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THE PREDICTION OF HYDROGEN EVOLUTION REACTION FROM DYNAMIC MAGNETIC FIELD ASSISTED WATER ELECTROLYSIS ARTIFICIAL NEURAL NETWORK

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Abstract

This study explores the prediction of Hydrogen Evolution Reaction (HER) performance in Dynamic Magnetic Field (DMF) assisted water electrolysis using Artificial Neural Networks (ANN). The integration of ANN models with experimental data from DMF-assisted electrolysis provides valuable insights into the complex interplay between magnetic fields and electrochemical processes. The results show significant enhancements in HER rates compared to conventional electrolysis, with static magnetic fields also contributing to performance improvements. The ANN models developed exhibit high accuracy in predicting HER performance under varying DMF rotational speeds, as evidenced by low Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and high R-squared values, demonstrating their strong predictive power and reliability. However, caution is advised regarding overfitting, and future research should focus on incorporating techniques like regularization and cross-validation to enhance model generalization. This study lays the foundation for further optimization of efficient hydrogen production technologies in the context of sustainable energy solutions.

Keywords: *Artificial Neural Network, Hydrogen Evolution Reaction, Water Electrolysis, Dynamic Magnetic Field, Prediction*

1. INTRODUCTION

The burgeoning interest in renewable energy sources and sustainable hydrogen production has prompted extensive research into enhancing efficiency and predicting performance using advanced computational techniques. Artificial intelligence (AI) and machine learning (ML) algorithms have emerged as powerful tools for modeling complex systems and optimizing various processes in the energy sector [1]. In recent years, numerous studies have demonstrated the efficacy of AI and ML approaches in predicting key parameters and optimizing operations related to energy conversion and hydrogen production.

Green electrochemical Hydrogen is considered as the cleanest renewable chemical energy source. However, the green hydrogen production still left carbon footprints especially in the electrocatalyst material exploration such as Platinum (Pt) and Iridium-oxide (IrO_2) [2]. High electron density material such as Pt is required to drive efficient HER on cathode which can provide stable inner Helmholtz plane [3]. The stable inner and outer Helmholtz plane are required for the formation of stable diffusion layer to ensure continuous ion transfer [4]. External magnetic field assisted electrolysis has been emerged to provide electrode-electrolyte interface modification without material modification. The presence of external magnetic field exposure modifies the water physical properties.

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The combination of electromagnetic force (EMF) with magnet has the potential to enhance hydrogen production in water electrolysis. Optimization of EMF application has been achieved by utilizing green light, leading to further improvements in efficiency [5]. The coupling of EMF and green laser surpasses the autoprotolysis potential, where water molecules autonomously act as both acids and bases, facilitating proton (H^+) transfer between them [6]. Consequently, ionization occurs at a lower potential, accelerating the achievement of HER. Another coupling experiment involved collimated sunlight, which, when combined with EMF, increased the HER rate by 53% compared to conventional saltwater electrolysis [7]. This enhancement in HER rate is attributed to sunlight polarizing water molecules, thereby activating the dipole effect already induced by EMF.

The magnetic field exposure generates magnetohydrodynamics (MHD) phenomenon during electrolysis. MHD modifies water intermolecular interaction in the diffusion layer which makes them perform better in current delivery and ion transfer [8]. When an electric current is passed through the water electrolyte, it causes ionization of the water molecules, resulting in the formation of hydrogen and oxygen gas at the electrodes [9]. The presence of a magnetic field influences this process by exerting a force on the charged particles (ions) in the electrolyte, leading to changes in the distribution and movement of ions [10]. This magnetic force can affect the efficiency and dynamics of the electrolysis process, influencing factors such as the rate of gas production, electrode wear, and energy consumption.

One notable area of research involves the application of AI and ML techniques to predict hydrogen production performance in electrolysis systems. For instance, a study by Davoodi *et al.* (2023) utilized machine learning algorithms to develop predictive models for electrolyzer efficiency, porous carbon uptakes, and hydrogen yield, considering factors such as operating conditions, electrode materials, and catalyst properties [11]. Their findings revealed significant improvements in prediction accuracy compared to traditional analytical methods, highlighting the potential of ML in optimizing electrolysis processes for efficient hydrogen generation.

