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Evaluation of the Factors Determining Hydrogen Embrittlement in Pipeline Steels: An Artificial Intelligence Approach

Abhishek Subedi
Department of Mechanical Engineering, Kathmandu University, Nepal. E-mail: abhishek.subedi@ku.edu.np

Alessandro Campari
Department of Mechanical and Industrial Engineering, NTNU, Norway. E-mail: alessandro.campari@ntnu.no

Antonio Alvaro
SINTEF Industry, SINTEF, Norway. E-mail: antonio.alvaro@sintef.no

Biraj Singh Thapa
Department of Mechanical Engineering, Kathmandu University, Nepal. E-mail: bst@ku.edu.np

Nicola Paltrinieri
Department of Mechanical and Industrial Engineering, NTNU, Norway. E-mail: nicola.paltrinieri@ntnu.no

Hydrogen is an emerging energy carrier with inherent environmental benefits. It has the potential to decarbonize industrial applications that require high-grade heat. In addition, hydrogen allows centralized clean energy production and distribution to remote end-use sites. For a smooth transition to hydrogen technologies, it is important to guarantee a safe and reliable distribution system. Hydrogen could be transported through the existing widespread pipeline network. Nevertheless, most pipeline steels were not designed for hydrogen service and are prone to hydrogen-induced degradation, which could result in sudden component failures and undesired releases with severe consequences. Hydrogen embrittlement depends on the interplay of three factors, i.e., the mechanical loading, the operating environment, and the material properties. The synergistic interaction of these parameters has significant safety implications. This study introduces a machine learning approach to evaluate the role of these factors in the occurrence of hydrogen-induced damages. Several pipeline steels have been assessed for embrittlement under different environmental and loading conditions. An extensive database has been created, and a decision tree model has been trained to predict the hydrogen embrittlement of materials. The main advantages of this model are its "white box" nature and simple interpretability. This artificial intelligence approach can ensure the safe application of hydrogen systems and allow advancements in inspection planning and predictive maintenance.

Keywords: Hydrogen embrittlement, Pipeline steel, Artificial intelligence, Machine learning, Decision tree, Inspection planning, Predictive maintenance.

1. Introduction

The need to decarbonize the energy sector demands extensive renewable energy production and its widespread utilization. However, the intermittent supply and the management of surplus energy represent significant setbacks for a renewable-based global energy landscape. In this scenario, hydrogen is emerging as a potentially clean and sustainable energy carrier. In 2021, hydrogen production capacity was 500 MW, and it is expected to reach 240 GW by 2030. The growing demand will require large-scale centralized production and extensive distribution networks. The ongoing global projects aim at exporting 12 Mt of hydrogen per year by 2030 (IEA, 2022). Hydrogen could be transported through the existing pipelines for natural gas, taking advantage of this capillary network. Despite this, the inherent properties of hydrogen can degrade pipeline steels through hydrogen embrittlement (HE) (Wang et al., 2021). Atomic hydrogen tends to penetrate the metal lattice of steels, deteriorate their mechanical properties, and induce cracking in otherwise high-performance materials, thus resulting in undesired releases with severe consequences. This issue can be mitigated through risk-informed inspection and maintenance planning (Campari et al., 2022).

HE results from the synerigistc interaction between mechanical parameters (residual and applied stress, strain rate, etc.), operating environment (temperature, pressure, hydrogen purity, etc.), and material factors (microstructure, composition, presence of welds, etc.) (Campari et al., 2023). Several publications analyze the influencing factors for HE in pipeline steels. Despite these studies, three research questions arise: how do loading conditions, operating environment, and material properties interact to determine HE magnitude in pipeline steels? What parameters are more significant for the HE susceptibility of materials? How can machine learning allow the investigation of this synergistic interplay, thus facilitating maintenance planning of equipment operating in gaseous hydrogen environments?

This study aims to fill this gap in knowledge by evaluating the impact of various environmental, material, and mechanical factors on the occurrence of hydrogen-induced damages using a machine learning (ML) approach. An extensive database that collects the results of tensile tests conducted in relevant hydrogenated environments has been created to train and evaluate the ML model. In the next section, fundamental knowledge regarding HE in pipeline steel is briefly provided. Then, the methodology and the machine learning model are explained. Finally, the main findings are presented and critically discussed to make recommendations for advancement in inspection planning and predictive maintenance of hydrogen transport pipelines.

