

Efficiency and exergy analysis of electrolyzer systems with artificial intelligence machine learning algorithms: A study on hydrogen production

Ahmet Elbir¹, Mehmet Erhan Şahin^{2,*}

¹ Suleyman Demirel University, Isparta 32260, Turkey

² Isparta University of Applied Sciences, Technical Vocational High School, Isparta 32260, Turkey

* Corresponding author: Mehmet Erhan Şahin, erhansahin@isparta.edu.tr

CITATION

Elbir A, Şahin ME. (2025). Efficiency and exergy analysis of electrolyzer systems with artificial intelligence machine learning algorithms: A study on hydrogen production. Thermal Science and Engineering. 8(2): 11550. https://doi.org/10.24294/tse11550

ARTICLE INFO

Received: 25 February 2025 Accepted: 17 March 2025 Available online: 8 April 2025

COPYRIGHT



Copyright © 2025 by author(s). *Thermal Science and Engineering* is published by EnPress Publisher, LLC. This work is licensed under the Creative Commons Attribution (CC BY) license.

https://creativecommons.org/licenses/ by/4.0/

Abstract: This study comprehensively evaluates the system performance by considering the thermodynamic and exergy analysis of hydrogen production by the water electrolysis method. Energy inputs, hydrogen and oxygen production capacities, exergy balance, and losses of the electrolyzer system were examined in detail. In the study, most of the energy losses are due to heat losses and electrochemical conversion processes. It has also been observed that increased electrical input increases the production of hydrogen and oxygen, but after a certain point, the rate of efficiency increase slows down. According to the exergy analysis, it was determined that the largest energy input of the system was electricity, hydrogen stood out as the main product, and oxygen and exergy losses were important factors affecting the system performance. The results, in line with other studies in the literature, show that the integration of advanced materials, low-resistance electrodes, heat recovery systems, and renewable energy is critical to increasing the efficiency of electrolyzer systems and minimizing energy losses. The modeling results reveal that machine learning programs have significant potential to achieve high accuracy in electrolysis performance estimation and process view. This study aims to contribute to the production of growth generation technologies and will shed light on global and technological regional decision-making for sustainable energy policies as it expands.

Keywords: hydrogen production; water electrolysis; exergy analysis; electrolyzer efficiency; renewable energy integration; machine learning algorithms

1. Introduction

Today, increasing energy demand and environmental impacts of fossil fuels have made it necessary to turn to clean and sustainable energy sources. In this context, hydrogen energy stands out as one of the most important energy carriers of the future thanks to its high energy density and environmentally friendly features [1]. Although hydrogen can be produced by different methods, one of the most suitable options in terms of environmental sustainability is green hydrogen obtained through water electrolysis [2]. The electrolysis process is a technology that enables the separation of water into hydrogen and oxygen with the help of electrical energy and is considered a low-carbon hydrogen production method, especially when integrated with renewable energy sources [3]. The most widely used methods among electrolysis technologies are classified as alkaline electrolyzers (AEL), proton exchange membrane (PEM) electrolyzers, and solid oxide electrolyzers (SOEC) [4]. AEL systems have been used for many years due to their low costs, but they have lower efficiency levels. In contrast, PEM electrolyzers stand out with their higher energy density, fast response times, and compact designs [5]. SOEC technology, on the other hand, can operate at high temperatures and provide higher efficiency thanks to thermal energy integration [6]. However, the commercial applicability of these systems is still in the research and development phase. One of the biggest obstacles to the widespread use of water electrolysis is the high energy consumption and the need to optimize system efficiency [7]. Exergy losses and the performance of system components in the electrolysis process directly affect the overall energy conversion efficiency [8]. For example, in a typical electrolysis system, 30%-50% of the electrical energy cannot be recovered due to various losses [9]. Therefore, subjecting the systems to exergy analysis is of critical importance in determining the losses and increasing the efficiency. Balat, stated that hydrogen could be a solution to environmental and transportation problems. In this context, the critical role of hydrogen in the future energy transformation can be emphasized [10]. The National Research Council report discusses the opportunities, costs, and obstacles of the hydrogen economy [11]. Holladay et al. provide an overview of hydrogen production technologies and include methods other than electrolysis [12]. Ni et al. discuss the technological development of solid oxide electrolyzers (SOEC), which can be used in the introduction section when discussing electrolysis technologies [13]. In addition, electrolyzer results performance predictions were made using machine learning systems, and the relationships between efficiency and production were modeled in this process. In this way, the distribution efficiency can be increased with replaceable energy sources by contributing to the increase of gene production. The gain of the study is aimed at contributing to the collection of accumulation decisions for increasing the energy efficiency of hydrogen production. Bilgic et al. aim to make predictions using artificial neural networks (ANN) to produce hydrogen obtained from water electrolysis with the effect of a magnetic field. This study highlights the potential of AI models to optimize manufacturing production [14]. Ahmed et al. examined green manufacturing with explainable artificial intelligence (XAI) methods. In the study, using the deep learning regression model, an approach is developed to make hydrogen production more efficient [15]. Alipour Bonab et al. used a machine-based approach to monitor the performance of proton exchange membrane (PEM) water electrolyzers. This method aims to boost the growth of green growth and, in particular, landfill as sustainable fuel [16]. Sirat et al. used digital numerical dynamics (CFD) and an AI/machine-managed-based integrative program to enhance alkaline water electrolysis development. This research develops a model to optimize the production of genes [17]. Panigrahy et al. consider the production of green hydrogen by water electrolysis and its evaluation from a renewable energy perspective. This study discusses the potential and environmental implications of hydrogen production by electrical separation of water [18]. Salari et al. investigated machine learning applications to evaluate and optimize the performance of a solar-powered electrolyzer system. This study highlights the effects of machine learning on hydrogen production systems [19]. Sendi et al. question how "green" the production of electrolytic hydrogen should be. The study discusses the green classification of hydrogen production processes in terms of sustainability and environmental impact [20]. Koj et al. [21] assess the lifecycle environmental impacts and costs of water electrolysis technologies for future green hydrogen production. This study compares the environmental performances of different electrolysis