Furthermore, the integration of AI-based predictive models with dynamic magnetic field (DMF) assistance in water electrolysis represents a cutting-edge approach to enhance hydrogen evolution reaction (HER) kinetics and overall system efficiency. Recent study on the implementation of Double Deep Q network (DDQN) deep reinforcement learning model to assists DMF water electrolysis has been successfully find the magnet rotation tuning strategy [12]. The magnetic rotation tuning strategy was critical to solve the efficiency problem imposed by fixed rotational speed DMF which cannot significantly improve the efficiency above 500 RPM [13]. Study by Abdelkareem. (2023) reports the prograss of ANN application in hydrogen production including the feasibility to predict HER performance under varying magnetic field intensities and frequencies [14]. By leveraging the capabilities of ANNs, the study achieved accurate predictions of HER rates and electrolysis efficiency, paving the way for optimized hydrogen production through magnetic field assisted electrolysis.

In addition to electrolysis systems, AI and ML techniques have been applied to various energy conversion processes, including solar energy harvesting, wind power generation, and biomass conversion. For example, a recent review by Jorge *et al.* (2022) comprehensively surveyed the application of machine learning in solar photovoltaic (PV) systems, highlighting its role in predicting solar irradiance, optimizing PV performance, and enhancing grid integration [15]. Similarly, studies by Malakouti *et al*. (2023) and Gupta *et al.* (2022) demonstrated the utility of AI algorithms in predicting wind turbine performance and optimizing biomass conversion processes, respectively [16], [17]. Both studies illustrate AI's efficacy in forecasting wind turbine performance and AI's role in optimizing biomass conversion processes.

Overall, the convergence of AI, ML, and energy research holds immense promise for advancing sustainable hydrogen production and renewable energy technologies. By harnessing the predictive capabilities of AI-based models, researchers can accelerate the development of efficient and cost-effective solutions to meet the growing demand for clean energy worldwide. This paper aims to contribute to this endeavor by exploring the prediction of HER from DMF-assisted water electrolysis using ANN. This study explores the development of predictive models using machine learning techniques which has not explored by [11]. Study [11] focused on investigating the effects of magnetic fields on HER kinetics and electrolysis efficiency using experimental methods. In contrast, the current study aims to bridge this gap by leveraging ANN models to predict HER performance under varying magnetic field conditions. By combining experimental data on DMF-assisted water electrolysis with machine learning algorithms, this study seeks to enhance our understanding of the complex interplay between magnetic fields and electrochemical processes.

2. MATERIALS AND METHODS

Figure 1 illustrates the design and development of the experimental apparatus [4, 11, 23]. The experimental setup consisted of a DMF assisted water electrolysis system comprising an electrolyzer unit, magnetic field generator, power supply, and data acquisition system. The schematic diagram of the experimental setup can be seen in figure 1. The electrolyzer unit consisted of two graphite rode electrodes (anode and cathode) immersed in a NaCl electrolyte solution. The electrolyte was consists of 500 ml distilled water with 50 gram NaCl. The magnetic field generator was positioned in close proximity to the electrolyzer to apply DMF during the electrolysis process. The generator consists of a 0,15mT Neodyimium N52 magnet attached to a 9V DC motor. The generator was placed in between the cathode another fixed magnet. The tested magnetic rotational speed variation was 0 RPM, 500 RPM, and 1000 RPM. The 12V 1.5A power supply provided the necessary electrical energy for water electrolysis. The data acquisition system was Arduino UNO R3 (Arduino, Italy) microcontroller which connected to MQ-8 Hydrogen sensor (FishEye, China) recorded real-time hydrogen concentration data in parts per million (PPM).