2. Hydrogen embrittlement in pipeline steels

Pipeline steels consist of several steel grades, which vary on microstructure, strength, alloying elements' content, and manufacturing process. H_2 distribution via pipeline exposes steels to compressed gaseous hydrogen from the inside and to chemical reactions (associated with cathodic protection) which produce atomic hydrogen from the outside. Hydrogen atoms can enter the metal lattice, thus affecting the material properties and even inducing cracking. In particular, it can diffuse through the steel and interact with grain boundaries and structural defects, such as dislocations and vacancies. These interactions tend to facilitate the initiation of microcracks and enhance their growth over time. For these reasons, steel becomes more prone to failure and fracture when exposed to hydrogen (Gangloff and Somerday, 2012). Figure 1 shows the simplified mechanism of material degradation due to HE.

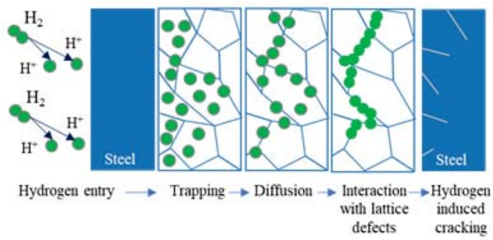

Fig. 1. Hydrogen embrittlement mechanism

Hydrogen has a low volumetric energy density of 10.8 MJ/Nm^3 (NIST, 2023), which imposes storage and transport under high pressure. However, a high hydrogen partial pressure increases the applied stress and triggers hydrogen-induced degradation. Sievert's law states that the solubility of hydrogen in metals is proportional to the square root of its partial pressure. In other words, the total hydrogen concentration within the metal increases with pressure (Campari et al., 2023). The temperature has a mixed effect on HE susceptibility. For most ferritic steels, HE is maximum at around room temperature and diminishes as the temperature rises or decreases. The likelihood of hydrogen-induced cracking is higher because hydrogen has higher diffusivity at room temperature than at cryogenic temperatures and remains trapped for enough time to accumulate (unlike at high temperature) (Lee, 2016).

In most cases, the use of high-strength steels is not recommended for hydrogen application as HE generally becomes more severe in high-strength materials because of stress amplification near defects (Somerday and San Marchi, 2008).

Microstructure is also an important aspect in determining hydrogen embrittlement susceptibility. X70 and lower grades steels have longitudinal bands of pearlitic-ferritic mix, while X80 and higher grades steels have a fine-grained mixture of ferritic-bainitic or ferritic-acicular ferritic microstructure. It is proven that the acicular ferritic structure is more sensitive to HE than the ferritic-pearlitic one because of the greater hydrogen diffusivity (Pulvinage, 2021). Steel of Grade A and B, and X42 tend to reach the saturation at hydrogen pressure ranging from 6.9 MPa to 13.8 MPa (San Marchi and Somerday, 2012), while the saturation pressure of the higher grades remains to be assessed. Steels with grade higher than X80 have been developed for natural gas transport in harsh environments. These pipelines have thinner walls, contain down to one-third of C, have higher weldability, thus meeting all the design requirements. The welding process will creates residual stresses and change in microstructure of the welded area and the heat-affected zone (HAZ), eventually resulting in the formation of brittle phases. The high-strength and low ductility of martensite makes these microstructures highly susceptible to HE (Thompson and Bernstein, 1977). The selection of the optimal properties for pipeline materials depends on their operating conditions. The American Petroleum Institute has classified the steel grades for pipeline application in the standard API 5L (2013), specifying their minimum yield strength.

Finally, the chemical composition of the steel is measured in terms of carbon equivalent content. The correlation of Dearden-O'Neill, widely used to compare plain carbon and carbon-manganese steels, is given by Eq. 1.

$$CE = C + \frac{Mn}{6} + \frac{Cr + Mo + V}{5} + \frac{Ni + Cu}{15} \tag{1}$$

According to European Industrial Gases Association, for hydrogen applications, the CE should be limited to 0.35 to avoid the formation of martensite during welding (EIGA, 2004). In addition, San Marchi and Somerday (2007) suggested that sulfur and phosphorous contents should be lower than 0.01 and 0.015, respectively. In general, the optimal combination of macro-mechanical properties is obtained by balancing alloying elements, and controlling the manufacturing processes, grain refinement, and heat treatments.

