental concepts and adsorption processes on metal surfaces

The process of adsorption on the metallic surfaces has been playing a fundamental role in many fields, such as corrosion inhibition, remedies, catalysis, material science, etc. [4]. These processes govern the relationships that exist between molecules and metallic substrates at the atomic and molecular levels. Based on the strength and nature of the interaction, there are two types of adsorptions, physisorption and chemisorption. Physisorption is defined as the type where weak Van der Waals forces interact with an adsorbate molecule on the surface, and this leads to a process that is non-specific and reversible, without much alteration in the electronic structures of the adsorbent or adsorbate [27]. Chemisorption is characterized by strong covalent or ionic bonds between the adsorbate and metal atoms, which frequently change important aspects of the electronic properties, and the process entails a stronger fixation, often irreversible [28]. The type and size of adsorption are affected by many other factors, including surface properties of the metal (e.g., crystallographic orientation and roughness), electronic configuration of the adsorbate, temperature and pressure conditions, as well as the surrounding medium [29]. Metals, such as transition metals, with vacant d-orbitals often exhibit strong chemisorption behavior as they have the ability to accept electron density from adsorbate molecules and back donate to the antibonding orbitals of the adsorbates, which increases the stability associated with adsorbed molecules. Mechanisms of adsorption are necessary when assessing effective corrosion inhibitors since these will adsorb themselves onto metal surfaces to provide protection by blocking entrance for corrosive species, such as oxygen or chloride ions, to the metal surface [5]. DFT and MD simulations have been widely used to study the adsorption processes at the atomic level and provided insights into adsorption energies, electron density distributions, and molecular orientations on metal surfaces [21]. At the experimental level, surface characterization techniques such as scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), or atomic force microscopy (AFM) are most frequently used to confirm theoretical findings and study the morphology and composition of adsorbed layers. Combined experimental and computational methods much improved the understanding of adsorption processes, which will point the next stage to the better delivery of future advanced materials and inhibitors for a specific application.

2.1.1 Role of the inhibitor-metal interaction in reducing corrosion rates

As a result of their ability to produce protective layers that shield metal surfaces from corrosive species, the interactions of corrosion inhibitors with metal surfaces play an important role in decreasing the rates of corrosion [4]. These interactions happen by adsorption of inhibitor molecules onto metal surfaces, either by physical adsorption (physisorption) or chemical adsorption (chemisorption), depending on the nature of both the inhibitor and the metal substrate. In physisorption, the interaction is weak and reversible; it is because there are mainly Van der Waals forces

involved, and hence it is dependent on the change in temperature as well as the environment. Chemisorption has been held up by stronger covalent or ionic bonds, to a significant degree, increasing the stability of the protective feature power of the inhibitor. In a more ideal manner, such types of effective inhibitors possess functional groups such as heteroatoms (N, O, S), π-electron systems, and aromatic rings facilitating strong interactions with vacant d-orbitals at metal surfaces [30]. These functional groups donate electron density to the metal surface while simultaneously accepting back-donation of electrons, resulting in a stable adsorption layer that prevents diffusion of aggressive ions such as Cl and SO_4. More active surfaces will be available for corrosion reactions, and thus, the corrosion rate will generally be reduced upon adsorption. Besides, the inhibitor exposes metal interaction to consider modification of the double-layer structure at the metal-electrolyte interface, which affects electrochemical processes like anodic metal dissolution and cathodic oxygen reduction. This has been studied by the application of computational techniques such as density functional theory (DFT) and molecular dynamics (MD) simulations, which help in understanding the process at molecular levels by providing insights into adsorption energies, electron density distributions, and mechanisms of bond formation [31]. Furthermore, several other experimental methods, such as electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, and surface analysis techniques like scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy, have all been extensively used here to validate and characterize the inhibitor-metal interactions. All in all, the strength and characteristics of the inhibitor-metal interaction are the primary determinants of the efficiency of the corrosion inhibitors since they encompass the stability and the coverage of the protective layer against corrosion processes and lengthen the lifetime of the metal structures.

2.2 Adsorption isotherms

2.2.1 Langmuir, Freundlich, and other models of inhibitor adsorption

Adsorption isotherms are mathematical expressions used to characterize the interactions between adsorbates, mostly corrosion inhibitors, and metallic surfaces, with the aim of characterizing adsorption processes to find out its nature, strength, and mechanism, which are the main key performance indicators for inhibitors in corrosion mitigation [21]. Language and Deutsch are some of the most commonly utilized isotherm models; however, some others, like the Temkin, El-Awady, and Flory-Huggins isotherms, can also be put forward in relevant applications. The Langmuir adsorption isotherm is characterized by monolayer adsorption on a homogeneous surface having adsorption sites that are energetically identical, with no interaction between adsorbed molecules [32]. Aside from Langmuir and Freundlich, there are other types of isotherms that are related to the complexities found in adsorption. The Temkin isotherm, for instance, takes into consideration lateral interactions of the adsorbed species and postulates that the energy of adsorption decreases linearly as the surface coverage increases [33]. The El-Awady model introduced a few adsorptions along with those of Langmuir, useful for the systems that involve multiple adsorptions [34]. The Flory-Huggins also devours the level of adsorbed species as per the surface area of the metal, which is especially useful in the case of large inhibitor molecules. All those adsorption models play an essential role in thermodynamic parameters estimation, including adsorption equilibrium constant K, Gibbs free energy change (ΔGads), spontaneity, and stability of adsorption [35].

A negative ΔGads value indicates a spontaneously occurring adsorption, with values around −20 kJ/mol being designated to physisorption and those close to −40 kJ/mol or even higher considered as chemisorption. Because each system can be different regarding the inhibitor, metal surface, and electrolyte involved in the study, it can also be said that the selection of a specific adsorption isotherm depends on the system being investigated [4]. The typical experimental techniques to obtain raw data for adsorption isotherms could be electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, or gravimetric weight-loss method, which then are modeled to fit such isotherms to reveal the type of adsorption mechanism [36]. Thus, including theoretical models in experimental data will demonstrate a complete scene of how adsorption takes place while using corrosion inhibitors and facilitate inhibitors' mixtures for increased protection against corrosion.

2.2.2 Correlation of theoretical data with experimental findings

The correlation between theoretical data and experimental data is by far the most promising route toward the validation of computational models and their mechanistic understanding of many chemical and physical processes, including corrosion inhibition [37]. Theoretical means like density functional theory (DFT) and molecular dynamics (MD) simulations provide predictive theoretical models by culminating in extensive descriptions of electronic structures, energy states, and molecular interactions of the systems at atomic or molecular dimensions. These models predict different properties such as adsorption energies, binding affinities, and stability of inhibitor-metal interactions under different conditions [17]. However, prediction accuracy is determined by the correctness of assumptions, force fields, and parameters upon which simulations were run. Hence, experimental correlation or data validation with theoretical data is necessary for establishing that models are meaningful in real life. Touching on the performance of corrosion inhibitors and the relative adsorption features on metal surfaces, the techniques used include electrochemical measurements and surface analysis (SEM, XPS), to mention just a few, and weight loss tests [38]. Electrochemical techniques—potentiodynamic polarization and electrochemical impedance spectroscopy (EIS)—could give insight into the corrosion rate and inhibition efficiency, including the mechanism of action of inhibitors through the quantitative measures taken on the differences in electrochemical properties in the presence of inhibitors. Results from these experimental approaches can be judiciously compared with theoretical predictions, such as adsorption energies or interaction energies predicted from computational models in one way to validate the accuracy of the theoretical approach. One important example of this correlation is adsorption isotherms compared to theoretical predictions for adsorption strength with experimental measurements of surface coverage at different inhibitor concentrations. For corrosion inhibitors, the theoretical calculation should predict the most favorable adsorption modes, whereas the experiment should check the actual degree of surface coverage and inhibitor efficiency [4]. In addition, the comparison of thermodynamic parameters, such as adsorption free energy (ΔGads) and activation energy (Ea), between the theoretical models and the experimental data may help evaluate the spontaneous and the efficient nature of adsorption as well as the strength of the inhibitor-metal interaction [39]. From theoretical to experimental results, one can expect differences due to the presence of impurities, input of temperature, and computational methods. They can be interested in how much further one needs to develop theories and what one needs to examine for better reliability of the prediction.

Ultimately, theoretical and experimental approaches together give a broad overview of the corrosion inhibition so that it will be useful for designing efficient inhibitors and developing better tactics to control corrosion in the industrial application.

2.3 Electron-level interactions

2.3.1 Charge transfer mechanisms during adsorption

The charge transfer mechanisms are most commonly employed to assess the adsorption of corrosion inhibitors on metal surfaces [40]. The inhibition process is again a sort of adsorption phenomenon between inhibitor molecules and the metal surface, in that electron density gets transferred either from the metal to the inhibitor (physisorption) or from the inhibitor to the metal (chemisorption). This degree and nature of charge transfer largely govern the efficiency of the inhibitor. During physisorption, the major interaction between the surface and the inhibitor arises from Van der Waals forces, and hence, the electron transfer is practically insignificant. On the other hand, chemisorption is found to be the interaction where there is a cation-anion bond between the functional group of an inhibitor molecule and a metal surface. It often involves the transfer of charge from the metal to the molecule of the inhibitor and may alter its electronic structure to favor better corrosion inhibiting properties [41]. Charge transfer can be assessed through various computational mechanisms, among which DFT is found to be most effective in modeling the electronic structure of the system at the molecular level [42]. In this theory, DFT calculations give an insight into energy levels, orbital interactions, and potential for charge redistribution between the metal surface and inhibitor molecules, crucial information for developing more effective inhibitors.

2.3.2 Visualization of molecular orbitals, electron density, and reactivity using DFT

As explained in the previous sections, DFT is very useful for charge transfer during adsorption and then analysis through molecular orbitals, reactivity, and electron density. DFT thereby constitutes a holistic modeling approach toward electronic structure elucidation of the molecular systems in question by calculating the energies of the highest occupied molecular orbitals (HOMO) and that of the lowest unoccupied molecular orbital (LUMO), which is essential to the understanding of charge transfer processes. The HOMO-LUMO gap is an important measure of reactivity—in most cases, small gaps correspond to high reactivity and a good ability to donate and/or accept electrons during the process of adsorption [43]. Normally, in studies on corrosion inhibitors, low HOMO-LUMO molecules are reported to be more reactive and much more efficient for adsorption on the metal surface to inhibit corrosion [44]. DFT computations also enable visualization of the electron density distribution, which elucidates the sharing of electron density between the inhibitor and metal and thus provides an understanding of the bonding nature [45].

Mulliken partitioning will help in visualizing electron density distribution in a molecule by quantifying the distribution of the electronic charge over different atoms in the molecule [46]. This study is crucial to fathoming the donor-acceptor interactions of the inhibitor with the metal surface. This study is also used to compute reactivity descriptors such as electrophilicity and nucleophilicity indices using DFT, which give an idea regarding the reactivity of the molecules in specific media. DFT can thus provide a complete picture of the working mechanism of inhibitors at the electronic level,

enabling one to identify functional groups responsible for corrosion inhibition [17]. This is the reason why DFT is an excellent tool for both the prediction of corrosion inhibitors and the design of new molecules with future corrosion resistance properties.

3. Functional groups and molecular structures

3.1 The role of functional groups

The role of functional groups in the adsorption efficiency of corrosion inhibitors is the adsorption mechanism determination of the inhibitor and interaction at the metal surfaces [44]. It has been well established that polar functional groups, particularly hydroxyl (-OH) or carboxyl (-COOH) groups, are prominent candidates in promoting adsorption onto metal surfaces [47]. Hydroxyl acts as a very strong electron donor such that it easily brings about an interaction with the surface metal atom or ions by the formation of hydrogen bonds, thereby intensifying the binding of the inhibitor to the surface [44]. Likewise, the carboxyl group is also an important requirement, as its oxygen atoms build up a stable coordination bond with the metal ions by developing electrostatic and covalent oxime interactions with them [48]. These polarized groups increase the strength of the anchoring of the metal to the inhibitor, and the protective hydrophobic barrier that is produced decreases the metal's corrosion rate [49]. This will frequently increase an inhibitor's overall energetic value for adsorption, making it a more effective means of protecting metal against corrosion. It is evident, therefore, that the selection of functional groups is very critical in effecting better inhibition and performance of inhibitors under given specific environmental conditions.