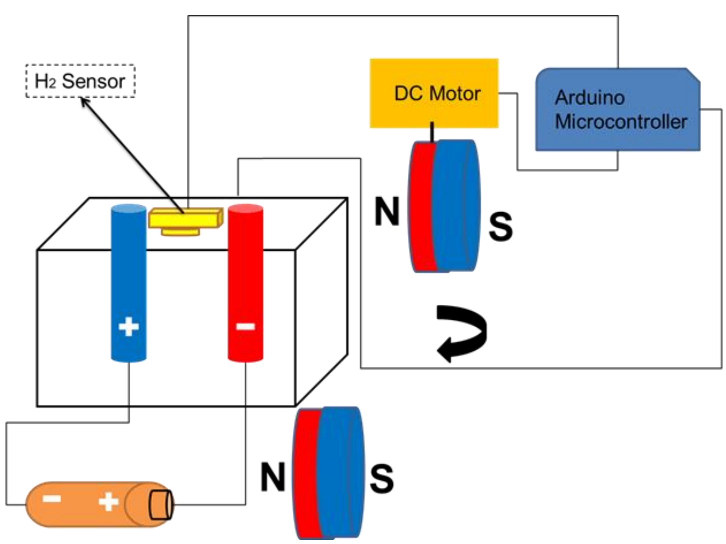

Figure 1. DMF assisted Electrolysis Experimental Setup

This study provides an ANN model for predicting HER performance in the DMF-asissted electrolysis process. Whole process from the model building, training, evaluation, and data visualization were performed using Python programming language. Initially, experimental data from the electrolysis process were loaded from a CSV file. The data were then preprocessed by separating features and the target variable, which were denoted as 'X' and 'y,' respectively. A train-test split was performed on the dataset, with 80% of the data used for training and 20% for testing. Feature standardization was applied to ensure zero mean and unit variance in both the training and testing sets. Subsequently, an Artificial Neural Network (ANN) regression model was trained using the MLPRegressor class, with two hidden layers, the rectified linear unit (ReLU) activation function (equation 1), the Adam optimizer, and a maximum of 1000 iterations. The model was evaluated using mean squared error (MSE) in equation 2, root mean squared error (RMSE) in equation 3, and R-squared (R2) metrics for both the training and testing sets (equation 3). Finally, the actual versus predicted HER performance was visualized using scatter plots for both the training and testing sets to assess the model's performance visually.

$$f\left(x\right) = \max\left(0, x\right) \tag{1}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2 \tag{2}$$

$$RMSE = \sqrt{MSE} \tag{3}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{n}\left(y_i - \overline{y}\right)^2} \tag{4}$$

In this study the ANN architecture that used was multilayer perceptron with randomized weight. The bias was also applied to the ANN model. The architecture of the ANN is served in figure 2 which consists of one input layer, two hidden layers, and one output layer. The input layer comprises of 10 neurons represent 10 previous time series data (t-1 to t-10). This followed by 2 hidden layers with 6 and 5 neurons which connected to a single output neuron in the output layer. The output neuron represents the prediction result in the next time step (t+1). The visual representation of the ANN architecture is shown in figure 2.

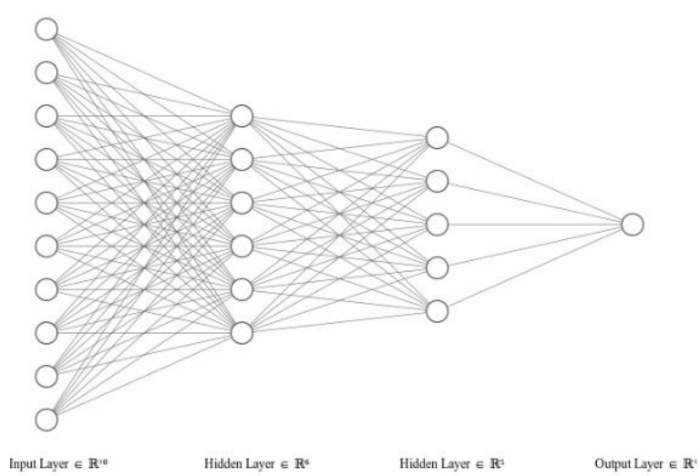

Figure 2. The multilayer perceptron ANN Architecture for prediction task formatting

The ANN model was trained using the collected experimental data, with a portion of the dataset reserved for validation and testing. The training process involved iteratively adjusting the model parameters to minimize the discrepancy between predicted and actual HER performance. The trained model was then evaluated using the validation dataset to assess its predictive accuracy and generalization capabilities. The performance of the trained ANN model was evaluated based on its ability to accurately predict HER performance under various DMF rotational speeds. The Metrics for the evaluation were MSE, RMSE, and R2 were computed to quantify the model's performance across different evaluation criteria.

In the HUASB reactor, there are two types of growing media: attached media and suspended media. The attached growth media is a container for the growth of microorganisms and is filled with bioball material. The clarifier is equipped to accept the liquid and solid after the generated gas has been separated in the gas liquid solid separator (GLSS) and collected in the biogas collector.