3. Methodology

The methodology proposed to predict the HE effect in pipeline steels and to evaluate the main susceptibility factors is divided into three steps, i.e., the database creation and pre-processing, the identification of the target attribute, and the training and evaluation of the ML classifier.

3.1. *Database creation and pre-processing*

The database collects the results of tensile tests conducted on pipeline steels. All these data have been gathered from peer-reviewed journals and publicly disclosed industrial reports, such as the "Technical Reference for Hydrogen Compatibility of Materials" (San Marchi and Somerday, 2012). As first step presented in this work, in-situ slow-strain rate tests (SSRT) with gaseous hydrogen charging are the only experiments considered. The original database was composed of 132 tests and 35 features, which relate to environmental conditions, material properties, and mechanical loading parameters. The missing values have been filled in with the following assumptions:

- Ambient temperature is 22 °C;
- Strain rate equals to 0.0001 s^{-1};
- Stress concentration factor for notched specimens equals to 5.5;
- Nominal chemical composition in ASME B31.12 (2019) is assumed;
- Average yield and ultimate tensile strengths are assumed according to ASME B31.12

The features associated with hydrogen purity, the presence of tungsten, and the presence of pre-charging have not been deemed relevant since they had the same value for each test. Hence, they have been eliminated during the pre-processing phase. Table 1 presents the structure of the final database.

Table 1. Features and example categories of the database

Feature	Type	Unit	Categories
Pressure	Numerical	MPa	3; 6.9; 7; 10; 12; etc.
Temperature	Numerical	$^{\circ}$C	20; 22; 25; 40; etc.
Material ID	Categorical		X42; X52; X60; X80; X100; Grade A; Grade B; etc.
Fe content	Numerical	%	98.77; 98.29; 98.54; 98.13; etc.
Cr content	Numerical	%	0.038; 0; 0.058; 0.13; 0.07; etc.
Ni content	Numerical	%	0.016; 0.04; 0; 0.14; etc.
Mn content	Numerical	%	0.82; 1.31; 1.66; 1.68; etc.
Mo content	Numerical	%	0.01; 0.013; 0.31; 0.15; etc.
Nb content	Numerical	%	0.003; 0.012; 0.048; 0.062; etc.
Ti content	Numerical	%	0.004; 0.05; 0; 0.01; etc.
V content	Numerical	%	0.008; 0.04; 0.01; 0.09; etc.
Al content	Numerical	%	0.004; 0.012; 0.04; 0.03; etc.
Cu content	Numerical	%	0.022; 0.075; 0.31; 0.12; etc.
Si content	Numerical	%	0.014; 0.29; 0.03; 0.22; etc.
C content	Numerical	%	0.26; 0.113; 0.07; 0.05; etc.
Sn content	Numerical	%	0.005; 0.01; 0; etc.
Co content	Numerical	%	0.0045; 0; etc.
S content	Numerical	%	0.026; 0.001; 0.015; 0.01; etc.
N content	Numerical	%	0.004; 0; etc.
P content	Numerical	%	0.02; 0.019; 0.006; 0.013; etc.
Microstructure	Categorical		Ferritic; Bainitic; Pearlitic; etc.
Base metal / Weld / HAZ	Categorical		Base; Girth weld; Cross weld; Inter-critical HAZ; etc.
Yield strength	Numerical	MPa	626; 605; 551; 520; etc.
Ultimate tensile strength	Numerical	MPa	693; 946; 1027; 1251; etc.
Stress concentration factor	Numerical		1; 2.1; 3.3; 5.5; etc.
Strain rate	Numerical	s^{-1}	0.0001; 0.0003; 0.00016; etc.

3.2. *Target identification*

The Embrittlement Index (EI) and the Total Elongation Loss (TEL) are two different indexes obtained from tensile tests that allow quantifying the susceptibility to hydrogen embrittlement of metallic materials. This study uses the EI as the target attribute to evaluate the HE effect in pipeline steels. EI is defined as the difference between the reduced area at fracture obtained from SSRT in gaseous H_2 and in a reference environment, divided by the reference reduced area.

$$EI = \frac{RA_{ref} - RA_{H_2}}{RA_{ref}} \cdot 100 \tag{2}$$

where RA_{ref} and RA_{H_2} represent the reduced area at fracture in a reference environment and hydrogen, respectively. Air or inert gases (e.g., He or Ar) can be used as a reference since they do not interact with the steel. RA is defined as follows:

$$RA = \frac{A_i - A_f}{A_i} \tag{3}$$

where A_i and A_f represent the initial and final fracture areas, respectively.