3.2 Influence of heteroatoms

Heteroatoms like nitrogen, sulfur, oxygen, and phosphorus are important types of atoms in corrosion inhibition, providing efficacy to inhibitors [50]. Inhibitors enhance metal surface interaction through coordination bonds or by altering the electronic properties of inhibitor molecules [51]. For instance, nitrogen atoms have lone pairs and are strong electron donors that could coordinate with metal cations from heterocyclic compounds [52]. Since sulfur makes very strong bonds with metals, especially with transition metals, it is often included in corrosion inhibitors [53]. Besides contributing high adsorption and efficiency, the sulfur atom of thiol (–SH) or that of thiazole groups is useful [54]. Oxygen in carbonyl, hydroxyl groups, and so on also increases the reactivity of the inhibitor by donating electron density to the metal surface [55]. Phosphorus-containing inhibitors, often incorporating phosphonate groups, find usage over a wide spectrum in the protection of metals and widely used application phenomena at high-level stability and corrosion resistance [56]. Heterocyclic compounds such as imidazoles, benzothiazoles, and pyridines have been found that the adsorbability of these inhibitors on the metal surfaces for protective layers forming is boosted by including some heteroatoms, especially nitrogen and sulfur. Thus, it is known that benzothiazole derivatives show good performances of corrosion inhibition. Such nitrogen as well as sulfur atoms not only donate electrons but also generate stable complexes with metal ions.

3.3 Structural optimization

Molecular geometries, stability, and other structural properties of the corrosion inhibitors are studied, as these are important in affecting their adsorption behavior

and performance [57]. The shape and size of the inhibitor molecule dictate how well it approaches the metal surface for adsorption. For example, a planar structure is preferred for strong adsorption and good stability of the adsorption process due to efficient π-π stacking interactions between the inhibitor and the metal surface [58]. Molecules, on the other hand, with large or branched structures, may have reduced adsorption because they get hindered sterically and do not effectively interact with the metal surface. Besides that, molecular stability is an important factor to guarantee that the inhibitor maintains integrity in harsh environmental conditions, like acidic or very high temperature environments [59]. Structural optimization involves terms that rather concern optimizing the electronic properties of the molecule itself to enhance the activity of the inhibitor, for example, by computer modeling to predict how each and every change in molecular structure affects the adsorption energy and mini efficiency of its use using density functional theory (DFT) and such methods. These optimization approaches offer both strong adsorption and good molecular stability, hence developing stronger inhibitors that protect over time against corrosion in applications where these metals become necessary.

4. Environmental and surface effects on adsorption

4.1 Environmental factors

Environmental variables such as pH, temperature, and electrolyte composition play a key role in the adsorption behavior and performance of corrosion inhibitors [53]. The effect of the environment's pH directly relates to the dissociation and protonation of functional groups within the inhibitor molecules, which then allows these functional groups to enable interaction with the surface of the metal [60]. In acidic environments, for example, these inhibitors are often more effective and accepted by basic functional groups (amines or thiols) because they can donate electrons and form stable complexes with metal cations [61]. In contrast, acidic functional groups (e.g., carboxyl or hydroxyl groups) in an alkaline solution are preferred because they present ionic bonding with metal ions [62]. Another factor is temperature, which induces the molecular motion, hence increasing the desorption rate of the inhibitors [63]. The strength of attraction may decrease as the increase in temperature leads to greater thermal energy disruption of the bonds between the inhibitor and the metal surface [64]. Also, the electrolyte composition, with respect to ions such as chloride or sulfate, may affect the efficiency of the inhibitor [65]. For example, chloride ions are known to catalyze localized corrosion, which thus hampers the effect of the inhibitors. The presence of competing ions can boost or depress the inhibitor's ability to add onto the metal surface due to their charge and size. These are the necessary environmental factors in knowing the inhibitor performance optimization at different operational conditions.

4.2 Metal surface characteristics

The characteristics and features of the metallic surface also go a long way in the adsorption of corrosion inhibitors onto them [66]. Surface roughness and surface defects severely influence the cut-off of inhibitor molecules. With texture, roughness, or rough surfaces, the available surface area for adsorption may increase, thereby decreasing the threshold limit for utilizing the efficacy of the inhibitor [67].

Localized sites developed by small-scale defects such as grain boundaries, vacancies, and dislocations will facilitate or hinder adsorption according to the character of interaction that exists between metal and inhibitor [68]. These localized defects influence the nanoscale geometry of the reaction sites by creating many varieties of contact points at the interface on both sides of the obstacles. Another factor of importance is the crystallographic orientation of the metallic surface since different crystal planes show different extents of reactivity. For example, the (111) plane of a metal is often less reactive, so it may adsorb inhibitors less strongly than the more reactive (100) or (110) planes [69]. One more important factor for the adhesion of inhibitors is the surface energy of the metal, which is affected by the crystallographic structure and contaminants present on the surface. The more the surface energy, the more the adhesion of inhibitor molecules, because the surface will cooperate better with polar functional groups present on the inhibitor molecules [70]. Thus, surface attributes must be considered in combination as they may influence the corrosion inhibition process. They would have to be considered when an effective inhibitor needed to be selected or designed.

4.3 Time-dependent behavior

The next most critical factor is the temporal behavior of corrosion inhibitors. Molecular dynamics (MD) simulation helps understand the different interactions of inhibitors and metal surfaces over time [21]. It allows modeling the time-variation of the translational and angular orientations of inhibitor molecules as they stick to the surface. This modeling offers a more realistic comprehension of the inhibitor behavior under changing conditions, as it also changes with time; the adsorption may evolve or fully stabilize after some time in conditions where the inhibitor may undergo some chemical transformation, surface contamination, or oxide formation. Therefore, by MD simulation, the exhibition of time evolution for inhibitor molecules in relation to metal surface interaction gives information concerning how long-lasting and stable would be that protective layer [71]. Furthermore, the time-related studies can estimate the desorption rates of inhibitors, thus providing information about the kinetics of the adsorption process. This is very useful for industrial applications, where one often induces the status of corrosion for long durations. Thus, simulating the MD model can help optimize the inhibitors' format by making clear whether or not the adsorption layer behaves stably and in a durable manner over long periods as they would be exposed to in a general real-world environment.

5. Applications of corrosion inhibitors

5.1 Synthetic inhibitors

These inhibitors are the best thing to happen to mankind because they have been used in almost all industries for the tested purpose of reducing corrosion [72]. Synthetic inhibitors are usually made from organic and inorganic chemicals that form protective covers on the metals' surfaces so that they do not corrode due to the surrounding media [73]. Commonly utilized synthetic inhibitors include amines, thiols, phosphonates, and compounds containing heteroatoms like nitrogen (N), oxygen (O), sulfur (S), and phosphorus (P) [74]. Synthetic inhibitors such as imidazolines and derivatives are extensively popularized by the oil and gas industry's oil

and gas industries by using these in pipeline systems and equipment employed in operations subject to acidic conditions, such as acid picking or enhanced oil recovery. Phosphate-based inhibitors are preferred among cooling systems because they are effective against scaling and corrosion achieved by circulating water [75]. Several case studies have proven how economical synthetic inhibitors can be effective. For example, the efficiency of the use of benzotriazole in copper systems has significantly enhanced performance, thereby minimizing maintenance costs and downtime [76]. However, as they are toxic and cause bioaccumulation and persistence in the environment, synthetic inhibitors face scrutiny and regulations in industries with stringent environmental guidelines. In response to industries seeking sustainability measures, the synthetic inhibitors are optimized for performance and assessed in terms of their environmental impacts as a balance between efficiency and safety.

5.2 Eco-friendly and plant-based inhibitors

An increase in consciousness about environmentalism and sustainability has triggered research into the greener and more natural plant-derived inhibition, possibly in place of synthetic chemicals [77]. These naturally derived ones from plant extracts, essential oils, and bio-based molecules are biodegradable, nontoxic, and renewable. These plant-based inhibiting agents have often had functional groups like hydroxyl (-OH), carboxyl (-COOH), and heteroatoms, which are often responsible for the adsorption of the metal surface and create a complete barrier to the action of corrosion [53]. Reports show that particular extract sources like *Azadirachta indica* (Neem), *Ocimum sanctum* (Basil), and *Lawsonia inermis* (Henna) proved to be the best corrosion inhibitors in acidic and neutral environments [78, 79]. This base is rich in alkaloids, flavonoids, and tannins, which show excellent inhibition properties [80]. It has been reported that the performance of some natural inhibitors is comparable to those of the synthetic kind [81]. For instance, neem showed inhibition efficiency as high as 90% on mild steel in hydrochloric acid solutions [82].

The environmental impact of biorational inhibitors is much smaller as compared to synthetic types. Safety considerations encompass aquatic and terrestrial ecosystems; they are cost-effective applications chiefly because of the raw material availability. However, there are certain challenges that should be overcome, such as standardization of the natural extracts, reproducibility of results, and interference from impurities for large-scale industrial application. Thus, comparative studies between synthetic and eco-friendly inhibitors reveal trade-offs between performance, cost, and sustainability. For instance, the quicker adsorption kinematics and greater durability of some synthetic inhibitors provide a contrast to plant-based inhibitors that are greener and have much lower rates of long-term environmental risks. Advances in green chemistry and nanotechnology nowadays promise better performance of natural inhibitors for oil and gas industries, as well as for marine applications and water treatment plants.

6. Emerging trends and future directions

6.1 Machine learning in corrosion studies

Integrating machine learning (ML) in corrosion research indicates a revolutionary leap in corrosion inhibitor formulation [16]. Machine learning techniques such

as artificial neural networks (ANNs), random forest, and support vector machines (SVMs) are being used to develop predictive models created on the coupling of molecular descriptors with environmental parameters and inhibitor performance [25]. By the process of analyzing large datasets accumulated from experimental and theoretical studies, machine learning algorithms can easily recognize the emerging trends and optimize the inhibitor structures at an unprecedented level of accuracy and speed. For instance, adsorption efficiency and corrosion rates can be predicted using molecular weight, dipole moment, and heteroatom presence as input parameters. The training dataset produces a well-defined model for structural comparison: without curated datasets from quantum chemical studies and experimentation results, models would have a limited ability to generalize to different inhibitor types and environments. So, on the one hand, ML becomes the means for discovering new inhibitors with superior activity; on the other hand, it saves considerable time and costs compared to traditional trial-and-error approaches. On the other hand, dataset standardization, model interpretability, and the need for a large, high-quality dataset were all outstanding topics for further study.

6.2 Integrating computational and experimental methods

The combination of research, computational, and experimental approaches has finally proved to be a tremendous hybrid approach for corrosion inhibitor research [83]. Density functional theory (DFT) and molecular dynamics (MD) simulations have been able to offer insights at molecular levels on adsorption mechanisms, electron transfer events, and interaction energies of inhibitors on metal surfaces [21]. Validation and enhancement of these methods with experimental data increase their accuracy and reliability for pragmatic and scalable solutions [21]. For instance, DFT calculations provide theoretical values for parameters like that of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) due to their relations with inhibitor reactivity. Theories encourage experimental methods such as electrochemical impedance spectroscopy (EIS) and surface characterization techniques such as scanning electron microscopy (SEM) and atomic force microscopy (AFM) in proving predictions and measuring real-life performance. The last few years have witnessed remarkable successes in hybrid approaches. For instance, the synergy of DFT simulations with experimental methods based on weight loss has identified naturally occurring plant extracts as highly active green inhibitors [84]. Such integration reduces research cycles and increases the potential for reproducibility in successful approaches. This will pave the way for the efficient screening and optimization of corrosion inhibitors.

6.3 Advanced theoretical approaches

Advances in computational chemistry and physics promise next-generation theoretical approaches for studying corrosion inhibition. Indeed, by going beyond conventional ones, specific methods such as Time-Dependent DFT (TD-DFT), molecular dynamics ab initio, and quantum Monte Carlo simulations open an avenue to more accurate modeling of dynamic processes at the inhibitor-metal interface. These account for time-dependent behaviors, electronic excitations, and solvent effects, which are crucial for understanding how an inhibitor will perform according to realistic conditions [85]. Other modeling efforts explore applications of reactive force fields (ReaxFF) and coarse-grained simulations to address penalties imposed

by the treatment of large-scale systems while still retaining molecule-level accuracy. These enable the researchers to simulate long-term adsorption behaviors and corrosion processes for deeper insights into the stability of inhibitors concerning their interactions with surfaces. Future advances in machine-learning-enhanced quantum simulations should further reduce computation costs and improve accuracy in predictions, and the constant evolution of these theoretical approaches should 1 day fill existing knowledge gaps while accelerating the discovery of high-performance, sustainable corrosion inhibitors.