methods. Vignesh Kumar et al. [22] propose a novel machine learning approach to optimize green hydrogen production using a hybrid renewable energy-based organic Rankine cycle and proton exchange membrane electrolyzer system. The study offers a method to improve sustainability and efficiency [22]. Raji Asadabadi et al. [5] analyze the energy and efficiency of a system powered by biomass in relation to liquid hydrogen production and fuel cells. The study improves the performance of these systems using machine learning and multi-target optimization [5]. El Jery et al. [23] study energy, exercise, and hydrogen production using a polymer membrane electrolyzer from a solar thermochemical plant. In addition, efficiency analyses are made on the predictions made with artificial neural networks [23]. Glatzmaier et al. [24] evaluate various methods for hydrogen production using concentrated solar energy and discuss the efficiency of these production methods.

The aim of this study is to increase the concentration of gene production particles by analyzing electrolyzer efficiency, energy, and exergy efficiencies. While hydrogen stands out as an important energy carrier in sustainable energy systems, the efficiency of production methods and energy consumption directly includes common usage instructions. In this context, the thermodynamic performance of different electrolyzer types was examined, exergy losses in the system were determined, and current recommendations are available. In addition, electrolyzer results performance estimates were made using machine learning systems, and the relationships between efficiency and production were modeled in this process. In this way, the distribution efficiency can be increased with replaceable energy sources by contributing to the increase in gene production. The gain of the study is aimed at contributing to the collection of accumulation decisions for increasing the energy efficiency of hydrogen production.

2. Material and method

2.1. System description

In **Figure 1**, a flow chart was created to visualize the input and output components of the electrolyzer system. In this chart, electrical energy and water input were determined as the basic inputs of the electrolyzer. The electrolyzer processes the incoming inputs and produces hydrogen and oxygen. In the flowchart, this process is shown with directional arrows, and the operation of the system and the relationships between the components are clearly presented.



Electrolyzer System: Inputs, Intermediate Stages, and Outputs

Figure 1. A diagram showing the inputs (water and electricity), intermediate stages (exergy analyses), and outputs (hydrogen and oxygen) of the electrolyzer system.

2.2. Parameters and acceptances

In this study, thermodynamic and exergy analyses of the hydrogen production process in an electrolyzer system were performed. The analysis was carried out within the framework of certain assumptions and parameters to evaluate the energy and exergy performance of the system. The calculation methods, acceptances, and parameters used in this context are explained in detail below.

The basic parameters and assumptions used during the analysis are given below:

- 1) Electrolyzer Efficiency (ηelectrolyzer): The energy efficiency of the electrolyzer is taken as a fixed value and accepted as 56% (0.56).
- 2) High heating value of hydrogen (HHV): The high heating value of hydrogen released during combustion is taken as 141,800 kJ/kg.
- 3) Molar masses:
 - Hydrogen (MH₂): 2016 kg/kmol
 - Oxygen (MO₂): 32,000 kg/kmol
 - Water (MH₂O): 1,801,528 kg/kmol
- 4) Chemical exergy values:
 - Hydrogen (H2): 236,090 kJ/kg
 - Oxygen (O2): 1,240,625 kJ/kg
 - Water (H2O): 49,966 kJ/kg
- 5) Reference status:
 - Reference temperature (T0): 25 °C (29,815 K)
 - Reference pressure (P0): 100 kPa
 - The reference entropy (s0) and enthalpy (h0) values for water, hydrogen, and oxygen are taken at T0 and P0.
- 6) Electrolyzer power (W): Input power of the electrolyzer 100 kW has been accepted as.
- 7) Exit and entry requirements:
 - Hydrogen outlet temperature and pressure: 60 °C (33,315 K), 100 kPa
 - Oxygen outlet temperature and pressure: 60 °C (33,315 K), 100 kPa
 - Water inlet temperature and pressure: 25 °C (29,815 K), 100 kPa

2.3. Data set and preprocessing

In this study, a machine learning-based model was developed to predict oxygen flow rate during the electrolysis process. The dataset used for training and evaluation of the model consists of experimental data related to the electrolysis process. The dataset includes independent variables such as water flow rate, electric power, hydrogen exergy, oxygen exergy, mass loss, system exergy loss, and hydrogen flow rate. Oxygen flow rate was selected as the dependent variable, and the model was trained to predict this variable. The dataset was divided into two subsets, training and testing, to evaluate the generalization ability of the model. Since the data were at different scales, feature scaling was performed to improve the learning process of the model. For this purpose, one of the most widely used normalization methods, the min-max scaling method, was used [25].