The susceptibility value has been labelled into two classes: "High" and "Low", in compliance with the classification provided in the report NASA/TM-2016–218602 (Lee, 2016). The class "High" (H) is defined by an EI higher than 50% and comprehends materials not recommended for hydrogen applications under the specified testing conditions. On the other hand, the class "Low" (L) includes the tests that resulted in EI lower than 50%. The "Low" susceptibility does not guarantee the suitability of a material for hydrogen pipelines under the specified operating conditions since the H_2 environment can degrade several other mechanical properties, such as fracture toughness and fatigue performance. A complete evaluation of hydrogen-induced degradation considering different mechanical performances, especially in presence of cracks, is required before employing a material for H_2 transport.

3.3. *Machine learning simulation*

A Decision Tree Classifier (DTC) has been trained to predict HE susceptibility. The algorithm divides the materials into two classes, depending on the EI value. A classification model is used rather than a regression because HE depends on several other factors, such as internal defects and material orientation during testing, that cannot be used to draw general conclusions about the susceptibility of a material. The training and evaluation process is shown in Figure 2.

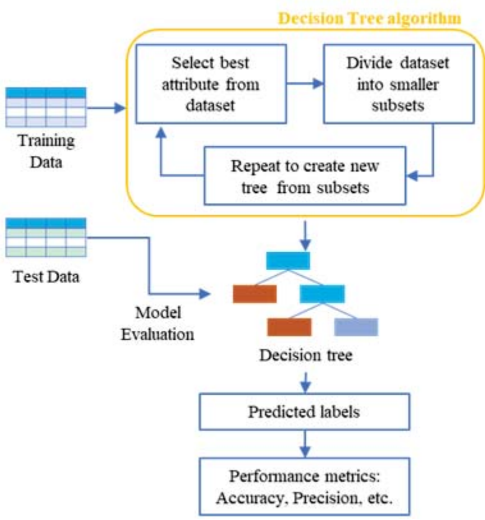

Fig. 2. Flow diagram of the Decision Tree Classifier

The database is divided into two sub-databases in a ratio of 70:30 to train the algorithm and test the model. The 70% dataset is used to create a decision tree. This algorithm uses if-else conditions to split the dataset into different classes. Each internal node constitutes a test on an attribute, each branch is the outcome of the test, and each leaf represents a class label. For classification problems, it uses either Entropy, Gini Index or Information Gain metrics to determine the best nodes. In any case, the objective is to reduce the randomness and obtain more homogeneous regions wherein datasets belong to similar classifications. Along with the development of splitting, the tree becomes complex and can develop noise and causes overfitting of the tree. Hence, the model can limit its prediction capability to the training dataset, without being able to generalize other unseen datasets. A forward pruning concept is used to reduce this risk. It limits overfitting by eliminating trees that have lower predictive power. This can be controlled by limiting the maximum depth of the decision tree and the minimum number of samples per decision space. Through several splits, a flowchart-like structure is achieved. It stops at a point where a further split is either not possible or it meets the defined requirements for classification (Dai et al., 2016). The remaining 30% dataset is used to evaluate the model. In this study, the Orange Data Mining software has been used to train and test the decision tree (Demšar et al., 2013).

4. Results and discussion

Three evaluation metrics (i.e., accuracy, precision, and recall) have been calculated to assess the performance of the DTC algorithm. Accuracy represents the fraction of correct predictions and is calculated using Eq. 4. Precision, calculated through Eq. 5, represents the fraction of true positive predictions, and recall, obtained through Eq. 6, indicates the fraction of positive labels that are correctly predicted (Juba and Le, 2019).

$$CA = \frac{TP + TN}{TP + TN + FP + FN} = 0.825 \quad (4)$$

$$Precision = \frac{TP}{TP + FP} = 0.824 \quad (5)$$

$$Recall = \frac{TP}{TP + FN} = 0.825 \quad (6)$$

where TP and TN indicate the ”Low” susceptibilities and the ”High” susceptibilities correctly predicted, respectively, while FP represents the ”High” mislabeled as ”Low” and FN indicates the ”Low” mislabeled as ”High”. The confusion matrix for the DTC model is shown in Figure 3.