7. Bridging theory to practice

7.1 Industrial implications

The transition between the computational insights and the greenery applications in corrosion protection has taken a phenomenal leap toward improving industrial processes in creating efficient and cost-effective corrosion inhibitors [86]. Such processes replace the lengthy and costly conventional methods that consist of testing and re-testing with mainly theoretical models such as density functional theory (DFT) and molecular dynamics (MD) simulations to find out the molecular architectures, mainly the functional groups, that promote efficiency in adsorption on metal surfaces. The computational tools yield a detailed understanding of what takes place with respect to the inhibitor-metal interaction in terms of charge transfer mechanisms, binding energies, surface coverage, etc. [87]. Accumulation of such information can benefit industrial scenarios in correlating performance with the inhibitor. Such information has been applicable to the oils and gas, automotive, and marine industries by leading to new inhibitors that have been designed specifically for extreme conditions such as high salinity, high temperatures, and acidic environments [88]. Some cases illustrating this kind of success story include computationally optimized heterocycles in pipeline protection systems, wherein inhibitors designed through DFT calculations have shown performance advantages over cost benefits as compared to traditional chemicals. Moreover, hybrid schemes are gaining wider acceptance, whereby formulating computational predictions with experimental validation has enabled corrosion prevention solutions to be applicable to various operational environments in ways that are scalable and reliable.

7.2 Challenges and opportunities

Even though much has been achieved, making computational scalability a possible reality in practice is still a thorn in the flesh for many. Predictive, sometimes, computational methods for inhibitors may be applicable to molecular-level predictions of their performances, but in most cases, this builds on much simpler models that hardly represent the complexities of some industrial systems, such as the effects of impurities, surface heterogeneity, or even environmental variability [89]. This gap can be closed through advanced simulations of methods such as reactive molecular dynamics (ReaxFF) coupled with experimental methods validating predictions under realistic operating conditions. Moreover, simulating large-scale systems is extremely expensive in computation time, which sets limits to scaling with the new HPC and machine learning approaches, perhaps to reduce computational overhead and even increase accuracy [90]. Their approach to inhibitor design for the future

involves interdisciplinary partnerships among computational chemists, materials scientists, and engineers for bringing hybrid frameworks that draw on theoretical and experimental knowledge. Interdisciplinary efforts would lead to much more advanced formulations of inhibitors that could be eco-friendly and plant-based material alternatives that prove to possess all the efficacy benefits of current alternatives and overall support global sustainability goals. By encouraging partnerships between academia and industry, new avenues are opened for realizing large-scale industrial applications of computationally designed inhibitors, promising gains in cost savings, improvements with respect to material lifetime, and a declining footprint on the environment.

8. Examples of inhibitors of adsorption on metal surfaces

8.1 Adsorption of ethanethiol (Etha) on Ni (100), Ni (110), and Ni (111) surfaces

Figure 1 shows the adsorption of ethanethiol on Ni (100), Ni (110), and Ni (111) surfaces. Adsorption of ethanethiol on the Ni (100), (110), and (111) surfaces shows significant differences in interaction strength and the attendant transformation due to the orientation of the surfaces. On the Ni (100) surface, ethanethiol shows strong and stable adsorption as a flat, symmetrical, and moderately energy-deformed structure. The Ni (110) surface is more open and sparsely occupied, so it results in more binding sites but with the adsorption energy being slightly lower as compared to (100), yet with small structural changes as evident from the very low deformation energy. The Ni (111) surface, the densest and most closely packed, gives rise to stable adsorption of minimal deformation energy, equivalent to the adsorption strength of (100) surfaces. On the other hand, these surfaces are promising for strong as well as stable

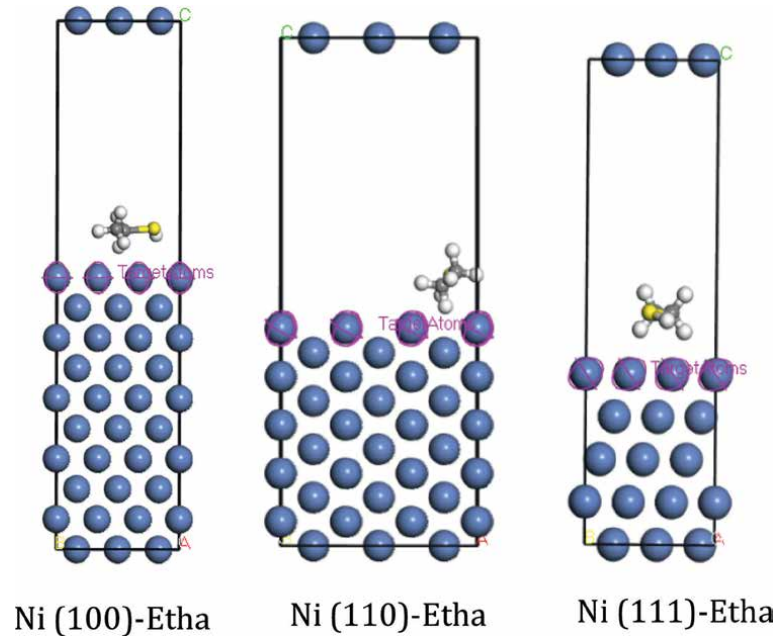

Figure 1.
Shows the adsorption of ethanethiol on Ni (100), Ni (110), and Ni (111) surfaces.

adsorption for applications such as catalysis, surface functionalization, and sensing, with the (110) surface being suitable for dynamic systems where less rigid molecule-surface binding is desirable.

8.2 Adsorption of ethanethiol on Au (100), (110), and (111) surfaces

Ethanethiol adsorption reveals striking differences, some of which can be surface orientation dependent on all of Au (100), (110), and (111) surfaces. The ethanethiol shows pronounced affinity toward the gold (110) surface in terms of markedly highest adsorption energy and lowest deformation energy, which helps to establish robustness in interaction and structural compatibility. The Au (111) surface, characterized by being densely packed, has less adsorption energy but promises stable binding, which is suitable for applications requiring minimal surface change. The adsorption strength is about average for Au (100), which means that both interaction and deformation are considered equally, being suitable for dynamic adsorption-desorption systems. These findings demonstrate the effect of surface orientations on adsorption processes that can be tailored for catalysis, sensing, or molecular immobilization. Indeed, these results would suggest that Au (110) is its preferred surface for any system requiring a strong yet permanent molecular interaction, while Au (100) and (111) would present versatility in conditions that were not as demanding. **Figure 2** shows the adsorption of ethanethiol (Etha) on Au (100), Au (110), and Au (111) surfaces.

The results in **Table 1** below confirm that there is a stronger interaction of ethanethiol with Au surfaces as compared to the Ni surfaces, as can be observed in the more negative value of total and adsorption energies for Au. Among all Ni surfaces, (100) and (111) orientations show an almost similar value of adsorption strength (−25.31 eV), which is a little stronger than the (110) surface (−25.06 eV). For Au, the (110) surface displays the strongest interaction (−27.70 eV), followed by (111) (−26.40 eV) and (100) (−26.21 eV). The rigid adsorption energy is close to the

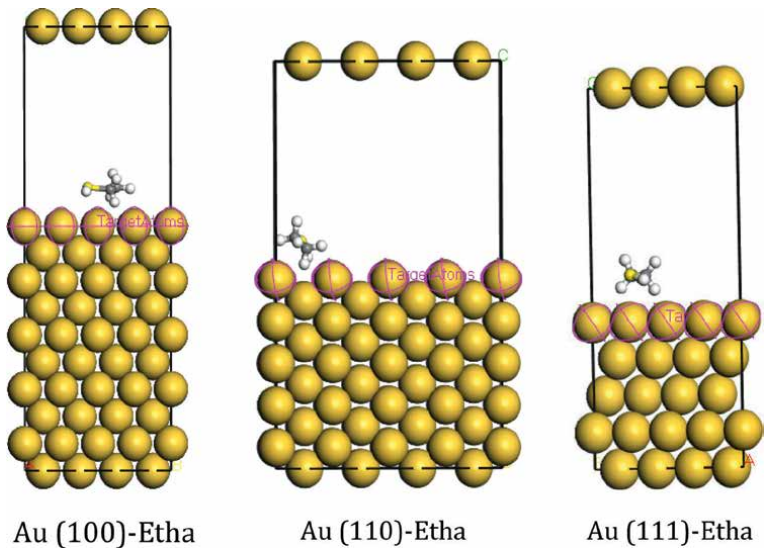

Figure 2.
Shows the adsorption of ethanethiol on Au (100), Au (110), and Au (111) surfaces.

Structures	Total energy	Adsorption energy (eV)	Rigid adsorption energy (eV)	Deformation energy (eV)
Ni (100)-ethanethiol	−30.47	−25.31	−25.06	−0.26
Ni (110)-ethanethiol	−30.22	−25.06	−24.98	−0.07
Ni (111)-ethanethiol	30.46	−25.31	−25.28	−0.03
Au (100)-ethanethiol	−31.37	−26.21	−25.87	−0.34
Au (110)-ethanethiol	−32.86	−27.70	−27.73	−0.03
Au (111)-ethanethiol	−31.56	−26.40	−26.31	−0.09

Table 1.
Adsorption of ethanethiol on Ni and Au surfaces.

adsorption energy since its differences are very small, indicating limited structural modification upon adsorption. Deformation energy is, as a whole, low (<0.1 eV), meaning that ethanethiol causes rather minor changes in either the surface or the molecule, having slightly higher deformation for Au (100) (−0.34 eV) and Ni (100) (−0.26 eV). These results demonstrate how varying surface crystallographic orientation affects interaction strength, with the (110) surfaces being particularly interesting. These findings are very relevant for applications, for example, in catalysis, surface functionalization, and sensor design, where strong and durable adsorption is required. Au surfaces, especially the (110) orientation, appear well suited for this purpose and, as such, could increase efficiency in energy storage, environmental sensing, and molecular recognition technologies.

9. Conclusion

This chapter integrates the fundamentals of the most important advancements in corrosion science with computerization and sustainable practice. Findings suggest a pronounced need to explore corrosion mechanisms at the molecular level to concoct effective inhibitors, while such research has been extensively supported by computational techniques like ab initio, molecular dynamics (MD) simulations, and density functional theory (DFT) analyses, so too has unparalleled knowledge about the interaction of inhibitors and metal surfaces derived from these avenues toward cost-effective, environmentally friendly solution development. The prospective corrosion inhibition efficiencies brought about by the incorporation of computational tools are invaluable since not only do they reduce experimental costs, but they also offer rapid screening of inhibitor candidates with excellent precision. This presents another facet of the shift in paradigm for sustainable corrosion management, which is being marked by principles of green chemistry, including bio-based, biodegradable inhibitors. Future research should concentrate on developing comparative advanced predictive models through machine learning and artificial intelligence, thereby improving efficiency and accuracy in the design of inhibitors while reducing their environmental impact. The use of eco-harbor composite materials in place of synthetic polymeric materials also makes an important contribution to the global effort to reduce hazardous chemicals, thus creating a cleaner, healthier environment. It is indeed very relevant to the very high significance of bridging the gap between experimental and computational studies in the achievement of holistic solutions to corrosion challenges.

Overall, it complements the trend of interesting engagement between progressive computational tools and sustainability-driven research.

Computational techniques will directly converge with a great synergy into achieving several SDGs by designing SDG 9 (Industry, Innovation, and Infrastructure), SDG 12 (Responsible Consumption and Production), and SDG 13 (Climate Action) goals. For instance, processing naturally, plant-sourced, eco-friendly, biodegradable corrosion inhibitors would aid researchers in avoiding toxic, petroleum-based chemicals, meeting SDG 12 for the development of such products. For instance, computational methods have been extensively employed to study plant extracts and bio-based inhibitors to predict efficacy and environmental impacts before such efforts come to actual costs of extensive experimental testing and resource consumption and even laboratory waste. Advances from innovative applications of computation in corrosion prevention technology confer on this intervention support to sustainable industrial infrastructure under SDG 9. This allows pollution-free and integrated inhibitors for a longer lifespan and greater strength for important infrastructure such as pipelines, bridges, and energy systems. Their reduced maintenance and material wastage costs align cost-efficiently under the umbrella of SDG 13, as an indirect outcome would be reduced greenhouse gas emissions because of less activity on the industrial processes and material replacements needed. These computational methods will also optimize the corrosion inhibitors tailored for offshore wind turbines and solar panel frameworks that will promote clean energy alternatives further. Overall, this is a green, economical way of conducting corrosion science for the benefit of the entire planet.

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Conflict of interest

The author declares no conflict of interest.