3. RESULTS AND DISCUSSION

The water electrolysis test results show the HER performance different among the external magnetic field exposures. The 2 hours test reveals DMF exposure increases the HER rate by 2 folds from the conventional electrolysis test. The static magnetic field also has a significant contribution which lifts the HER rate by 1.5 folds. However, figure 3 shows no significant difference between 500 and 1000 RPM DMF. This shows the presence of interchanging magnetic field is more important than the intensity of the magnetic field itself.

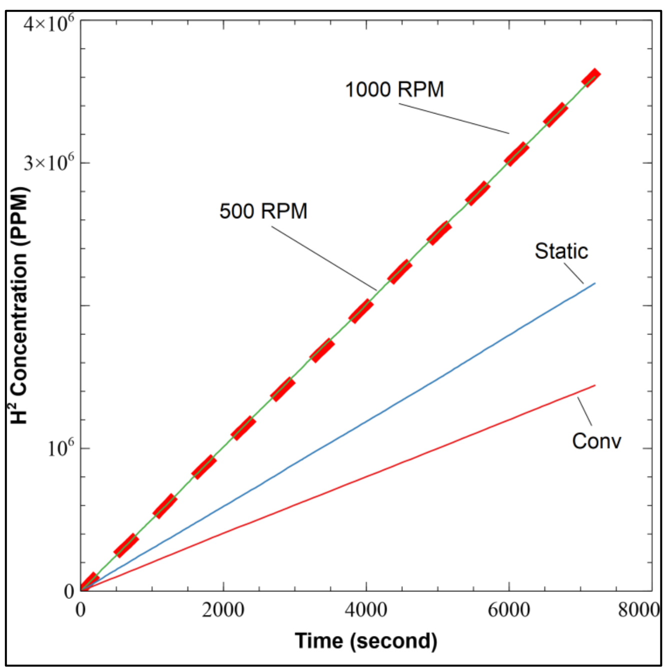

Figure 3. The water electrolysis experiment results to assess HER performance

During the linear incremental pattern of the Hydrogen Evolution Reaction (HER), the rate of hydrogen gas production increases steadily as the applied potential becomes more negative. This pattern is observed in electrochemical experiments where the electrode potential is gradually adjusted, leading to a corresponding increase in the reaction rate. In the linear incremental region, the HER follows Faraday's law of electrolysis, where the amount of hydrogen gas evolved is directly proportional to the quantity of electricity passed through the electrolyte [18]. As the electrode potential becomes more negative, the driving force for proton reduction increases, resulting in a higher rate of electron transfer and hydrogen gas generation [19]. This linear relationship between applied potential and HER rate is characteristic of well-behaved electrochemical systems.

The results of the ANN model training for predicting HER performance of conventional electrolysis indicate highly accurate predictions. This is evidenced by the extremely low Mean Squared Error (MSE) values for both the training 2756741.64 and testing 2737587.91 sets. The accurate prediction can be seen by the actual HER vs predicted HER performance plot in the top side of figure 4. Root Mean Squared Error (RMSE) values further confirm this accuracy, with values of 1660.34 for training and 1654.57 for testing, suggesting minimal deviation between the actual and predicted HER performance. Additionally, the high R-squared values of 0.99998 for training and 0.99998 for testing indicate that the model explains almost all the variance in the data, demonstrating its strong predictive power and reliability.

The ANN model also achieve the same performance with very low MSE values 6284829.64 for training and 6075879.73 for testing on static magnetic field assisted electrolysis data. This indicates minimal average squared differences between actual and predicted HER performance. Correspondingly, the RMSE values are also low, with 2506.96 for training and 2464.93 for testing, implying small deviations between predicted and actual values. Moreover, the high R-squared values of 0.99998 for training and 0.99998. As a result, predicted vs actual data of static magnetic field electrolysis is very close as shown in the bottom side of figure 4.