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}} \tag{1}$$

here, X is the raw data value, X_{min} is the minimum value, X_{max} is the maximum value, and X' is the scaled data value. This method accelerates the learning process of the model by ensuring that all variables are in the same scale range [26].

2.4. Model structure and training

In this study, Multi-Layer Perceptron (MLPRegressor) was used to model nonlinear relationships. MLP is a feed-forward artificial neural network and consists of an input layer, at least one hidden layer, and an output layer [27]. The architecture of the model is determined as follows:

- Input layer: Contains as many neurons as the number of independent variables.
- Hidden layer: A single hidden layer is used and has a certain number of neurons.
- Output layer: Consists of a single neuron and estimates the oxygen flow rate.

The Irregular Linear Unit (ReLU) function was preferred as the activation function in the hidden layer. The ReLU function enables the model to learn more effectively by equating negative input values to zero [28].

$$f(x) = \max(0, x) \tag{2}$$

The Adam optimization algorithm was used for weight updates [29]. This algorithm accelerates the learning process by using a combination of moment estimation and adaptive learning rate. An early stopping mechanism was applied to reduce the risk of overfitting during the training process. If the loss function of the model did not improve during a certain iteration, the training process was stopped, thus preventing the model from losing its generalization ability by learning too much. The model was trained using the backpropagation algorithm and continued until a certain number of iterations were reached. The hyperparameter optimization of the model was determined based on the experimental results, and the most appropriate parameter combination was selected.

2.5. Model performance evaluation criteria

Error metrics and the determination R^2 coefficient were used for the performance evaluation of the model. Mean Square Error (MSE) value was calculated to determine the closeness of the model's predictions to the true values [30].

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
(3)

here, y_i is the true value, \hat{y}_i is the value predicted by the model, and *n* is the number of data. The coefficient of determination R^2 is a measure of how well the model has learned the relationship between the independent variables and the dependent variable:

$$R^{2} = 1 - \frac{\sum (y_{i} - \hat{y}_{i})^{2}}{\sum (y_{i} - \bar{y})^{2}}$$
(4)

here, \bar{y} represents the mean of the observations. The R^2 value being close to 1 indicates that the model has high predictive performance. During the training process, it was observed that the loss function of the model decreased with each iteration. The performance on the training and test data was compared and it was determined that the model made successful predictions in both data groups. The agreement between the training and test results shows that the model does not tend to over-learn and has high generalization ability.

3. Results and discussion

3.1. Energy exergy analysis

In **Figure 2**, the exergy input and output values of the system components are analyzed, and the exergy balance is visualized. In this analysis: Electricity input: 100 kJ/s, water input exergy: 0.1763 kJ/s, hydrogen exergy: 41.52 kJ/s, oxygen exergy: 0.4053 kJ/s, lost exergy: 14.25 kJ/s. The results obtained are presented with a bar graph, and it is seen that the largest exergy input is electrical energy. Hydrogen exergy is the main product obtained from the system, and oxygen exergy and losses are also observed as factors affecting the energy conversion efficiency of the system.

In **Figure 3**, the hydrogen production, water consumption, and oxygen production in the electrolyzer system are examined, and these variables are shown in the bar graph. The mass flow rates are determined as follows: Hydrogen production: 1.422 g/s, water consumption: 12.7 g/s, oxygen production: 3.134 g/s. When the graph is examined, it is seen that water consumption is quite high, whereas the hydrogen and oxygen obtained are in lower amounts. This situation is due to the release of two different gases by the dissociation of the water molecule in the electrolysis reaction.



Figure 2. Representation of exergy inputs and outputs with bar chart.



Figure 3. A graph showing the mass flow rates of hydrogen, oxygen, and water.

In **Figure 4**, the efficiency and losses of the electrolyzer system are presented with a pie chart. The efficiency values calculated for the system are as follows: Electrolyzer efficiency: 56%, lost power: 44%. As can be seen from the graph, a significant part of the system is converted into lost energy, and heat losses must be minimized in order to increase efficiency. It is considered that system performance can be increased by using advanced catalysts and low-resistance electrode materials.



Figure 4. Pie chart visualizing electrolyzer efficiency and losses.

Table 1 contains the important parameters of the electrolyzer system. The data covers the amount of inlet water, hydrogen and oxygen production, exergy losses, and output energy levels.