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Chapter 4

Advances in Corrosion Monitoring Techniques

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Abstract

Corrosion is an industrially and economically challenging environmental material degradation process that has a profound impact on human lives, with a staggering annual global cost of about 2.5 trillion dollars. Corrosion monitoring is a management practice of strategically averting corrosion harm to safeguard tangible assets. This chapter presents a review report on the general advantages of corrosion monitoring as well as the principles, advantages, and disadvantages of the various up-to-date monitoring techniques and kinds of facilities that are used for monitoring, providing insights into the advanced and emerging monitoring technologies. The report shows that, presently, there are several different corrosion monitoring techniques and more in emergence that may not be equally beneficial for every application, so it is essential to carefully evaluate, select, and implement them to effectively track the corrosion processes of assets across different environmental conditions. It is crucial for all structural assets, especially those with various corrosion rates at different surface locations and that are made of metallic and/or non-metallic components such as steel, aluminum, concrete, ceramics, and glass in corrosive settings. Corrosion monitoring is essential for assets that require total removal, repair, or replacement. Corrosion monitoring is purposed to proactively identify potential corrosion risks and take necessary measures to ensure the integrity of our assets and safe working environments. Artificial intelligence, with machine learning capabilities, stands out as an emerging technology with the potential to transform corrosion monitoring and control to previously unachievable levels with traditional monitoring techniques.

Keywords: corrosion risks, corrosion management, corrosion monitoring, benefits, techniques, selection, advanced technologies, advantages

1. Introduction

Corrosion is an industrially and economically expensive environmental material-degradation process that has a multifaceted impact on every person, community, country, and the entire world, with a monumental total estimated annual global cost of 2.5 trillion dollars, equivalent to about 3.4% of the global gross domestic product

annually [1]. The corrosion management policy offers a methodical framework for identifying corrosion-related hazards as well as for creating and implementing effective risk control measures. The benefits that can be attained by effective corrosion management include reduced leaks, increased plant availability, decreased unscheduled maintenance, decreased deferral costs, and statutory or corporate compliance with safety, health, and environmental laws [2, 3]. The corrosion management process offers the focus and action plan details on how to best use human, capital, and material resources to [2]:

i. Reduce corrosion maintenance and repair costs for corroded materials, the quantity of products lost due to corrosion damage, and extend the useful life of manufactured products or assets.

ii. Analyze risk and responsibility by metal type, and examine appropriate metal parts processing and handling guidelines by assessing present risks in production, shipping, storage, and processing; figuring out the repercussions of failures in each area; and lowering risk by using new packaging and corrosion protection technologies.

iii. Examine the potential for new coatings, alloys, and corrosion inhibitors by implementing best practices and innovative corrosion protections and preventatives for more corrosion-resistant goods.

iv. Examine every step of the manufacturing and delivery processes to cover the entire range of corrosion control for improved corrosion protection.

Corrosion management includes choosing the right materials, applying protective coatings, using cathodic protection, adding inhibitors, and conducting regular inspections, etc. for structural systems [3, 4]. All corrosion protection actions are supported by corrosion monitoring data to take early action against all corrosion issues. Corrosion monitoring is therefore a crucial corrosion management process of gathering, observing, and assessing data on the degree of corrosion-induced degradation in a material such as metal, concrete, wood, etc., or the corrosivity of the environment surrounding the material to know the levels of their degradation through specific corrosion-probing techniques or devices in infrastructures, plants, buildings, bridges, and other engineered systems [2–5]. Usually changes in corrosion rates are used to evaluate the level of degradation of materials, but changes in several other parameters, such as weight loss, mechanical properties, physical properties, chemical properties, and integrity loss of material, such as esthetic value and cracking, are also used in evaluating degradations of materials [6, 7]. Corrosion monitoring can help in several other ways, such as [3, 4, 6–9]:

i. Determining corrosion rates, identifying potentially hazardous conditions, locating structural defects, and discovering material non-compliances.

ii. Providing an early warning that damaging process conditions exist.

iii. Diagnosing a particular corrosion problem and identifying its cause.

iv. Evaluating the effectiveness of a corrosion control or prevention technique.

v. Determining optimal application of corrosion control or prevention technique.

vi. Providing management information relating to the maintenance requirements and ongoing condition of the plant.

vii. Providing performance data and a basis for life prediction.

Corrosion monitoring is usually applied where:

i. High-pressure, high-temperature, flammable, explosive, and toxic processes exist.

ii. There is a high probability of corrosivity in equipment.

iii. Corrosion rate may have changed due to changes in operating conditions.

iv. Corrosion inhibitors are in use.

v. There is a high concentration of corrosive constituents in the process.

vi. Process feedstock is changed.

vii. Plant output or operating parameters are changed from design specifications.

viii. Evaluation of corrosion behavior of alloys is necessary.

ix. Induced potential shifts are used to protect systems and/or structures.

x. There is a vital concern about product contamination due to corrosion.

Almost any industry where corrosion prevention is a top priority can benefit from corrosion monitoring. Examples include the oil and gas sector, such as in pipelines, vessels, flowlines, gathering systems, water wash systems, drilling mud systems, desalters, chemical injection systems, processing, and water systems; the refining sector, such as in crude overheads, sour water strippers, cooling systems, amine systems, and vacuum towers; the pulp and paper sector, such as in boiler systems, digesters, and white liquor; utilities, which include effluent systems, boiler water systems, cooling systems, and make-up water systems; and the petrochemicals or other chemicals/processing sectors, such as in cooling systems and process systems. There are several methods of corrosion techniques, and two or more of the techniques are usually integrated in corrosion monitoring systems to offer a broad foundation for data collection. The alloy system, operational parameters, and actual process fluid all affect the precise techniques that can be employed [9–12].

The aim in this chapter is to provide knowledge advances from credible literary sources on corrosion monitoring techniques, with regards to the different monitoring techniques, types of facilities or equipment in use for corrosion monitoring, the techniques' applicability to different environmental settings, the overall advantages of corrosion monitoring, and where corrosion monitoring is needful, with insights into emerging technologies.

2. Methodology

The information in this chapter was compiled, condensed, and refined for improved readability and comprehension using a variety of journals, theses, and other credible literary sources published between 2012 and 2025.

2.1 Corrosion monitoring techniques

Corrosion monitoring techniques are classified as direct or indirect techniques. Direct techniques refers to approaches that measure corrosion rates or associated parameters directly on the surface of the material. These methods provide information regarding the corrosion process in real-time or almost real-time. Some of the popular direct methods for corrosion monitoring include [10–19]:

2.1.1 Visual monitoring

In this technique, physical inspection by personnel for corrosion is carried out, either without or with various aids such as dyes, magnification, borescopes, etc. to improve visibility. The advantages of the technique are that it is simple, relatively quick, and can be done during regular maintenance. The drawbacks of the technique are that it only detects corrosion after sufficient amounts of corrosion products form, access is required for personnel to the system or part under corrosion, there is the possibility of not detecting corrosion that is hidden by dirt and overlapping parts, and it does not offer continuous monitoring [13–17].

2.1.2 Weight loss coupons

Weight loss coupons are standardized test samples used to evaluate the effects of corrosion on metals or alloys under certain conditions. These coupons are usually flat, small, and rectangular in shape. They are made of the same material as the metal under evaluation and are exposed to the same environmental conditions as the building or equipment they represent. The type and rate of corrosion that occurs in a system can be monitored and measured using corrosion coupons. By placing the coupons in a field or laboratory test environment, the material's corrosion as represented by the coupons in the environment can be acquired. Corrosion coupons are often positioned in a system's specific section, such as a vessel or pipeline, and usually left there for a set period of time, which could be a few weeks or several months. After the exposure period, the corrosion coupons are removed and inspected to determine the kind of corrosion and its extent by evaluating variables such as surface morphology, weight loss, or modifications in material properties. The benefits of the weight loss coupons technique are that it is simple and inexpensive; it can be used in any environment, including gases, liquids, solids, and particulate flow; corrosion deposits can be seen and examined; visual inspection can be carried out; weight loss and corrosion rate can be easily calculated; inhibitor performance can be easily evaluated; and localized corrosion can be marked and measured. Because weight loss coupons can be made from any commercially available alloy, this method is incredibly flexible. Additionally, a wide range of corrosion phenomena, such as stress-assisted corrosion, bimetallic (galvanic) corrosion, differential aeration, and heat-affected zones, can be explored with the use of suitable geometric designs. They provide a trustworthy way to confirm the efficacy of corrosion prevention methods like the use of coatings and

inhibitors. The drawbacks of the weight loss technique are that it is time-consuming, as it requires lengthy exposure times, and its inability to provide real-time data. Furthermore, results from this technique are often delayed since the weight loss coupons need to be retrieved and examined in a laboratory, and the technique does not identify localized or early-stage corrosion; instead, it merely offers an average corrosion rate across the exposure period of the coupons [10–19].

2.1.3 Electrical resistance monitoring

This monitoring technique uses variations in a metal's electrical resistance to determine how quickly it is corroding. This method requires direct touch with the metal surface. This method involves conducting intrusive electrical resistance monitoring by inserting tiny metal probes or electrodes into the system or piece of equipment under observation. These probes are made of the same material as the metal under evaluation. Surface alterations caused by corrosion result in variations in electrical resistance. The electrical resistance of the probes is regularly measured using advanced technology. By keeping an eye on these resistance changes, corrosion severity and pace can be determined. Higher numbers indicate less corrosion, whilst lower resistance levels suggest a higher rate of corrosion. Intrusive electrical resistance monitoring enables the early detection of corrosion problems by supplying real-time data on corrosion activity. It is widely used in applications such as storage tanks, pipelines, and critical infrastructure where rapid corrosion reaction and continuous monitoring are crucial. The benefits of coupons are all present in electrical resistance probes. They are available in a wide range of element geometries, metallurgical makes, and sensitivities; they can be flush mounted to perform pigging operations without removing them; they can be used to set off an alarm; they react rapidly to corrosion disturbances and can be used to obtain direct corrosion rates while they are installed in-line until their operational life is over; and their diverse range of sensitivities can allow the operator to select the most sensitive one that is compatible with the needs of the process. Their main drawbacks are sensitivity to temperature changes, which can affect resistance measurements, and limitation to monitoring only uniform or nearly uniform corrosion. They are also less appropriate for short-term corrosion studies since they need prolonged exposure to identify significant corrosion trends [10–19].

2.1.4 Inductive resistance probes

These are probes that work by measuring changes in the electrical impedance of metals to determine the corrosion rate. Unlike intrusive probe types, these probes do not need to come into close touch with the metal surface. The electromagnetic theory underpins the operation of these probes. They are made of a coil that creates a magnetic field around the metal or component that is being monitored. As the metal corrodes, its electrical resistance changes in value and causes changes in the magnetic field. The inductive resistance probe detects these changes and transforms them into corrosion data. This monitoring technique is particularly useful in situations where physically inserting probes into a system is not practicable nor acceptable. For instance, it is effective in monitoring the rusting of exterior objects like buildings or pipes. Inductive resistance probes identify corrosion activity in real time to enable continuous monitoring. By tracking variations in electrical impedance, it can determine the rate and degree of corrosion. Higher impedance values frequently indicate lower rates of corrosion, while lower values suggest a higher rate [14–19].

2.1.5 Linear polarization resistance

In the linear polarization resistance technique, a metal's resistance to corrosion is measured. The technique works on the principle that when little electrical charge is applied to the metal's surface in a range of E_{corr} ± 25 mV, the current that follows (I_{corr}) is measured using the Stern-Geary relation given by (1) to (3) to help determine the rate of the metal corrosion [12].

$$I_{corr} = \frac{\beta_a \beta_c}{2.3(\beta_a + \beta_c)} \frac{\Delta_i}{\Delta_E}. \tag{1}$$

The polarization resistance R_P, is given by rate between the applied current and the potential response DE as

$$R_p = \frac{\Delta_E}{\Delta_i} = \frac{\beta}{I_{corr}} \tag{2}$$

$$\beta = \frac{\beta_a \beta_c}{2.3(\beta_a + \beta_c)} \tag{3}$$

Where, Δ_i is the applied current (mA), Δ_E is the potential response (mV), I_{corr} is corrosion intensity in μA/cm^2, R_p is the polarization resistance in kΩ, β is the value of 13 to 52 mV in the most metal/media systems, β_a is the anodic Taffel constant, and β_c is the cathodic Taffel constant. Higher polarization resistance levels indicate a slower rate of corrosion, while lower values suggest a faster rate. This method is widely used in corrosion research and monitoring systems. The technique is an easy and non-destructive way to detect corrosion in real time. It is commonly used to assess the effectiveness of corrosion control strategies and identify any changes in corrosion rates over time in a number of applications, such as storage tanks, pipelines, and metal structures. One benefit of the technique is that it allows for instantaneous corrosion rate measurement. This is a more effective instrument than electrical resistance or coupons, where metal loss is the primary metric and exposure time is necessary to calculate corrosion rate. The technique's drawback is that it only works well in aqueous electrolytic conditions that are reasonably clean and could not work well in conditions with limited electrolyte conductivity. Also, in gases or water/oil emulsions, where electrode fouling can make readings impossible, LPR will not function [13–19].

