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The use of Artificial Intelligence to assist in the analysis of corrosive materials in nuclear reactors

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1. Introduction

Currently, corrosion in nuclear reactor materials represents a major challenge to the structural integrity of these systems. Due to the complexity and non-linear nature of the physicochemical variables involved, traditional methods have limitations in corrosion analysis, especially given the wide variety and complexity of experimental data[1].

As an alternative to this problem, Artificial Intelligence emerges, capable of assisting in pattern identification and supporting scientific discovery through data analysis. Large volumes of data, combined with machine learning, have been very useful in applications related to energy storage, as they constitute one of the main foundations of the functioning of systems based on Artificial Intelligence [2].

In nuclear reactors, materials are subjected to extreme conditions, such as high temperatures, high pressure, radiation, and aggressive environments, favoring different corrosion mechanisms [3][4]. Furthermore, the simultaneous presence of CO_2, H_2S, and chloride ions intensifies the degradation of passive films, highlighting the need for more advanced analytical approaches [5].

In this scenario, the integration between experimental data and machine learning allows for the identification of critical variables, improves predictions, and assists in understanding the physicochemical mechanisms of corrosion. The combination of experimentation, computational modeling, and Artificial Intelligence has proven to be a promising strategy for analyzing corrosive processes in nuclear systems [6][7][8].

As an objective, this article was researched to present alternatives for the use of Artificial Intelligence with machine learning, which assist in studies and identifications regarding corrosive materials in nuclear reactors.

2. Methodology

The application of Artificial Intelligence does not replace experimentation, but acts as a complementary tool in the analysis of data obtained by electrochemical and microstructural techniques. Data like corrosion rate, electrochemical impedance spectroscopy (EIS), corrosion potential, and characterization of passive films are used as inputs for machine learning models. These data are obtained through controlled experimental systems, for example, three-electrode electrochemical cells [9]. For data input, one can use the general equation of metallic corrosion, corresponding to the basic anodic reaction of corrosion [10], such as Eq. 1:

$$M \rightarrow M^{n+} + ne^{-} \quad (1)$$

Where:

- M= metal;
- n= number of electrons;
- e^-= electrons.

Iron is oxidized, such as Eq. 2: $$Fe \rightarrow Fe^{2+} + 2e^- \quad (2)$$

As a phenomenon highly dependent on the interaction between multiple factors such as chemical composition, microstructure, and environmental conditions [11] corrosion can be analyzed with the aid of machine learning techniques. This approach enables the effective identification of non-linear patterns and complex relationships among these variables, which are often not captured by traditional models [12]. Furthermore, learning methods allow for the identification of corrosive behavior clusters, contributing to the classification of materials and environments according to their risk levels.

Physics-informed machine learning incorporates differential equations and physical laws directly into the training of neural networks, reducing the exclusive reliance on large volumes of experimental data [13]. In the context of corrosion, this approach allows for the integration of electrochemical fundamentals into AI models, contributing to greater reliability in predicting corrosive phenomena and understanding material degradation mechanisms.

Thus, AI assists in data interpretation and the investigation of corrosive phenomena, promoting multidisciplinary integration and contributing to the development of more efficient solutions for nuclear environments.

3. Results and Discussion

The 316L stainless steel, widely used in nuclear systems, exhibits corrosion resistance due to the formation of a chromium-rich passive film. However, its stability strongly depends on the environment. The presence of chloride ions and H_2S can promote the breakdown of the passive film, increasing electrochemical activity and corrosion rate [14]. The behavior of 316L stainless steel was studied in a solution containing NaCl, CO_2, and H_2S. Thus, when analyzing how these elements affect the protective passive film of the steel, the results showed that:

- the pitting potential (Epit) is not altered;
- the passive current (Ipass) increases significantly with the increase in H_2S concentration;
- there was greater electrochemical activity and greater degradation of the passive film.

This occurs because H_2S undergoes oxidation and produces sulfur (S^0) ($H_2S \rightarrow S^0$), which increases the anodic current and promotes defects in the passive film. Thus, Cl^- ions locally weaken the passive film of the 316L steel, allowing the penetration of sulfur originating from H_2S oxidation. This process favors the formation of metallic sulfides and defects in the protective oxide, making the film more conductive, less stable, and more susceptible to corrosion [15]. To demonstrate the electrical changes that the passive film undergoes due to these defects promoted by Cl^- and H_2S, the equation below assists in this analysis, such as Eq. 3:

$$d_{sc} = \frac{\varepsilon\varepsilon_0}{C}\gamma \quad (3)$$

Here, the calculation estimates the electrical thickness of the passive film.

Where:

- d_{sc}= space charge layer distance;
- C= oxide capacitance;
- ε= dielectric constant.

This equation helps to demonstrate that the passive film undergoes electrical changes due to the defects promoted by Cl^- and H_2S.