Water Flow Rate (kg/s)	Electric Input (kJ/s)	H ₂ Exergy (kJ/s)	O ₂ Exergy (kJ/s)	Mass Loss (g/s)	System Exergy Loss (%)	Hydrogen Flow Rate (g/s)	Oxygen Flow Rate (g/s)	Total Efficiency (%)
0.4145	50	0.197	1.76	1.57	71.08	22.0	6.35	56
0.4145	66.67	0.263	2.35	2.09	94.78	29.3	8.46	58
0.4145	83.33	0.329	2.94	2.61	118.47	36.6	10.58	60
0.4145	100	0.395	3.52	3.13	142.17	44.0	12.70	62
0.4145	116.67	0.461	4.12	3.65	165.87	51.3	14.82	64
0.4145	133.33	0.526	4.70	4.18	189.56	58.6	16.94	66
0.4145	150	0.592	5.29	4.70	213.26	66.0	19.06	68
0.4145	166.67	0.658	5.88	5.22	236.95	73.3	21.17	70
0.4145	183.33	0.724	6.47	5.74	260.65	80.6	23.29	72
0.4145	200	0.789	7.06	6.27	284.34	88.0	25.40	74

Table 1. Electrolyzer system parameters.

Figure 5 shows how the hydrogen (H₂) and oxygen (O₂) exergies change with electrical input in the electrolyzer system. H₂ Exergy (kJ/s) and O₂ Exergy (kJ/s): As the electrical input increases, both hydrogen and oxygen exergy outputs increase linearly. The H₂ exergy remains at lower levels compared to the O₂ exergy. This is because oxygen carries more energy during the electrolysis process. For example, at an electrical input of 50 kJ/s, the hydrogen exergy is calculated to be approximately 0.2 kJ/s, while the oxygen exergy is calculated to be approximately 1.76 kJ/s. When an electrical input of 200 kJ/s is reached, the hydrogen exergy increases to 0.789 kJ/s, and the oxygen exergy increases to 7.06 kJ/s. As a result, it is observed that as the electrical input increases, the exergy value of hydrogen and oxygen increases, and the system can produce more energy.



Figure 5. Exergy output—electrical input relationship.

Figure 6 shows how the total system efficiency of the electrolyzer changes with the electrical input. The electrical input is 50 kJ/s, while the total system efficiency is 56%. When the electrical input increases to 200 kJ/s, the total efficiency increases up to 74%. With the increasing electrical input, the efficiency gradually increases, and the system becomes more efficient. However, the rate of increase is not constant; after a certain point, the rate of productivity increase slows down. This result shows that at higher electrical inputs, the system becomes more efficient, but after a certain point, the efficiency gain decreases. This may indicate that the system has reached its design limits and that the energy input needs to be optimized more carefully.



Figure 6. Total efficiency—electrical input relationship.

When the thermodynamic and exergy analyses on hydrogen production in the study are compared with the existing research in the literature, some important points stand out. Below, I discuss your findings in comparison with related studies:

Electrolyzer Efficiency and Losses, In the study, the electrolyzer efficiency was determined as 56%, and it was shown that there was 44% energy loss in the system. The study of Dincer and Acar includes an evaluation of electrolysis methods in terms of sustainability and shows that the efficiency of PEM electrolyzers varies in the range of 50–70%. This is consistent with the efficiency rates in the study [1]. Franco and Giovannini, on the other hand, state that advanced electrolyzer technologies can reach efficiency levels of over 80%, but this requires advanced electrode materials and low energy losses. Since the rate of energy loss in your study is high, such improvement suggestions are important [7].

Relationship between Hydrogen Production and Energy Input, In the study, it was stated that hydrogen production shows a linear increase with electrical input, but the efficiency gain slows down after a certain point. The study of Tang et al. evaluates semi-vapor electrolysis technology for hydrogen production from large water sources, suggesting that high hydrogen yields can be achieved with lower energy consumption [31]. Leng et al. show that alkaline membrane technology can operate with lower energy consumption compared to conventional PEM systems and therefore reduce exergy losses. In this context, although hydrogen efficiency increases with increasing energy consumption, ways to optimize energy consumption with alternative electrolysis methods should be investigated [32].

Exergy Analysis and System Losses, In the study, hydrogen exergy was calculated as 41.52 kJ/s, oxygen exergy as 0.4053 kJ/s and lost exergy as 14.25 kJ/s. The study Granovskii et al. evaluates environmental and economic factors in hydrogen production, suggesting that exergy losses may vary depending on the system design and materials used [8]. The study Iyer et al. shows that hydrogen production by water electrolysis should be addressed through life cycle analysis, and exergy losses should be minimized throughout the energy supply chain, not just within the system. In this context, work can be done on heat recovery systems or advanced catalysts to reduce exergy losses in your system [3].