2.1.6 Electrochemical impedance spectroscopy

Impedance measurements are used in electrochemical impedance spectroscopy, a corrosion monitoring technique for examining the corrosion process of metals. It is a sophisticated technique that offers important insights into corrosion processes and is founded on electrochemical principles. This method involves applying a little alternating current at various frequencies to the metal surface. An impedance spectrum is obtained by measuring the electrical response that results. We may learn about a variety of electrochemical activities occurring on the metal surface from this spectrum, including corrosion reactions and protective coating generation. One can ascertain crucial factors like corrosion rate, protective coating integrity, and corrosion inhibitor

efficacy by analyzing the impedance spectrum. Additionally, it can identify localized pitting or corrosion. A flexible method for gathering qualitative and quantitative data on corrosion processes is electrochemical impedance spectroscopy. It enables us to comprehend the intricate behavior of metals in situations that are acidic [15–19].

2.1.7 Electrochemical frequency modulation

The way metals erode can better be understood by using a corrosion monitoring technique called electrochemical frequency modulation (EFM). A little alternating current is applied to the metal, and the variations in its electrochemical response are monitored. By concentrating on the frequency modulation of the current, EFM enables us to ascertain crucial elements such as the type and pace of corrosion. This method can distinguish between several corrosion types, such as uniform corrosion and localized corrosion, and it offers quantitative data regarding the degree of corrosion. The capability of EFM to track corrosion in real time and identify variations in corrosion rate is one of its benefits. This non-destructive technique works well in a variety of settings, such as high-temperature systems and aqueous liquids. EFM is frequently used in both industrial and research contexts to analyze the performance of protective coatings, determine the factors driving corrosion rates, and gauge the efficacy of corrosion inhibitors [12–19].

2.1.8 Harmonic analysis

This technique examines specific signal frequency components to determine how metals deteriorate. This technique finds harmonic frequencies linked to corrosion processes by analyzing the metal's electrical response. Numerous details regarding the rate and intensity of corrosion can be gleaned from the amplitudes and phases of these harmonic components. This method can be used to identify various forms of corrosion, including pitting and localized corrosion, and to monitor how corrosion behavior varies over time. Aqueous liquids, industrial settings, and climatic conditions are just a few of the locations in which this non-destructive method can be applied. In summary, it is a technique for monitoring corrosion that concentrates on particular frequency components to comprehend the corrosive behavior of metals. It can identify the types and rates of corrosion by examining these components. This non-destructive technique helps assess and enhance corrosion prevention strategies [12–20].

2.1.9 Electrochemical noise

In this technique, the corrosion processes are examined by sporadic variations of the associated electrical impulses from the corrosion processes to know the corrosion status quo of metals. Direct contact with the metal surface is necessary for this technique. Electrodes or probes are inserted into the apparatus or system under observation in order to track electrochemical noise. The tiny electrical impulses produced by metal surface corrosion processes are picked up by these electrodes. The rate of corrosion, localized corrosion, and other significant corrosion-related characteristics can be learned about by examining the random fluctuations in these signals, sometimes referred to as electrochemical noise. Corrosion mechanisms and the efficacy of corrosion management techniques can be learned about by examining features such as signal amplitude, frequency distribution, and duration. Localized corrosion can inflict significant damage with modest overall corrosion rates, making electrochemical noise

monitoring particularly useful for identifying and evaluating this type of corrosion. It can be used in a variety of contexts, such as industrial settings, atmospheric conditions, and water solutions, and it offers real-time monitoring capabilities. Although the technique may identify both localized and general corrosion, it is highly costly to set up and run, and results may be distorted by external signal noise sources. The material or system being monitored must be shut down in order to install and retrieve data, and the data received using this technology may be challenging to interpret [10–19].

2.1.10 Galvanic monitoring

In this technique, the instantaneous corrosion current of the metal or alloy is measured using the galvanic monitoring technique, also known as zero resistance ammetry (ZRA). ZRA probes expose the process fluid to two electrodes made of different metals. There is a natural voltage (potential) difference between the electrodes when submerged in solution. The rate of corrosion on the more active electrode pair is correlated with the current produced by this potential difference. The electrode pairs for bimetallic corrosion, pitting and crevice attack, corrosion-assisted cracking, corrosion by highly oxidizing species, and weld deterioration can all be monitored galvanically. The most common uses for galvanic current measurement are in water injection systems where the concentration of dissolved oxygen is a major concern. Galvanic currents and, thus, the rate at which steel process components corrode are significantly increased when oxygen seeps into such systems. When gaskets or deaeration systems leak, galvanic monitoring systems can detect the presence of oxygen in the injection waters [10–19].

2.1.11 Potentiodynamic polarization

This is a corrosion monitoring technique in which a metal's resistance to corrosion is evaluated. It entails adjusting the metal's potential while monitoring the relationship between its corrosion current and voltage. The metal is usually subjected to various potentials during potentiodynamic polarization, and the currents that result are measured. This obtained information aids in the understanding of the corrosion behavior of the metal. Crucial corrosion characteristics can be ascertained by examining the polarization curve, which illustrates the link between current and potential. These include the polarization resistance, which shows the metal's capacity to withstand corrosion, and the corrosion potential, which shows the metal's propensity to corrode. We can assess a variety of corrosion events, including passivation, pitting, and general corrosion, using potentiodynamic polarization. It offers insights into the efficacy of corrosion control techniques and assists in identifying critical potentials where corrosion is likely to occur [10–19].

2.1.12 Thin layer activation and gamma radiography

In this technique, radioactive substances are utilized to evaluate the structural integrity and corrosion of material components. The process of thin-layer activation involves applying a thin coating of a radioactive substance to the surface of the material component. Radiation from this radioactive substance reacts with the material component and the byproducts of corrosion. The amount and location of corrosion on the material's surface can then be ascertained by measuring the radiation that is released. In contrast, gamma radiography uses a gamma ray source to examine the interior structure of the material component. Any interior corrosion or degradation can be

identified through measurement of the transmitted gamma rays intensity passing through the material component. Both gamma radiography and thin-layer activation can provide detailed internal structural images of material components. Gamma radiography enables interior corrosion or degeneration to be evaluated; thin layer activation aids in the understanding of surface corrosion. These techniques are particularly helpful for monitoring the progress of localized corrosion in a material component, especially when the component is intricate and difficult to access without causing harm to it. However, these techniques are restricted to only materials that can be penetrated by radiation and call for certain tools and safety measures against radiation [10–19].

2.1.13 Electrical field signature method

This is a non-intrusive technique that assesses the corrosion of a metal without coming into contact with the metal. Rather, it measures and examines the changes in the electrical field brought on by corrosion processes. This technique involves only placing sensors or probes close to the metal surface without making direct contact. The electrical field fluctuations brought on by corrosion reactions occurring on the metal surface are detected and analyzed by these sensors. Crucial details about the type of corrosion, its rate, and even localized corrosion can be learned by examining these electrical field signatures. This method gives information about how the metal is corroding and enables real-time monitoring. The technique is capable of continuous corrosion monitoring using satellite communication. It is appropriate for monitoring pits on huge structures or locations where direct access to the metal surface is challenging due to its non-intrusive nature. It is, however, expensive and labor-intensive to install and cannot detect corrosion pits that are less than 0.8 mm in size [13–19].

2.1.14 Acoustic emission

This is a non-intrusive technique in which noises that material components produce are used to assess how they are corroding. In this technique, sensors or other equipment are placed on or near the surface of the material component to capture the sounds made during corrosion. These sounds could be related to cracking, hydrogen leakage, or material deterioration. Many details regarding the corrosion features, including the rate and extent of damage, can be gleaned from the characteristics of these noises, including their frequency, volume, and duration. For the detection and tracking of interior material changes, such as localized degradation, acoustic emission is especially helpful. It is suitable for a variety of materials, including metals, composites, and coatings, and it offers real-time monitoring. On the side of advantages, the technique is non-destructive, can be used on in-service equipment, and provides localized thickness measurements, while its drawbacks are the need to access both material sides and the limitation to monitoring only thickness loss due to corrosion [10–19].

2.1.15 Magnetic flux leakage technique

This is a popular nondestructive technique for detecting corrosion anomalies in pipelines. Steel's magnetic qualities serve as the foundation for the sensing principle. In the absence of defects, magnetic flux lines would primarily flow through the interior of the ferromagnetic material when it is magnetized near saturation under the applied magnetic field; in contrast, bending and leakage of magnetic flux lines will occur at corrosion or defect sites. An electromagnet typically creates the magnetic

field, and a Hall-effect sensor is employed to find magnetic flux leakage. The multi-flux leakage technique is limited for material surface and near-surface detection, but it works well for large-area examination. To identify the shapes of faults and differentiate between internal and external defects, improvements are required [10–16].

2.1.16 Multi-frequency electromagnetic technique

Another popular non-destructive corrosion monitoring technique is electromagnetic-based sensing, in which a transmitter coil and a receiver coil make up the sensor. There are numerous variations of this monitoring approach, which is based on Faraday's law of induction. The multi-frequency electromagnetic inspection sensor for pipeline integrity and corrosion detection is one example. The technique works on the principle that an alternating current excites the transmitter coil, and the resulting alternating magnetic field causes eddy currents to flow through the nearby conductive pipes. A voltage with a phase shift from the primary electromagnetic field is induced in the separate reception coil by the transmitter's primary electromagnetic field and a secondary field created by eddy currents in the pipes. The electrical conductivity, magnetic permeability, and defect existence of the material all affect the phase shift and magnitude change. Low-frequency electromagnetic scans can be used to calculate the thickness of pipe metal, while high-frequency electromagnetic scans can distinguish between inner wall characteristics because of the skin effect [10–16].

2.2 Indirect techniques

Indirect corrosion monitoring techniques are those techniques used to evaluate a material's corrosion behavior in an indirect manner. These techniques rely on secondary indicators that offer information about the corrosion process rather than directly monitoring corrosion rates or damage. These methods involve measuring things like electrical resistance, weight or size changes, surface roughness or color changes, mechanical property changes, or the propagation of ultrasonic waves. The following are a few indirect methods of corrosion monitoring [13–19]:

2.2.1 Corrosion potential

Corrosion potential is one corrosion monitoring technique that aids in assessing the probability of corrosion on metal surfaces. The corrosion potential is the difference in electrical potential between the metal surface and its surroundings. It is a non-intrusive technique, and it assists in assessing whether the metal will corrode or remain safe. To quantify it, we use reference electrodes or other non-contact methods. By monitoring the corrosion potential over time, we may identify any changes that may indicate a higher risk of corrosion or the effectiveness of corrosion prevention strategies. If the corrosion potential shifts toward more positive or negative values, it indicates changes in the metal's corrosion behavior [13–19].

2.2.2 Hydrogen flux monitoring

This non-invasive method aids in comprehending the amount and behavior of hydrogen gas, which can exacerbate corrosion. To monitor hydrogen flux, sensors or probes are placed near the material surface to identify and measure the flow of hydrogen gas. These sensors monitor the way hydrogen moves through the material or is

released during corrosion. Monitoring the hydrogen flux provides important information on the presence, concentration, and interactions of hydrogen with the material. This information can be used to evaluate the effectiveness of corrosion control methods and understand the risk of corrosion caused by hydrogen. Hydrogen flow monitoring is particularly useful for materials that are vulnerable to hydrogen embrittlement or in environments where hydrogen gas is present, like in the oil and gas industry. This method aids in material selection, design considerations, and the use of preventive measures to lessen the consequences of hydrogen-induced corrosion [12–19].

2.2.3 Chemical analyses

The process of analyzing and assessing the chemical alterations that take place in a corroding system is known as chemical analysis in corrosion monitoring. It entails researching the chemical makeup of corrosive solutions, examining corrosion byproducts, and determining the many chemicals that contribute to the corrosion process. Chemical analyses use a variety of methods, including [10–21]:

i. *Corrosion product analysis*: Examining the characteristics and nature of the corrosion products that are produced during corrosion is part of this technique. These products are identified and analyzed using methods such as scanning electron microscopy and X-ray diffraction.

ii. *Electrochemical analysis*: In this technique, electrochemical parameters such as pH, potential, and ion concentration are evaluated in order to determine how a material is affected by the corrosive environment. For electrochemical analysis, techniques like ion chromatography and potentiometry are employed.

iii. *Spectroscopic analysis:* This technique involves the detection and quantitative measurement of certain chemical species or components present in the corrosive environment, using spectroscopic techniques such as atomic absorption spectroscopy, Raman spectroscopy, and infrared spectroscopy to understand the rate of corrosion that is taking place.

iv. *Wet chemical analysis:* In this technique, the concentration of specific ions or compounds in the corrosive solution is determined using titration techniques and chemical reagents to have insight into the level of corrosion of specific material components in that corrosive solution. For instance, the concentration of chloride is measured using silver nitrate titration.