		Predicted	
		High	Low
Actual	High	TN=79.2%	FP=15.4%
	Low	FN=20.8%	TP=84.6%

Fig. 3. Confusion matrix for the Tree Classifier

Although 82.5% of the total tests are correctly classified, it is important to emphasize that not all incorrect predictions have the same safety implications. Any classification of materials that are highly degraded by HE but are predicted to be tolerably affected is more critical than vice-versa. In this case, the wrong classification could lead to an improper material selection, which would increase the risk of failure in pipeline systems.

The features of the database are not equally important for the classification process. Hence, the two scoring methods have been used to rank the features based on the amount of information they provide and the influence they have in the automatized decision-making process. The ten top-ranked features are reported in Table 2, distinguishing between the Information Gain and the Gini Index.

Table 2. Comparative rank scoring of features

Rank	Information Gain	Gini Index
1	Material ID	Material ID
2	Mn content	Mn content
3	Cu content	Mo content
4	Mo content	Cu content
5	P content	P content
6	Pressure	V content
7	Base/weld	Pressure
8	V content	Cr content
9	Cr content	Base/weld
10	C content	C content

The top ten features for classification are the same regardless of the chosen scoring methods. The first ranked feature is the Material ID. However, seven out of ten top-ranked features are related to the chemical composition of the material. The contents of C, Mn, Cr, Mo, V, Cu, and Ni determine the carbon equivalent content, which strongly relates to the hydrogen compatibility of a material. Among those elements, Ni is the only one that does not appear among the ten top-ranked features. Hence, the definition of the CE complies with the significance of these features for the tensile properties degradation in materials exposed to hydrogen. After calculating the CE content for all these materials and again classifying the HE susceptibility based on this parameter, according to the screening method proposed by San Marchi and Somerday (2007), it has been found that the CE content can be greater than 0.35, and still being compatible for hydrogen applications (when ranked uniquely with respect to hydrogen-induced ductility loss). Similarly, the database indicates that the limits in S content (lower than 0.01) and P content (lower than 0.015) seem not to have significant implications on hydrogen-metal compatibility. Pressure is the only environmental factor that is considered highly significant for HE susceptibility, and it is not surprising since pressure is the driving force for hydrogen uptake into the metal. The presence of welds or HAZs is another highly relevant factor. The stress concentration and the strain rate (i.e., the loading factors) are in the eleventh and nineteenth positions, respectively. This proves that a proper selection of materials for hydrogen applications has the potential to reduce the magnitude of HE, thus minimizing the risk of component failures.

The Decision Tree is shown in Figure 4. It is composed of 29 nodes and 14 leaves. The root node is the Material ID, while the leaf nodes are the Strain rate, the Base/weld, the Smooth/notched, the Cr content, the Ultimate tensile strength, the Yield strength, the Pressure, the C content, and again Material ID. According to the DTC, smooth specimens of 42CrMo4, X42, X60, X65, and X120 steels are less affected by HE. In the case of notched specimens, a more complex dependence on the Cr content, UTS, and strain rate has been highlighted. The higher the UTS and the lower the strain rate, the greater will be the HE effect on tensile properties. On the other side, Grade A, Grade B, X52, X70, X80, and X100 are generally more affected by HE. For these ma-