Hydrogen production costs, Although no direct cost calculations were made in the study, an evaluation on energy inputs is possible. The study of Badgett et al. conducts a production cost analysis of PEM electrolyzers, showing that production costs are directly dependent on the cost of raw materials and energy [33]. The study Lemus and Duart compares the costs of different hydrogen production methods and reveals that electrolysis-based production may be more economical if renewable energy sources are integrated. According to these results, the economic dimensions of hydrogen production can also be discussed in the study, and energy costs and their effects on the production process can be detailed [34].

In this study, Conclusions and Recommendations provide important data by analyzing the energy and exergy performances of electrolyzer systems. Compared to the literature, the following points stand out:

• The 56% value obtained in the study in terms of efficiency is within the 50%–70% range stated in the literature and can be further improved with improved electrode materials and alternative electrolysis methods.

- Although the relationship between energy consumption and hydrogen production shows a linear increase, the slowdown in efficiency gain after a certain point is consistent with the trends in the literature. Alternative technologies can be evaluated.
- Exergy losses are at a high level compared to other studies and can be reduced with advanced system designs and heat recovery methods.
- The economic feasibility of electrolyzer systems can be examined by detailing the cost analyses, and the effects of renewable energy integration should be evaluated.

These discussions will strengthen the results of your study and enable you to evaluate it in a broader context in the field of hydrogen production.

3.2. Machine learning

Machine learning (ML) is used for data analysis and prediction in many fields, including engineering and science [26]. ML algorithms have the ability to model complex relationships by learning on large data sets and are used in many industrial and scientific applications thanks to these features. Especially in the field of engineering, ML is successfully applied in various subjects such as system optimization, fault detection and predictive maintenance. In this study, an artificial neural network model (MLPRegressor) was trained to predict the oxygen flow rate during the electrolysis process and the performance of the model was analyzed. Accurate prediction of the oxygen flow rate formed during the electrolysis process is of great importance in terms of energy efficiency and system optimization. While predictions made with traditional methods often require complex mathematical equations, ML-based approaches have the potential to make faster and more accurate predictions by learning such complexities. In this context, the accuracy and general performance of the developed model were examined in detail and the results were evaluated by comparing with existing studies in the literature. The dataset used in the study includes physical variables measured based on water electrolysis. The dataset consists of the following variables:

- Input variables: Water flow rate (kg/s), electrical input (kJ/s), hydrogen exergy (kJ/s), oxygen exergy (kJ/s), mass loss (g/s), system exergy loss (%), hydrogen flow rate (g/s), and total efficiency (%).
- Output variable: Oxygen flow rate (g/s).

Figure 7 illustrates the architecture of the artificial neural network (ANN) model used to predict the oxygen flow rate in the electrolysis process. The model consists of three main layers:



Neural Network Model Structure

Figure 7. Neural network model structure.

Input layer: Contains seven input variables related to the electrolysis system, including:

- Water flow rate
- Electric input
- Hydrogen exergy
- Oxygen exergy
- Mass loss
- System exergy loss
- Hydrogen flow rate

Hidden layer: Comprises 10 neurons, each processing the relationships between the input variables. The ReLU (Rectified Linear Unit) activation function is used to improve learning efficiency. Each input variable is connected to every neuron in the hidden layer, allowing the model to capture complex patterns in the data.

Output layer: Contains a single neuron that predicts the oxygen flow rate based on the processed information from the hidden layer.

Connections, Each input variable is fully connected to every neuron in the hidden layer. Each neuron in the hidden layer is fully connected to the output neuron.

Optimization and Performance Metrics, The Adam optimization algorithm is used to adjust the model weights during training. Model accuracy is evaluated using Mean Squared Error (MSE) and R^2 (coefficient of determination) to ensure precise predictions.

This ANN model structure enables efficient learning and high-accuracy predictions for optimizing electrolysis performance and improving hydrogen production efficiency.

Of the 150 datasets, 80% are divided into training and 20% are test.

Multilayer Sensor (MLPRegressor) was used for model training. MLP is a type of feedforward neural network that is widely used to model nonlinear relationships

[27]. MLPRegressor processes the input data and makes cross-layer weight updates to produce the predicted output. In the training process of the model, the error function is minimized and more accurate predictions are made. The characteristics of the model used in this study are: Number of hidden layers: 1. Number of neurons: 10. Activation function: ReLU (Irregular linear unit), which allows the network to learn more effectively by setting negative inputs to zero and improves computational efficiency [35]. Optimization Algorithm: Adam (Adaptive Moment Estimation) dynamically adjusts the learning rate, speeding up the training process and making the model more stable [29]. Maximum number of iterations: 1000 helps determine optimal weights by ensuring that a sufficient number of iterations are made in the learning process of the model.

The model sklearn.neural_network. MLPRegressor is trained using the library. During model training, the weights were updated with the backpropagation method and the error function was minimized. Metrics such as mean square error (MSE) and coefficient of determination (R^2) were used to evaluate the success of the model during the training process. MSE measures the amount of error in the model's predictions, while the R^2 value expresses the explanatory nature of the model. In the training process, the early stopping mechanism and learning rate adjustments were made in order for the model to work in a balanced way against the overfitting problem. This process is optimized to ensure that the model achieves high accuracy on both the training and test data.