2.2.4 Biological monitoring and analysis

This technique generally seeks to identify and quantify the presence of sulfate-reducing bacteria (SRBs), a class of anaerobic bacteria that consume sulfate from the process stream and generate sulfuric acid, a corrosive that attacks production plant materials.

2.2.5 Sand/erosion monitoring

In this technique, specially designed devices are used to measure sands and other slurry particles as well as erosion in a flowing system. The technique finds wide application in oil/gas production systems where particulate matter is present.

2.3 Main equipment or instruments of corrosion monitoring system

The industry, application, and degree of information required for corrosion analysis can all affect the equipment utilized in a corrosion monitoring system. Finding the best equipment for a particular monitoring project might be aided by speaking with corrosion specialists or specialized suppliers. The primary components of a corrosion monitoring system include [15–19, 22]:

i. *Corrosion probes/sensors*: These are available in various varieties, including galvanic corrosion probes, corrosion coupons, linear polarization resistance (LPR) probes, and electrochemical noise (EN) probes. They are installed with the purpose of measuring the corrosion rates in the system under observation.

ii. *Data loggers*: These devices gather and store data from the corrosion probes and also keep track of crucial variables like temperature, corrosion rate, humidity, and other environmental factors.

iii. *Transmitters*: A central monitoring system receives the data that the probes or loggers have gathered via transmitters. Depending on the monitoring system, they might be wired or wireless.

iv. *Central Monitoring system*: The data sent by the probes or loggers is received and processed by this system. In order to analyze, visualize, and present the data, it usually consists of hardware and software components. Engineers or operators can monitor corrosion trends, identify anomalies, and decide on maintenance and preventative plans with the aid of the central monitoring system.

v. *Reference electrodes*: To create a reference potential for precise corrosion measurements, reference electrodes collaborate with corrosion probes or sensors. Saturated calomel electrodes (SCE) and silver/silver chloride (Ag/AgCl) electrodes are common varieties.

vi. *Wiring and cabling*: Reliable connections between the probes, data recorders, transmitters, and the central monitoring system require appropriate wiring and cabling. These parts need to be made to be resistant to corrosion and to endure harsh climatic conditions.

vii. *Power supply*: For corrosion monitoring devices to function, a steady power supply is required. Depending on the particular configuration, batteries, AC power sources, or a combination of both may be used.

viii. *Ancillary equipment*: Depending on the needs and application, more equipment can be needed. For outdoor installations, these can include weatherproof enclosures; mounting brackets or clamps to hold the probes in place; calibration standards for routine sensor calibrations; and coating coupons or protective coatings for reference.

In order to select the most appropriate sensors, a series of evaluation criteria need to be considered.

The main criteria include the following: size suitability for the application need, ruggedness, required depth of scan/in situ loss of section (direct), reliability/

accuracy, life span, coupling/installment, mobility (direct), sensitivity, power consumption, the ability of the sensor to function in the requisite environment (aqueous or non-aqueous), and how well the sensor systems and/or component types have worked or not in history as designed for other projects [10–19].

2.4 Importance of corrosion monitoring

Corrosion monitoring is very important for the following reasons [2–19]:

i. Preservation of assets: The structural integrity of many assets, including materials, equipment, and structures, is preserved by avoiding significant breakdowns and prolonging their life through timely detection by monitoring and resolving corrosion problems.

ii. Ensuring safety: Failures brought on by corrosion can present major safety risks, especially in sectors like infrastructure, transportation, and oil and gas. Possible corrosion hazards can be proactively detected to take the required actions to guarantee a safe working environment through routine corrosion monitoring.

iii. Cost-efficiency: Costly replacements, repairs, and downtime can result from corrosion. Vigilant corrosion monitoring allows us to better plan maintenance tasks, put in place suitable corrosion management strategies, and ultimately reduce the expenses related to major repairs and asset replacements.

iv. Optimizing performance: Equipment and system performance and efficiency are adversely affected by corrosion. We can identify early indicators of deterioration and take corrective measures, such as replacements, repairs, or adjustments, to preserve peak performance by keeping an eye on corrosion levels.

v. Regulatory compliance: Corrosion has a negative impact on the efficiency and performance of systems and equipment. By monitoring corrosion levels, we can see early signs of deterioration and implement remedial actions, such as replacements, repairs, or changes, to maintain top performance.

vi. Environmental protection: Hazardous material spills or leaks due to corrosion can endanger the environment. We can find possible leakage sources, stop environmental contamination, and lessen the effect on nearby ecosystems by conducting careful corrosion monitoring. In conclusion, corrosion monitoring is essential for maintaining asset integrity, guaranteeing safety, cutting expenses, improving performance, satisfying legal requirements, and preserving the environment. By taking proactive measures to solve corrosion-related problems, we extend the life of our priceless assets and encourage effective and sustainable operations.

2.5 Advanced methods and emerging technologies

2.5.1 Fiber optics technique

This is an advanced method of corrosion monitoring by which temperature, strain, and corrosion-related alterations in the structure of assets are measured using optical fiber sensors. These sensors detect changes in light transmission brought on by

expansion, contraction, or chemical reactions from corrosion, among other changes in the material's properties. Structural health is monitored using a variety of designs, such as Distributed Optical Fiber Sensors (DOFS) and Fiber Bragg Gratings (FBG) [23–32].

The advantages of the fiber optic sensor technique are high sensitivity, real-time monitoring, and minimal maintenance requirements since fiber optic sensors are immune to electromagnetic interference, making them highly reliable in offshore environments where electronic noise can affect conventional sensors. In addition, fiber optic sensors can cover long distances, allowing for extensive structural monitoring with a single fiber network. In comparison to electrical-based sensors, fiber optic sensors are also non-destructive, have in-situ distributive measurements, long reach, small size, flexibility, geometric versatility, and light-weight, and are inherently immune to electromagnetic interference. They are also compatible with optical fiber data communication systems and safer when flammables are present. The limitations of the technique are that fiber optic sensors have high installation costs and require specialized expertise for deployment and data interpretation. Moreover, the complexity of integrating these sensors into existing infrastructure of assets can pose challenges, and physical damage to fiber optics can lead to signal loss or degradation [23–32].

2.5.2 Wireless corrosion monitoring

Wireless sensors are used by wireless corrosion monitoring systems to send corrosion data to a central monitoring station. In remote or dangerous settings where wired systems are unfeasible, these technologies are especially helpful. Benefits of the technology include low installation cost, the capacity to deliver real-time data from distant locations, and the elimination of the need for significant wiring. Additionally, the wireless capability enables monitoring in inaccessible locations. Passive wireless sensors are inexpensive and small enough to be widely used in the system of interest. Its drawbacks include the need for battery-operated sensors, which may not last very long, and the possibility of signal interference in specific settings [29–37].

2.5.3 Corrosion monitoring with IoT

In this technology, Internet of Things (IoT)-based systems, utilizing a network of wireless sensors, cloud computing, and data analytics, remotely monitor corrosion variables in real time. These devices wirelessly send data to a central monitoring unit on environmental factors such as temperature, humidity, and salinity, as well as structural health indicators like metal loss and electrochemical activity. It is then possible to use machine learning algorithms to identify patterns and anticipate possible malfunctions. This corrosion monitoring technology has the following benefits: it supports predictive maintenance by identifying corrosion risks before significant damage occurs, optimizing maintenance schedules, and minimizing operational disruptions; it provides remote accessibility, enabling engineers and managers to monitor asset structures from any location via cloud-based dashboards and mobile applications; and it enables continuous, real-time monitoring, reducing the need for manual inspections and downtime while offering predictive analytics for proactive corrosion management; and it enhances data accuracy and integration by combining multiple sensor inputs, offering a comprehensive view of corrosion progression. However, the technology has some drawbacks because it needs a dependable way to send data, which can be hard to achieve in environments with poor connectivity; connecting it to existing digital systems might need a lot of money and technical know-how; the sensors and

communication parts must be tough enough to withstand harsh environmental conditions, raising the initial costs; setting up and integrating it can be difficult; and strong cybersecurity measures are needed to keep the data safe [26–37].

2.5.4 Corrosion monitoring using artificial intelligence

Artificial intelligence is the equipment of computer system to mimic human capability by reacting intelligently in making decisions to solve problems on its own without or with minimal human intervention. The main objectives of artificial intelligence research include robotics, general intelligence, vision, automated planning, natural language processing, and knowledge representation. Deep learning, pattern recognition, neural networks, expert systems, evolutionary computation, machine learning, and discriminant analysis, metaheuristic optimization, swarm optimization, video processing, and computer vision are just a few of the artificial intelligence fields that have been in use especially for some research [38]. The different intelligence methods and their relationships are shown in **Figure 1** [38].

The most reliable and successful methods in corrosion engineering among such technologies are machine learning, deep learning, and pattern recognition. The use of artificial intelligence (AI) and machine learning to evaluate corrosion data and forecast corrosion behavior is growing. The advantages of applying AI in corrosion monitoring include the following [36, 39–43]:

i. Capability of generating accurate predictive models of corrosion behavior based on environmental variables such as temperature, pressure, and chemical

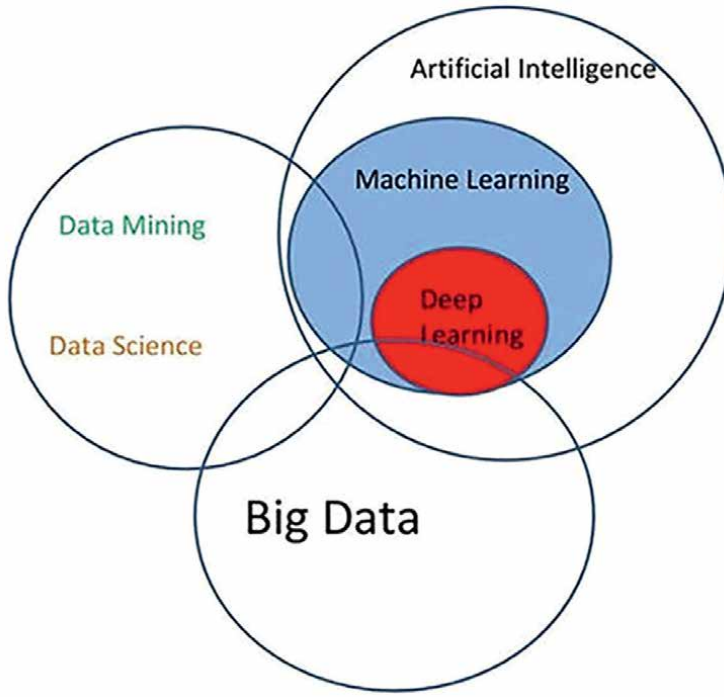

Figure 1.
Artificial intelligence techniques interrelation [38].

composition for greater understanding of corrosion mechanisms and forecasting of effects under various circumstances.

ii. AI-powered systems can continuously monitor corrosion signs in real-time for early diagnosis of corrosion-related problems.

iii. AI-driven warning systems integrated with IoT sensor networks can deliver immediate notifications, facilitating prompt action and intervention when anomalous corrosion-related circumstances are identified.

iv. Capability to identify tiny corrosion patterns that people might miss, like complex or localized types that could lead to rapid deterioration.

v. Large datasets from multiple sources (sensors, laboratory tests, and historical records) can be analyzed by AI algorithms, especially machine learning and deep learning, to find intricate patterns and relationships suggestive of corrosion. This allows for more precise predictions of corrosion rates and possible failures.

vi. AI in corrosion monitoring has several other benefits, including increased precision in corrosion rate prediction, early failure risk identification via real-time sensor data processing, and optimized maintenance plans, all of which reduce costs and increase safety of assets.

Although artificial intelligence with its machine learning capability holds promise for overcoming the shortcomings of traditional corrosion monitoring techniques by its ability to analyze vast amounts of data, spot patterns, and produce projections, the drawbacks of the technology are that it necessitates knowledge of data science and artificial intelligence, as well as vast datasets for training machine learning models [36, 38–42].