The behavior of 316L steel was also analyzed using electrochemical techniques such as potentiodynamic polarization, EIS and Mott-Schottky. In the same manner as the previous calculation, the results showed that the increase in H_2S concentration significantly raised the passive current (I_{pass}), indicating greater electrochemical activity and greater degradation of the protective passive film of the steel. The H_2S undergoes oxidation, forming elemental sulfur (S^0), which penetrates the passive film and favors the formation of metallic sulfides and structural defects in the oxide. The Mott–Schottky equation was used to calculate the defect density of the passive film, such as Eq. 4:

$$\frac{1}{C^2} = \frac{2}{q\varepsilon\varepsilon_0 N_d}\left(E - E_{fb} - \frac{kT}{q}\right) \quad (4)$$

and the donor density of the oxide, such as Eq.5 :

$$N_d = \frac{2}{q\varepsilon\varepsilon_0 \cdot slope} \quad (5)$$

The higher the N_d, the greater the amount of defects in the passive film.

The Mott–Schottky equation, which analyzes the electrical properties of the passive film on 316L stainless steel to calculate the defect density, is based on the following variables [16]:

- C - represents the capacitance of the passive film;
- q - elementary electron charge;
- ε - dielectric constant of the oxide;
- ε_0 - permittivity of vacuum;
- Nd - amount of electronic defects present in the oxide;
- applied electrochemical potential;
- E_{fb} - flat-band potential of the material;
- k - Boltzmann constant;
- T – absolute temperature in Kelvin;
- slope - semiconductor behavior of the protective oxide.

The increase in H_2S raises I_{pass}, reduces R_{ct} and increases N_d, indicating greater degradation of the 316L steel passive film [17]. These parameters can be used in Artificial Intelligence models to predict corrosion and material degradation in nuclear environments, with Machine Learning being suitable for the analysis of complex and non-linear processes [18].

Protective coatings used in third-generation reactors exhibit degradation over time, through electrochemical analyses, polarization curves, and electrochemical impedance spectroscopy [19]. These data can futurely serve as a baseline for Artificial Intelligence applications aimed at analyzing corrosive behavior and the evolution of coating degradation. Below is an example of an algorithm applied to solve an AI engine:

```
BEGIN
 Read corrosion_data;
 Consistency <- Verify_ consistency(corrosion_data);
 IF !Consistency then
   Correct(corrosion_data);
        Organize_by_sample(corrosion_data);
        Exposure_time(corrosion_data);
 END IF
Results <- Calculate_electrochemical_parameters_AI(corrosion_data);
Interpret_Results_AI(Results);
Classify_risk_level_AI(Results);
Generate_graph(Results);
END
```

The analysis of these phenomena allows for the identification of degradation patterns and the correlation of environmental variables with corrosive behavior, contributing to the understanding of the mechanisms involved. Similarly, protective coatings used in third-generation reactors exhibit degradation over time [20].

As an output of the AI system, electrochemical data can be automatically converted into potentiodynamic polarization curves, allowing for the correlation of potential, current density, and H_2S and CO_2 concentrations. Thus, the AI can identify changes in the corrosive behavior of 316L steel, using parameters such as the increase in passive current (I_{pass}) to indicate passive film degradation and predict corrosion evolution, as shown in Figure 1 (HE et al., 2009).

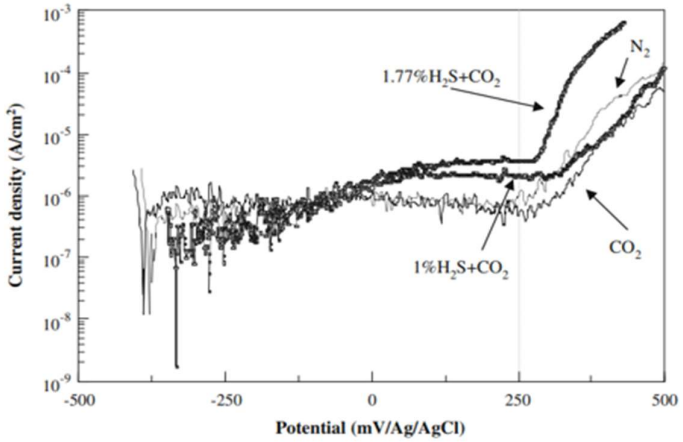


Figure 1 – passive current (I_{pass})

Furthermore, machine learning techniques allow for the identification of degradation trends and the prediction of material failures before critical problems occur. In nuclear systems, this approach assists in the continuous monitoring of corrosion through the integrated analysis of experimental and historical data, making AI a strategic tool to enhance operational safety [21][22].

4. Conclusions

The complexity of corrosive processes in nuclear environments imposes limitations on traditional analysis methods. Artificial Intelligence emerges as a tool capable of handling this complexity, allowing for the analysis of heterogeneous data and the identification of non-linear patterns. By integrating experimental data, physical knowledge, and machine learning techniques, it becomes possible not only to predict material behavior but also to understand the mechanisms that govern corrosion.

Thus, AI should not be viewed merely as a predictive tool, but as a supportive instrument for scientific discovery, contributing to the advancement of knowledge in the field of nuclear materials and to the development of safer and more efficient solutions. In this context, the adoption of Artificial Intelligence-based approaches tends to establish itself as a fundamental practice in nuclear materials engineering, especially given the growing volume of available experimental data. The ability to integrate different information sources and extract relevant knowledge allows for the optimization of analysis processes and the reduction of uncertainties associated with material degradation. Furthermore, the use of AI favors the development of more efficient monitoring and mitigation strategies, directly contributing to the operational safety and reliability of nuclear systems throughout their service life.

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