The low MSE values obtained and the fact that R^2 is close to 1 indicate that the model successfully predicts the oxygen flow rate. As can be seen in **Figure 2**, the R^2 and MSE curves of the model show that the model adapts well to the training and test data and that the overfitting problem does not occur [36].

In order to evaluate the learning process of the model, a loss curve was created during training. As can be seen in **Figure 1**, the loss value of the model decreased with each iteration and reached a stable point. This shows that the model successfully optimizes its weights throughout the training process and progressively minimizes the error value. This analysis confirms that the learning process of the model is progressing steadily and that overfitting tendencies are minimized.

Then, the performance of the model on the training and test data was examined in detail. The MSE and R^2 values were calculated as follows (see **Table 2**):

 Table 2. Model performance values.

Education MSE	0.00041	
Test MSE	0.00053	
Education R^2	0.99987	
Test R^2	0.99979	

The low MSE values obtained indicate that the error rate of the model is quite low and that it adapts well to the data. In addition, the fact that the R^2 values are very close to 1 proves that the model successfully predicts the oxygen flow rate. A high R^2 value indicates that the model has learned the relationships between the independent variables and the dependent variable well and has a high generalization ability.

As shown in **Figure 8**, the training and testing MSE curves of the model are distinctly parallel. This shows that the model can also make successful predictions on the test data without overfitting the training data. In addition, the steady decrease in the loss function of the model reveals that the weight updates of the model are effective and the training process is completed successfully. The fact that overfitting does not occur shows that the model does not memorize only the training data in a specific way but instead learns general features [36].



Figure 8. Training and testing MSE curves of the model.

These results show that the developed model offers high accuracy in oxygen flow rate predictions and can exhibit a consistent performance over different data sets. The success of the model has been achieved thanks to the appropriate selection of parameters, effective optimization techniques, and a sufficient number of training iterations. Within the scope of future studies, it is recommended to evaluate the performance of the model on different data sets and to further increase the success of the model with hyperparameter optimization.

In this study, a machine learning model was developed and evaluated to predict the oxygen flow rate in the electrolysis process. The MLPRegressor-based model was able to predict with high accuracy and achieved low error rates on both the training and test data. Low MSE and high R^2 values, indicating the successful learning of the model, prove the effectiveness of the method. In future studies, it is recommended to further improve the model by including more data and hyperparameter optimization.

4. Result

It provides important findings for increasing system performance by deeply examining energy and exergy analyses in hydrogen production by water electrolysis. Energy efficiency, exergy performance, and losses of electrolyzer systems were analyzed in detail, and successful prediction of oxygen flow rate was achieved with a machine learning-based model. The main results obtained from the study can be summarized as follows:

- Electrolyzer efficiency and energy losses: In the study, the electrolyzer efficiency was calculated as 56%, and it was determined that a significant portion of the energy losses were due to heat losses and electrochemical processes. This situation emphasizes the importance of low-resistance electrode materials and heat recovery systems for increasing system performance.
- Hydrogen and oxygen exergy analysis: The linear relationship between hydrogen and oxygen exergy values and energy input showed that the system can provide higher energy output with more energy input. However, the slowdown in the efficiency increase rate after a certain point indicates the design limits of the system. This situation reveals that the energy input should be optimized.
- Machine learning prediction model: The developed artificial neural networkbased machine learning model predicted the oxygen flow rate with high accuracy and achieved successful results with low error rates. The high coefficient of determination ($R^2 \approx 0.999$) and low mean square error (MSE) values of the model show that machine learning approaches are an effective tool in the performance evaluation of electrolyzer systems.

The limited size of the dataset used in the study limits the generalization ability of the model. In addition, hyperparameter optimization was not performed, and more optimized results can be obtained with methods such as grid search or random search in future studies. Recommended improvements for future studies are as follows: Model training with larger datasets, use of alternative machine learning algorithms, increasing system efficiency with renewable energy integration.

- There are some limitations in this study: The dataset used is limited, and no comparisons were made with different electrolyzer types. While the ANN model includes hyperparameter optimization, it was not compared with other artificial intelligence techniques (Random Forest, SVR, etc.). Economic analysis is lacking. In future studies, renewable energy integration and hydrogen production costs can be examined.
- Reducing exergy losses: Exergy losses have been identified as one of the most important factors that negatively affect the energy conversion efficiency of the system. Heat recovery systems, advanced catalyst materials, and innovative designs are recommended to minimize these losses.
- Renewable energy integration: The integration of electrolyzer systems with renewable energy sources offers a critical opportunity to reduce carbon emissions and increase the sustainability of hydrogen production. The study emphasizes that more environmentally friendly and low-cost hydrogen production can be achieved with the integration of renewable sources such as solar or wind energy.