3. Conclusion

A review report on advances in corrosion monitoring techniques has been presented, covering their pros and cons, areas of application, and overall advantages. The report shows that there are many corrosion monitoring techniques, and many more are emerging, and the application of any technique will depend on the accuracy level and reliability needed for specific applications, the type of corrosion, the environmental conditions, cost affordability, the level of automation involved, and monitoring capacity and speed. The review report shows that:

i. Corrosion monitoring is a crucial aspect of the corrosion control strategy in various industries. By measuring and analyzing corrosion-related parameters through corrosion monitoring, organizations can assess the extent of corrosion, predict its progression, and implement appropriate control measures.

ii. The classical corrosion monitoring devices include weight-loss coupons, spool pieces, electrical resistance probes, linear polarization probes, galvanic probes, hydrogen pressure probes, hydrogen electrochemical patch probes, electrochemical noise probes, and the field signature method, but all these techniques, while

useful, have limitations. The various limitations of these techniques include sensitivity limitation, potential for missed issues, scope limitation, inaccessibility challenges to the system or part being monitored, difficulty in monitoring localized corrosion, time-consuming and laborious processes, expertise requirements for accuracy, difficulty in real-time monitoring, and potential for some undetected corrosion and catastrophic failures.

iii. To address limitations of classical or traditional corrosion monitoring techniques, advanced or emerging corrosion monitoring technologies such as electrochemical probes, acoustic emission monitoring, fiber optic sensors, wireless IoT-based remote sensing systems, and artificial intelligence are now being considered. These techniques or technologies offer real-time data acquisition, higher sensitivity, and predictive maintenance capabilities, allowing for proactive corrosion management and risk mitigation. Industries can therefore better reduce the financial and safety risks related to corrosion and guarantee the longevity and functionality of their assets by investing in cutting-edge corrosion monitoring systems and procedures.

iv. Although the focus is now on cutting-edge corrosion monitoring systems and procedures, especially artificial intelligence, there are still issues with cost, system integration, and environmental adaptation, requirement of expertise personnel, etc. Future studies in these technologies of corrosion monitoring should therefore concentrate on: advancing wireless and energy-efficient sensor networks to improve real-time monitoring capabilities in remote offshore environments, developing cost-effective sensor technologies that balance affordability with high performance, enhancing artificial intelligence-driven predictive models to improve the accuracy of corrosion trend analysis and risk assessment, and enhancing personnel training in these technologies.

Conflict of interest

The authors declare that there are no conflicts of interest regarding this work.

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Chapter 5

Effect of Oilfield Chemicals on Corrosion in Downstream Units

Tariq Almubarak, Muthukumar Nagu and Shenbaga Murthy

Abstract

Corrosion is a natural degradation process wherein metals react with their environment, resulting in the formation of more stable compounds such as oxides, hydroxides, or sulfides. This process leads to considerable economic losses across industrial sectors due to material degradation and equipment failure. In the oil and gas industry, the issue is particularly critical, as metallic infrastructure is continuously exposed to aggressive environments during production, processing, and transport. While a range of mitigation techniques have been developed to limit corrosion, recent studies have shown that chemical treatments used in upstream operations can inadvertently contribute to corrosion in downstream facilities. The objective of this chapter is to evaluate the corrosion challenges observed in downstream units because of oilfield chemical use in upstream operations. Affected downstream systems include gas-oil separation plants, transmission pipelines, flowlines, trunklines, and refining units such as the Crude Distillation Unit (CDU), Vacuum Distillation Unit (VDU), Fluid Catalytic Cracking Unit (FCCU), and Hydrocracker Unit (HCU). Various upstream additives—such as asphaltene inhibitors, defoamers, biocides, hydrate inhibitors, scale inhibitors, and acidizing fluids—may persist in produced fluids and interact unfavorably with metallurgy and process conditions downstream. This chapter outlines the key oilfield chemicals used in upstream processes, highlights their potential to induce or exacerbate corrosion in downstream units, and discusses monitoring and mitigation strategies to minimize these effects.

Keywords: oilfield additives, downstream corrosion, refinery equipment, corrosion inhibitors, corrosion mechanisms, MIC, biocide, scale inhibitors, hydrate inhibitors, process fouling

1. Introduction

1.1 Corrosion

Corrosion remains a critical integrity concern across the oil and gas industry, affecting infrastructure performance, safety, and reliability. It is defined as the degradation of metallic materials due to chemical or electrochemical reactions with their environment. In operational settings, corrosion may occur in multiple forms, including uniform corrosion, pitting corrosion, crevice corrosion, and stress corrosion cracking [1, 2].

The underlying mechanisms involve several interrelated factors:

- Electrochemical interactions: Arise when a metal meets an electrolyte, such as water or brine, initiating anodic and cathodic reactions.
- Chemical reactions: Include direct attack by corrosive agents such as carbon dioxide (CO_2), hydrogen sulfide (H_2S), or dissolved oxygen.
- Environmental variables: Parameters such as temperature, pressure, and fluid velocity significantly influence corrosion rates.
- Material characteristics: The alloy composition and microstructure of a material determine its corrosion resistance.
- Fluid chemistry: pH, ionic strength, and the presence of contaminants (including bacteria) or dissolved gases in the fluid contribute to corrosion behavior.

1.2 Types of corrosion in oil and gas facilities

Various corrosion types commonly affect oil and gas infrastructure:

1. Uniform corrosion: A general attack across the entire metal surface, resulting in gradual thinning.
2. Pitting corrosion: A highly localized form of corrosion that results in small, deep pits. It frequently occurs in chloride-containing environments such as seawater or brine [3, 4].

1.2.1 Pitting mechanism

Pitting typically initiates at points of mechanical damage or passive film breakdown, especially in the presence of chlorides [5]. The process includes:

1. Initiation: A local anodic site forms, often at surface defects or inclusions [6].
2. Propagation: Electrochemical gradients between the pit and surrounding metal drive localized dissolution [7].
3. Pit growth: Metal loss deepens the cavity while the surrounding area remains relatively unaffected [8].
4. Stabilization: A self-sustaining microenvironment may develop within the pit, facilitating continued corrosion [9].
5. The severity of pitting is influenced by the cathode-to-anode area ratio, with higher ratios accelerating penetration.
6. Crevice corrosion: Occurs in shielded zones with limited fluid exchange, such as gasket interfaces or under deposits.

7. Stress corrosion cracking (SCC): Arises from the combined effects of tensile stress and corrosive agents, leading to brittle failure.

1.3 Key drivers of corrosion in oil and gas operations

Multiple environmental and operational factors contribute to corrosion risk [10–18], including:

1.3.1 CO_2 corrosion (sweet corrosion)

Carbon dioxide, when dissolved in water, forms carbonic acid, a moderately strong acid capable of initiating metal dissolution. The generalized corrosion reaction is seen in Eq. (1):

$$Fe_{(s)} + CO_{2\,(g)} + H_2O_{(l)} \rightarrow FeCO_{3\,(s)} + H_{2\,(g)} \tag{1}$$

1.3.2 CO_2 corrosion mechanism, Eqs. (2)–(5)

1. CO_2 dissolves in the aqueous phase, forming H_2CO_3.

2. H_2CO_3 dissociates into H^+ ions, driving anodic metal dissolution:

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

3.Cathodic reactions include

$$2H^+ + 2e^- \rightarrow H_2 \tag{3}$$

$$2H_2CO_{3\,(aq)} + 2e^- \rightarrow H_{2\,(g)} + 2HCO^-_{3\,(aq)} \tag{4}$$

$$2HCO^-_{3\,(aq)} + 2e^- \rightarrow H_{2\,(g)} + 2CO^{2-}_{3\,(aq)} \tag{5}$$

These reactions may result in iron carbonate ($FeCO_3$) scale formation. The protectiveness of this scale depends on environmental conditions such as flow velocity, temperature, and saturation index [19–23].

1.3.3 H_2S corrosion (sour corrosion)

Hydrogen sulfide reacts with iron to form iron sulfide (FeS), a reaction that is central to sour service corrosion, Eqs. (6)–(10):
The anodic reaction is:t

$$Fe \rightarrow Fe^{2+} + 2e^- \tag{6}$$

The cathodic reactions are:

$$H_2S_{(aq)} \leftrightarrow HS^-_{(aq)} + H^+_{(aq)} \tag{7}$$

$$HS^-_{(aq)} \leftrightarrow S^{2-}_{(aq)} + H^+_{(aq)} \tag{8}$$

$$2H^{+}_{(aq)} + 2e^{-} \leftrightarrow H_{2\,(g)} \tag{9}$$

The overall reaction is:

$$Fe_{(s)} + H_2S_{(aq)} \leftrightarrow FeS_{(s)} + H_{2\,(g)} \tag{10}$$

1.3.4 Oxygen corrosion

Oxygen contributes to corrosion by acting as both an oxidant and a depolarizer. In aqueous environments, oxygen accelerates electron loss from iron surfaces, enhancing corrosion. Its influence increases with temperature and dissolved oxygen concentration, particularly in carbon steel systems [24, 25].

2. Mitigation strategies

Corrosion control in oil and gas operations typically involves multiple layers of protection:

1. Material selection: Use of corrosion-resistant alloys or metallurgical modifications.

2. Coatings and linings: Barrier systems to shield surfaces from corrosive media.

3. Cathodic protection: Impressed current or sacrificial anode systems to suppress anodic reactions.

4. Chemical inhibition: Addition of corrosion inhibitors to modify electrochemical kinetics.

5. Process control: Operation within defined integrity windows by managing pressure, velocity, and temperature.

A clear understanding of corrosion mechanisms and site-specific risk factors allows for the implementation of targeted mitigation strategies, ensuring long-term asset integrity.

3. An overview of oil field chemicals and their effects

The use of oilfield chemicals in upstream operations is essential for ensuring flow assurance, controlling corrosion, minimizing scaling, and managing microbial activity. These additives include asphaltene dispersants, foamers, demulsifiers, biocides, scale inhibitors, paraffin inhibitors, hydrate inhibitors, corrosion inhibitors, fracturing fluids, completion brines, and packer fluids [26]. While effective in addressing challenges at the wellbore and surface facilities, residual quantities of these chemicals may persist in the produced fluids and carry over into downstream systems.

The transition from upstream to downstream involves significant shifts in operating conditions. Downstream units—such as gas-oil separation plants, pipelines,

flowlines, trunklines, and refining systems (e.g., Crude Distillation Unit (CDU), Vacuum Distillation Unit (VDU), Fluid Catalytic Cracking Unit (FCCU), and Hydrocracker Unit (HCU)) operate under elevated temperatures, varied pressures, and different metallurgies. These differences often make downstream systems more sensitive to chemical incompatibilities.

One major concern is the carryover of active or degraded chemical species into units not designed to handle them. For instance:

- Scale inhibitors may leave behind elevated levels of ions such as Ca^{2+}, Mg^{2+}, Ba^{2+}, and Sr^{2+}, which can alter scaling tendencies downstream and disrupt saturation indices.
- Corrosion inhibitors formulated with phosphorus-, sulfur-, or nitrogen-based groups can interact with downstream metallurgy, leading to under-deposit corrosion, localized attack, or fouling.
- Hydrate inhibitors like methanol or monoethylene glycol (MEG) may interfere with catalyst beds or cause operational instability in distillation and separation units.
- Biocides may either promote microbial resistance or form by-products that lead to metal surface attack.
- Demulsifiers and surfactants can affect interfacial tension, destabilize desalters, or form persistent films on metal surfaces, contributing to fouling or corrosion.

These chemical interactions may result from:

- Carryover in the production stream, especially when separation is incomplete.
- Contamination during transport or blending, including tank bottom sludges or mixing errors.
- Reuse or recycling of water or process fluids, which may retain residual concentrations of active chemicals.

When introduced into refining environments, these compounds may contribute to:

- Accelerated corrosion rates (especially pitting and crevice corrosion).
- Catalyst deactivation.
- Phase separation issues.
- Product quality degradation.
- Equipment fouling and increased maintenance frequency.

A deeper examination of these effects by chemical class is provided in Section 2.1.

3.1 Effect of oil field chemicals

Oilfield chemicals used in upstream operations may persist in produced fluids and enter downstream systems, where they can cause or accelerate corrosion. The impact of these chemicals varies depending on their composition, concentration, degradation behavior, and interaction with downstream metallurgy and operating conditions. The most implicated categories include corrosion inhibitors, scale inhibitors, biocides, and demulsifiers.

3.1.1 Corrosion inhibitors

Corrosion inhibitors are applied to protect metal surfaces by forming passive films or altering electrochemical kinetics. However, their residual presence in produced fluids can result in corrosion challenges in downstream refining units. These challenges are often linked to the composition and thermal stability of the inhibitor under high-temperature or multiphase conditions.

- *Imidazoline-based inhibitors*: commonly used in carbon steel protection, often include phosphorus or sulfur moieties. Under refining temperatures, these compounds may decompose or react with metal surfaces, forming fouling layers or contributing to under-deposit corrosion.
- *Quaternary ammonium compounds (QACs)*: adsorb onto metal surfaces, interfere with passive film formation, or affect oil-water separation.
- *Pyridine-based inhibitors*: effective in acidic environments but may influence microbial ecosystems, potentially increasing the risk of microbiologically influenced/induced corrosion (MIC).
- *Phosphonate-based inhibitors*: chemically stable and offer corrosion protection by chelating with metal ions. However, they may introduce phosphorus species that foul catalysts, contribute to soft scaling, or initiate localized pitting, particularly in areas with stagnant flow.