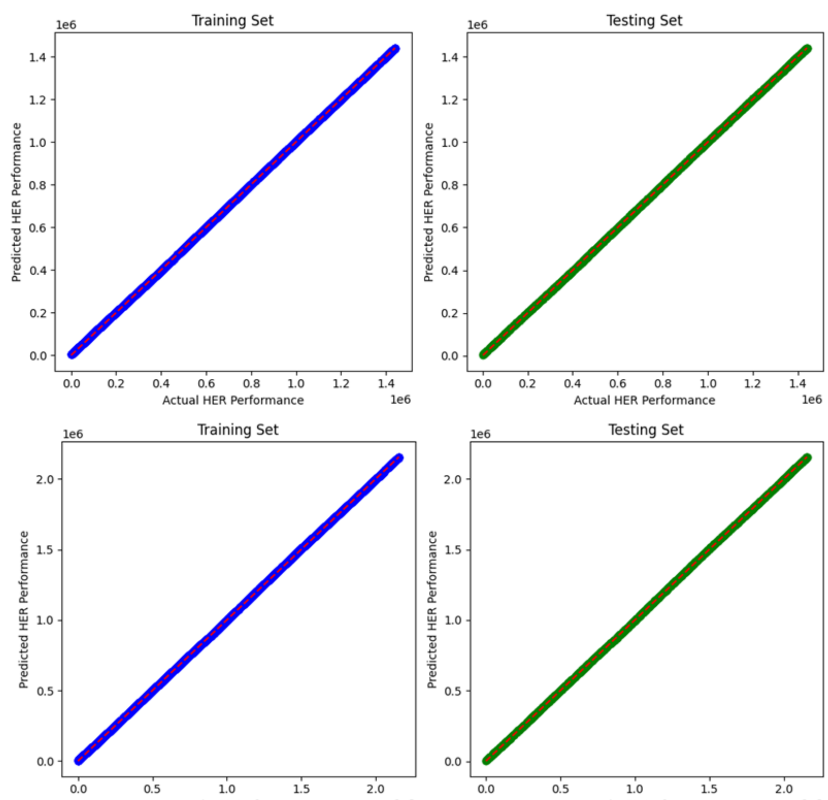

Figure 4. Actual HER vs predicted HER performance of conventional and static magnetic field assisted water electrolysis training and testing

Water electrolysis test results show the HER performance different among the external magnetic field exposures. The 2 hours test reveals DMF exposure increases the HER rate by 2 folds from the conventional electrolysis test. The static magnetic field also has a significant contribution which lifts the HER rate by 1.5 folds. However, figure 3 shows no significant difference between 500 and 1000 RPM DMF. This shows the presence of interchanging magnetic field is more important than the intensity of the magnetic field itself.

The prediction for 500 RPM DMF also have same performance character with low MSE values, with 15322165.19 for training and 15402615.61 for testing, indicating minimal average squared differences between predicted and actual HER performance across the dataset. The prediction results tighly fit the actual dataset as shown in the top side of figure 5. The RMSE values, at 3914.35 for training and 3924.62 for testing, further corroborate this finding, showing relatively small deviations between predicted and actual values. Moreover, the high R-squared values of 0.99999 for training and 0.99999 for testing reveal that the model explains almost all the variance in the data.