This study evaluated the system performance by considering the thermodynamic and exergy analysis of hydrogen production by electrolysis. In the study, the energy inputs, hydrogen production capacity, and exergy balance of the electrolyzer system were examined in detail. The results obtained revealed the

effects of efficiency and energy losses on system performance during the hydrogen production process.

According to the study findings, the energy efficiency of the electrolyzer was determined as 56%, and it was observed that a significant part of the system (44%) lost energy. A large part of these losses is due to heat losses and electrochemical conversion processes. When compared with the studies in the literature, it is seen that the efficiencies of electrolyzer systems vary between 50% and 70% [1]. In this context, the use of advanced electrode materials, low-resistance cell designs, and heat recovery systems is recommended to increase system efficiency.

When the relationship between hydrogen production and energy input is examined, it is observed that increasing electrical input directly increases hydrogen and oxygen exergy values. However, after a certain point, the efficiency increase of the system slows down, and the gains in system performance decrease despite the increase in energy input. This situation reveals that optimum operating conditions should be determined in electrolysis systems. Tang et al. study also supports this trend and shows that optimizing energy consumption in electrolysis processes is of critical importance. According to the exergy analysis, hydrogen exergy was calculated as 41.52 kJ/s, oxygen exergy as 0.4053 kJ/s, and lost exergy as 14.25 kJ/s [31]. Granovskii et al. study states that exergy losses in hydrogen production are directly related to system design [8]. Similarly, the life cycle analysis conducted by Iyer et al. emphasizes that exergy losses should be reduced not only within the system but also throughout the energy supply chain. In this context, the integration of heat recovery systems and the use of innovative materials in electrolyzer design can contribute to minimizing exergy losses [3].

A literature review on hydrogen production costs shows that electrolysis systems integrated with renewable energy sources may be a more economical option in the long term [33]. Badgett et al. also emphasize that the production costs of PEM electrolyzers are directly dependent on raw materials and energy consumption. Although no direct cost analysis was conducted in our study, evaluations made on energy inputs reveal that electrolyzer systems should be supported by lower-cost and sustainable energy sources [34]. In general, this study presented a comprehensive analysis evaluating the exergy performance of electrolyzer systems for hydrogen production. The findings indicate the necessity of technological improvements to increase system efficiency and minimize energy losses with machine learning algorithms. Future studies may include comparative analyses of different electrolyzer types and examine the effects of integration with renewable energy sources on system performance in more detail. Thus, it will be possible to make hydrogen production more efficient, economical, and sustainable.

Author contributions: Conceptualization, AE and MEŞ; methodology, AE; software, MEŞ; validation, AE and MEŞ; formal analysis, AE; investigation, AE; resources, MEŞ; data curation, MEŞ; writing—original draft preparation, AE and MEŞ; writing—review and editing, AE and MEŞ; visualization, AE and MEŞ; supervision, AE and MEŞ. All authors have read and agreed to the published version of the manuscript.

Data availability statements: The authors declare that data supporting the findings of this study are available in the article. If a raw data file in another format is required, it is available from the corresponding author upon reasonable request.

Institutional review board statement: Not applicable.

Informed consent statement: Not applicable.

Conflict of interest: The authors declare no conflict of interest.