Residual inhibitors may also affect weld zones or heat-affected areas, increasing susceptibility to pitting, crevice corrosion, or stress corrosion cracking.

3.1.2 Scale inhibitors

Scale inhibitors prevent the formation of mineral scales, particularly from ions such as Ca^{2+}, Mg^{2+}, Ba^{2+}, and Sr^{2+}. These chemicals function by interfering with nucleation or crystal growth mechanisms.

- *Phosphonate-based inhibitors*: widely used due to their thermal and chemical stabilities. However, they may form deposits at elevated temperatures, interfere with oxide film formation, and introduce phosphorus species that foul downstream catalyst systems.
- *Polyphosphate-based inhibitors*: more prone to hydrolysis, forming orthophosphate species that readily precipitate with divalent cations. This can lead to soft sludge formation, equipment fouling, and product contamination in downstream units.

Additionally, scale inhibitors may alter the saturation index of water systems or provide nutrients that encourage MIC, especially when in excess or not adequately separated prior to refining.

3.1.3 Biocides

Biocides suppress microbial activity to control MIC. However, when these compounds persist downstream, they may induce or worsen corrosion under certain conditions.

- *Glutaraldehyde-based biocides*: degrade into reactive aldehydes or acids that corrode metal surfaces.

- *Halogenated biocides*: including chlorine- and bromine-based oxidizers, may promote halide-induced pitting or react with organics to form corrosive by-products.

In addition, some biocides disrupt microbial ecosystems in a way that allows more corrosive species to dominate, further aggravating MIC risks. Moreover, MIC can be caused by both aerobic and anaerobic organisms. Sulfate-reducing bacteria (SRB), for example, are a major cause of localized corrosion in water-rich or stagnant environments, forming corrosive hydrogen sulfide as a metabolic by-product. Iron-oxidizing and slime-forming bacteria may create differential oxygen cells under biofilms that support localized attack. If biocide programs are not properly maintained or selected, microbial communities may shift to more resistant strains or adapt through protective biofilm formation.

Case histories from pipeline and desalter units have shown that overuse or improper cycling of biocides can lead to toxicity plateaus, where bacteria persist in sublethal conditions and become more resistant. Additionally, intermittent or pulse dosing without real-time microbial monitoring can result in poor efficacy. MIC-related failures are often underestimated due to their hidden and localized nature but can lead to costly unplanned shutdowns if not detected early.

3.1.4 Demulsifiers and surfactants

Demulsifiers are used to break water-in-oil emulsions. When carried downstream, they can interfere with separation processes and affect metal surfaces:

- Surfactant residues may destabilize desalter performance, reduce phase separation efficiency, and accumulate on heat exchanger surfaces.

- Certain demulsifier formulations may promote fouling or form biofilms, both of which can trigger localized corrosion.

Although the primary concern discussed in this section is corrosion, oilfield chemical carryover can also result in other operational issues such as catalyst poisoning, phase separation problems, and contamination of refinery products. These broader impacts are summarized in **Table 1**.

Chemical	Application	Potential effect in downstream units
Corrosion inhibitors	Prevent corrosion of equipment and pipelines	Corrosion of refinery equipment
Scale inhibitors	Prevent formation of scales in pipelines and equipment	Contamination of refinery products; fouling
Paraffin inhibitors	Prevent paraffin wax deposition	Separation problems in refinery units
Hydrate inhibitors	Prevent hydrate formation in pipelines and equipment	Catalyst poisoning; desalter upset
Demulsifiers	Break emulsions between oil and water	Water-in-oil carryover; separation inefficiency
Surfactants	Modify interfacial tension	Foaming; product contamination
Biocides	Suppress microbial growth	Corrosion; formation of toxic by-products

Table 1.
Common oilfield chemicals used in upstream operations and their potential effects in downstream refinery units.

3.2 Monitoring and inspection techniques

Effective corrosion management in downstream facilities requires a combination of real-time monitoring, routine inspection, and informed chemical selection. This section outlines standard monitoring techniques followed by dedicated subsections for each major oilfield chemical category, detailing best practices for selection and application to minimize corrosion and operational risks.

3.2.1 Corrosion inhibitor selection and application guidelines

To minimize downstream corrosion from residual corrosion inhibitors, the following practices are recommended:

1. Conduct thorough risk assessments and corrosion studies.
2. Evaluate compatibility with downstream metallurgy and produced fluids.
3. Monitor corrosion rates using coupons, probes, and fluid sampling.
4. Assess the chemical and thermal stability of the inhibitor under refining conditions.
5. Implement effective chemical management and injection control programs.

Key selection factors include:

- Type of metal surface being protected
- Type and concentration of corrosive species (e.g., CO_2, H_2S)
- Operating temperature and pressure

- Presence of other additives that may interact
- Potential to influence MIC or promote under-deposit corrosion

3.2.2 Scale inhibitor selection and application guidelines

Residual scale inhibitors can interfere with downstream scale balance, promote fouling, or trigger localized corrosion. To reduce such effects:

1. Perform water chemistry analysis and saturation index modeling.
2. Select inhibitors based on the predominant scaling ions (e.g., Ca^{2+}, Ba^{2+}, Sr^{2+}).
3. Distinguish between *phosphonate* (stable, but fouling risk) and *polyphosphate* (less stable, more reactive) formulations.
4. Assess the potential for phosphorus accumulation or catalyst interaction.

Key selection factors include:

- Nature of the scale (carbonate, sulfate, mixed)
- Fluid salinity, pH, and ionic strength
- Compatibility with corrosion inhibitors and surfactants
- Risk of MIC from nutrient contribution
- Stability under downstream process temperatures

3.2.3 Biocide selection and application guidelines

Biocides must be chosen carefully to avoid downstream corrosion *via* microbial shifts or reactive degradation products and the following is recommended:

1. Select biocides based on microbial population profiles and system conditions.
2. Avoid persistent overuse to prevent the development of resistant strains.
3. Verify breakdown pathways to avoid acidic or halide-based corrosion products.
4. Ensure compatibility with water treatment and separation systems.

Key selection factors include:

- Type of microorganisms (e.g., sulfate-reducing bacteria, iron-oxidizing bacteria (IOB), iron-reducing bacteria (IRB))
- Operating temperature, pH, and water content

- Potential for halide-induced pitting or MIC
- Environmental discharge limits and toxicity
- Interaction with other chemical additives

3.2.4 Demulsifier selection and application guidelines

Demulsifiers can cause issues when surfactant residues reach downstream units, impacting separation performance or enabling MIC. Below are some recommendations to keep in mind:

1. Formulate demulsifiers specific to crude characteristics and water chemistry.
2. Monitor desalter and separator performance for signs of carryover.
3. Evaluate surfactant persistence under refining conditions.
4. Assess potential for film formation or microbial colonization.

Key selection factors include:

- Type of emulsion (water-in-oil vs. oil-in-water)
- Water salinity, pH, and process shear
- Stability of surfactant under temperature and residence time
- Compatibility with corrosion inhibitors and separation units

3.2.5 Hydrate inhibitor selection and application guidelines

Hydrate inhibitors are deployed in upstream operations to prevent the formation of crystalline clathrate structures that can block pipelines and equipment. Common inhibitors include methanol, monoethylene glycol (MEG), and newer low-dosage hydrate inhibitors (LDHIs). These chemicals, when carried downstream, can interfere with equipment reliability, process stability, and environmental performance.

Methanol is effective at low temperatures and offers ease of injection, but it is flammable, volatile, and non-regenerable. When present in refining streams, methanol may cause catalyst deactivation or introduce volatility and flash point issues in product streams. In corrosion contexts, methanol may alter fluid pH or interact with other additives, influencing passivation behavior or promoting stress corrosion cracking under certain metallurgy.

MEG is non-flammable and can be recovered and reused through regeneration units. However, its higher viscosity and thermal stability make it harder to remove in downstream units, where it can lead to fouling or contamination of water circuits. Its breakdown products may also interfere with heat exchanger performance.

Guidelines for hydrate inhibitor management include:

1. Select the appropriate inhibitor based on thermodynamic modeling and downstream sensitivity.

2. Minimize over injection to limit downstream accumulation and interference.

3. Ensure compatibility with downstream catalysts and materials.

4. Evaluate regeneration or recovery strategies to minimize discharge and waste handling.

Operational changes such as depressurization or temperature ramping should be coordinated with hydrate inhibitor use to prevent retrograde formation or residue buildup.

4. Summary and recommendations

The unintentional carryover of oilfield chemicals into downstream processing units introduces a variety of corrosion-related risks, in addition to fouling, catalyst poisoning, and operational instability. While these chemicals are indispensable for managing upstream flow assurance, their interactions with downstream metallurgy, fluid chemistry, and separation systems demand careful oversight. This chapter examined the corrosive implications of residual corrosion inhibitors, scale inhibitors, biocides, and demulsifiers, and emphasized the need for integrated chemical selection, monitoring, and control strategies across the production value chain.

Key recommendations:

- Develop chemical selection guidelines tailored for upstream operations with downstream exposure in mind. Criteria should include stability under high temperature, degradation behavior, and reactivity with downstream materials and catalysts.
- Perform regular monitoring of fluid properties at key handover points, particularly for contaminants like phosphorus, sulfur species, residual surfactants, and microbial activity.
- Establish integrity operating windows (IOWs) for downstream units, with the defined limits for chemical residues, scaling ions, and corrosive species to guide operational decisions.
- Segment downstream assets into corrosion loops to localize monitoring efforts and target high-risk areas using appropriate probe or coupon technologies.
- Implement integrated chemical management programs that coordinate upstream chemical injection with downstream process impacts. Include compatibility testing between additives.
- Use corrosion-resistant alloys and internal coatings where carryover risk is high and corrosion rates exceed tolerable thresholds.
- Enhance communication between upstream and downstream teams, particularly in fields with high chemical treatment rates or variable production chemistry.

5. Future research directions

Ongoing research is needed to better quantify, predict, and mitigate the downstream effects of oilfield chemicals. Suggested directions include:

- Modeling chemical breakdown products and reactivity under refining conditions to predict corrosion pathways and fouling behavior.
- Developing smart monitoring systems capable of real-time detection of chemical residues and early-stage corrosion.
- Designing lower-impact chemical formulations with short-lived residues or enhanced downstream compatibility.
- Investigating additive interactions in mixed-chemical environments, especially in multiphase or transient flow regimes.
- Studying long-term impacts on catalyst systems and separation units to assess recovery and deactivation mechanisms linked to chemical carryover.
- Utilizing machine learning and AI-based tools to analyze corrosion monitoring data and predict failure points based on chemical usage patterns.
- Creating shared industry databases to track incidents related to chemical carryover, allowing cross-operator learning and predictive standardization.
- Investigating the environmental consequences of persistent additives post-refining, especially in wastewater treatment and flare systems.

These additional research areas are critical for developing holistic, cross-functional strategies that connect upstream chemical treatment practices with downstream corrosion control and sustainability.

Nomenclature

CDU	crude distillation unit
CO_2	carbon dioxide
FCCU	fluid catalytic cracking unit
H_2S	hydrogen sulfide
HCU	hydrocracking unit
HS^-	bisulfide ion
IOW	integrity operating window
LDHI	low dosage hydrate inhibitor
MEG	monoethylene glycol
MIC	microbiologically influenced/induced corrosion
QAC	quaternary ammonium compound
SRB	sulfate-reducing bacteria
VDU	vacuum distillation unit

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Metals deteriorate over time through chemical or electrochemical reactions with their environment, resulting in corrosion, a natural and often unavoidable process. Besides shortening the lifespan of metal parts, this phenomenon leads to significant financial costs, safety hazards, and maintenance challenges across various industries, including maritime engineering, transportation, construction, and the oil and gas sector. The enormous range of environmental variables to which metals are exposed, from saline water and acidic soils to industrial contaminants and air humidity, makes controlling corrosion a constant challenge. Additionally, it is challenging to implement a one-size-fits-all solution due to the varied compositions and surface properties of metallic materials. Although coatings, cathodic protection, alloying, and inhibitors are examples of traditional protective techniques that have demonstrated varied degrees of effectiveness, their environmental impact, longevity, and cost-effectiveness are frequently limited. The need for creative, long-lasting, and reliable corrosion management techniques is greater than ever, as contemporary applications require metal constructions to be more reliable and durable. This book presents research on corrosion and the challenges faced in controlling corrosion on metallic surfaces.

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