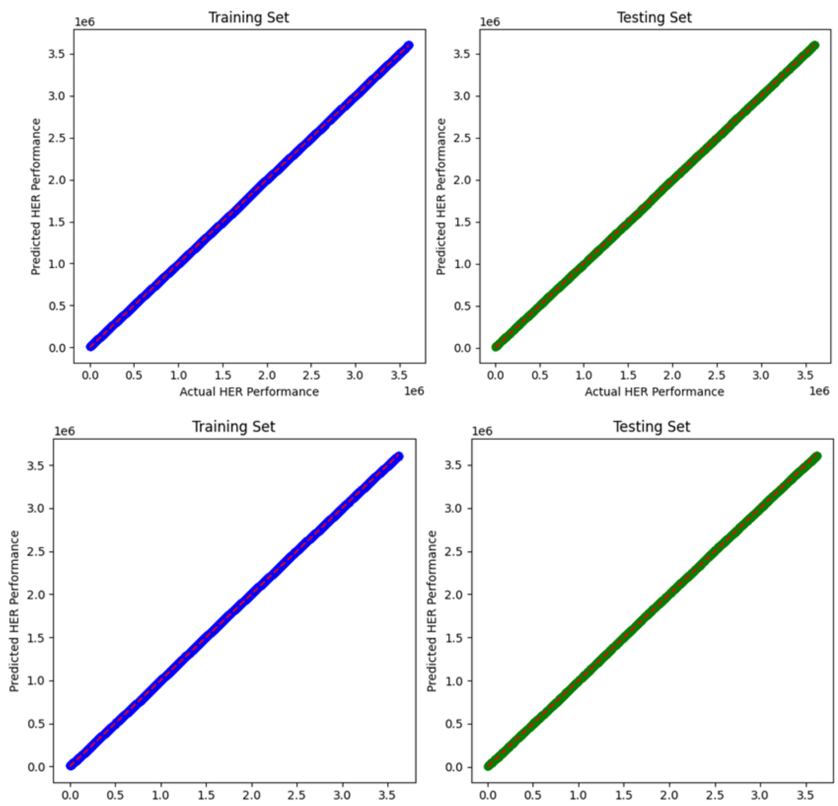

Figure 5. Actual HER vs predicted HER performance of performance of 500 RPM DMF and 1000 RPM DMF water electrolysis training and testing

The ANN model performance on the prediction of 1000 RPM DMF exhibit relatively high MSE values, with 22744822.22 for training and 24999052.79 for testing, indicating larger average squared differences between predicted and actual HER performance compared to previous experiments. The RMSE values, at 4769.15 for training and 4999.91 for testing, further confirm these observations, suggesting somewhat larger deviations between predicted and actual values. Despite this, the high R-squared values of 0.99998 for training and 0.99998 for testing indicate that the model still explains the vast majority of the variance in the data, highlighting its strong predictive capacity and reliability. The reliability can be seen from the tightly fit data in the bottom side of figure 5.

It is critical to interpret the tightly fit data within the context of model complexity and generalization. When an ANN exhibits tight fits to the training data, as indicated by high R-squared values and low error metrics like MSE and RMSE, it suggests that the model has effectively captured the underlying patterns and relationships present in the training data [20]. This can be beneficial in situations where the goal is to accurately predict outcomes within the training dataset itself. Therefore, the ANN model in this study have a good performance on HER prediction of conventional, static magnetic field assisted, and DMF assisted water electrolysis. However, caution is advised when interpreting such tight fits, especially in complex models with multiple hidden layers and parameters.

This study has produced an ANN model that capable to predict the HER rate correctly in a certain time evolution. However, the model is not free from the risk of overfitting associated with tightly fit ANN. Overfitting occurs when a model learns the training data too well, capturing noise and irrelevant patterns that do not generalize to new, unseen data [21]. As a result, the model may perform poorly when applied to real-world scenarios or new datasets, leading to decreased predictive accuracy. To address this issue, techniques such as regularization, dropout, early stopping, and cross-validation are commonly employed to prevent overfitting and improve the model's generalization ability [22]. Furthermore, recent literature emphasizes the importance of assessing model interpretability alongside performance metrics. While tightly fit ANN can achieve high accuracy in predictions, understanding the underlying mechanisms and features driving these predictions is crucial for model transparency, trustworthiness, and domain-specific insights. Techniques such as feature importance analysis, SHAP (SHapley Additive exPlanations) values, and model-agnostic interpretability methods are gaining prominence for gaining insights into ANN decision-making processes and identifying influential features [23]. Therefore, several improvements to avoid overfitting should be applied in the future to enhance the model accuracy and precision in predicting HER rate.

Prediction for 500 RPM DMF also have same performance character with low MSE values, with 15322165.19 for training and 15402615.61 for testing, indicating minimal average squared differences between predicted and actual HER performance across the dataset. The prediction results tighly fit the actual dataset as shown in the top side of figure 5. The RMSE values, at 3914.35 for training and 3924.62 for testing, further corroborate this finding, showing relatively small deviations between predicted and actual values. Moreover, the high R-squared values of 0.99999 for training and 0.99999 for testing reveal that the model explains almost all the variance in the data.

4. CONCLUSION

In conclusion, this study demonstrates the effectiveness of ANN in predicting HER performance in DMF assisted water electrolysis. The integration of ANN models with experimental data from DMF-assisted electrolysis provides valuable insights into the complex interplay between magnetic fields and electrochemical processes, revealing significant enhancements in HER rates compared to conventional electrolysis. The ANN models developed exhibit high accuracy in predicting HER performance under varying DMF rotational speeds, as evidenced by low MSE, RMSE, and high R-squared values, highlighting their strong predictive power and reliability. While caution is advised regarding overfitting, future research focusing on techniques like regularization and cross-validation can enhance model generalization. Overall, this study contributes to advancing our understanding of DMF-assisted water electrolysis, laying the foundation for optimizing hydrogen production technologies and addressing the global demand for clean energy through the convergence of AI and energy research.

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