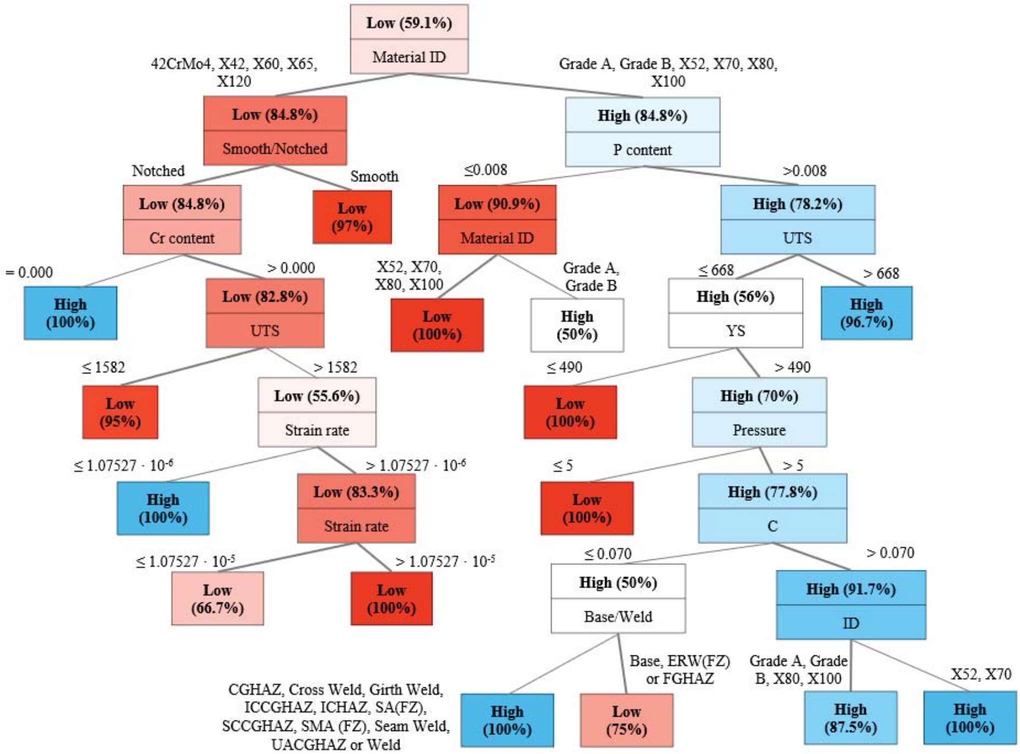

Fig. 4. Structure of the Decision Tree Classifier

terials the combination of UTS lower than 668 MPa and YS lower than 490 results in ”Low” susceptibility. Materials with higher YS can have ”Low” susceptibility if their operating pressure is below 50 bar. In general, high-strength materials, with P content greater than 0.008 %, exposed to a pressure above 50 bar are severely degraded by hydrogen.

From the analysis of the prediction, it turned out that the algorithm has wrongly classified X52, X65, X70, X80, and 42CrMo4 steels, while it was accurate in predicting the HE susceptibility of Grade A, Grade B, X42, X100, and X120 steels. The reasons of these misclassifications can be summarized as follows:

- Grade A, Grade B, X52, and X65 steels have limited test data in comparison to other materials and this lack of information hinders the classification process;
- The wrongly classified X70 and X80 steels are tested in welded areas and HAZs. Since the database contains only one test for each type of weld the evaluation is inherently unreliable;
- 42CrMo4 has been wrongly classified because it has been pre-charged, thus increasing the amount of hydrogen within the metal lattice and making it more affected by HE.

The dataset comprehends 54 ”High” and 78 ”Low” labels. This fact indicates that, based on this exemplified attempt, a significant amount of pipeline materials would not be compatible with hydrogen transport. The remaining steels need a thorough evaluation of fracture properties and fatigue performance before being used for H_2 transport. In addition, all these equipment items should be properly inspected and maintained to monitor their degradation over time and to preserve their structural integrity and fitness-for-service.

The performance of the classification model proposed can be improved by increasing the amount of data in the training dataset, especially concerning tests on welded areas and HAZs. The utilization of more complex and performing algorithms, such as Random Forest, Gradient Boosting Machine, or Artificial Neural Network, can also improve the classification accuracy (Campari et al., 2023).

5. Conclusions

A machine learning approach has been used to evaluate the synergistic interplay of environmental, material, and loading factors on pipeline steels and to classify them based on their HE susceptibility under certain operating conditions. A database of tensile test results has been created and used to train and evaluate a DTC model. The most important influencing factors have been examined and ranked based on the impact on hydrogen-induced degradation of mechanical properties. This approach showed potential in providing better understanding of the complex interaction between these factors. The results may hold significant implications for identifying proper pipeline steels for hydrogen applications. These findings can be helpful in designing new hydrogen-specific equipment but also in planning risk-informed inspection and maintenance activities in the existing pipeline infrastructure. The ML algorithm has proven to be reliable in predicting the HE severity (with 82.5% accuracy), despite the limited number of experimental tests available. However, the future development of more extensive datasets and the adoption of more sophisticated algorithms will be considered to increase the classification performance.

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