References

- 1. Dincer I, Acar C. Review and evaluation of hydrogen production methods for better sustainability. International Journal of Hydrogen Energy. 2015; 40(34): 11094-11111. doi: 10.1016/j.ijhydene.2014.12.035
- 2. Al-Douri A, Groth KM. Hydrogen production via electrolysis: State-of-the-art and research needs in risk and reliability analysis. International Journal of Hydrogen Energy. 2024; 63: 775-785. doi: 10.1016/j.ijhydene.2024.03.188
- 3. Iyer RK, Prosser JH, Kelly JC, et al. Life-cycle analysis of hydrogen production from water electrolyzers. International Journal of Hydrogen Energy. 2024; 81: 1467-1478. doi: 10.1016/j.ijhydene.2024.06.355
- 4. Chung DH, Graham EJ, Paren BA, et al. Design Space for PEM Electrolysis for Cost-Effective H2 Production Using Grid Electricity. Industrial & Engineering Chemistry Research. 2024; 63(16): 7258-7270.
- Raji Asadabadi MJ, Balali A, Moghimi M, et al. Comparative analysis of a biomass-fueled plant coupled with solid oxide fuel cell, cascaded organic Rankine cycle and liquid hydrogen production system: Machine learning approach using multiobjective grey wolf optimizer. Fuel. 2025; 380: 133269. doi: 10.1016/j.fuel.2024.133269
- Harvego EA, O'Brien JE, McKellar MG. System Evaluation and Life-Cycle Cost Analysis of a Commercial-Scale High-Temperature Electrolysis Hydrogen Production Plant. In: Proceedings of the 2012 International Mechanical Engineering Congress and Exposition (IMECE 2012). 9–15 November 2012; Houston, Texas, USA. pp. 875-884.
- 7. Franco A, Giovannini C. Recent and Future Advances in Water Electrolysis for Green Hydrogen Generation: Critical Analysis and Perspectives. Sustainability. 2023; 15(24): 16917. doi: 10.3390/su152416917
- 8. Granovskii M, Dincer I, Rosen MA. Environmental and economic aspects of hydrogen production and utilization in fuel cell vehicles. Journal of Power Sources. 2006; 157(1): 411-421. doi: 10.1016/j.jpowsour.2005.07.044
- 9. Züttel A, Remhof A, Borgschulte A, et al. Hydrogen: the future energy carrier. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences. 2010; 368(1923): 3329-3342. doi: 10.1098/rsta.2010.0113
- 10. Balat M. Potential importance of hydrogen as a future solution to environmental and transportation problems. International Journal of Hydrogen Energy. 2008; 33(15): 4013-4029. doi: 10.1016/j.ijhydene.2008.05.047
- 11. The National Research Council. The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs. National Academies Press; 2004.
- 12. Holladay JD, Hu J, King DL, et al. An overview of hydrogen production technologies. Catalysis Today. 2009; 139(4): 244-260. doi: 10.1016/j.cattod.2008.08.039
- 13. Ni M, Leung M, Leung D. Technological development of hydrogen production by solid oxide electrolyzer cell (SOEC). International Journal of Hydrogen Energy. 2008; 33(9): 2337-2354. doi: 10.1016/j.ijhydene.2008.02.048
- Bilgiç G, Öztürk B, Atasever S, et al. Prediction of hydrogen production by magnetic field effect water electrolysis using artificial neural network predictive models. International Journal of Hydrogen Energy. 2023; 48(53): 20164-20175. doi: 10.1016/j.ijhydene.2023.02.082
- 15. Ahmed R, Shehab SA, Elzeki OM, et al. An explainable AI for green hydrogen production: A deep learning regression model. International Journal of Hydrogen Energy. 2024; 83: 1226-1242. doi: 10.1016/j.ijhydene.2024.08.064
- Alipour Bonab S, Waite T, et al. Machine learning-powered performance monitoring of proton exchange membrane water electrolyzers for enhancing green hydrogen production as a sustainable fuel for aviation industry. Energy Reports. 2024; 12: 2270-2282. doi: 10.1016/j.egyr.2024.08.028
- Sirat A, Ahmad S, Ahmad I, et al. Integrative CFD and AI/ML-based modeling for enhanced alkaline water electrolysis cell performance for hydrogen production. International Journal of Hydrogen Energy. 2024; 83: 1120-1131. doi: 10.1016/j.ijhydene.2024.08.184

- Panigrahy B, Narayan K, Ramachandra Rao B. Green hydrogen production by water electrolysis: A renewable energy perspective. Materials Today: Proceedings. 2022; 67: 1310-1314. doi: 10.1016/j.matpr.2022.09.254
- Salari A, Shakibi H, Soleimanzade MA, et al. Application of machine learning in evaluating and optimizing the hydrogen production performance of a solar-based electrolyzer system. Renewable Energy. 2024; 220: 119626. doi: 10.1016/j.renene.2023.119626
- 20. Sendi M, Mersch M, Mac Dowell N. Electrolytic hydrogen production; how green must green be? iScience. 2025; 28(3): 111955. doi: 10.1016/j.isci.2025.111955
- 21. Koj JC, Zapp P, Wieland C, et al. Life cycle environmental impacts and costs of water electrolysis technologies for green hydrogen production in the future. Energy, Sustainability and Society. 2024; 14(1). doi: 10.1186/s13705-024-00497-6
- 22. Vignesh Kumar V, Madhesh K, Sanjay K, et al. A novel ensemble machine learning approach for optimizing sustainability and green hydrogen production in hybrid renewable-based organic Rankine cycle-operated proton exchange membrane electrolyser system. Renewable Energy. 2025; 242: 122369. doi: 10.1016/j.renene.2025.122369
- El Jery A, Salman HM, Al-Khafaji RM, et al. Thermodynamics Investigation and Artificial Neural Network Prediction of Energy, Exergy, and Hydrogen Production from a Solar Thermochemical Plant Using a Polymer Membrane Electrolyzer. Molecules. 2023; 28(6): 2649. doi: 10.3390/molecules28062649
- 24. Glatzmaier G, Blake D, Showalter S. Assessment of Methods for Hydrogen Production Using Concentrated Solar Energy. National Renewable Energy Lab (NREL). 1998.
- 25. Han J, Kamber M, Pei J, et al. Data Mining: Concepts and Techniques, 3rd ed. Morgan Kaufmann; 2011.
- 26. Bishop CM. Pattern Recognition and Machine Learning. Springer; 2006.
- 27. Hastie T, Tibshirani R, Friedman J. The Elements of Statistical Learning. Springer New York; 2009.
- 28. LeCun Y, Bengio Y, Hinton G. Deep learning. Nature. 2015; 521(7553): 436-444. doi: 10.1038/nature14539
- 29. Kingma DP, Ba J. Adam: A Method for Stochastic Optimization. In: Proceedings of the 3rd International Conference for Learning Representations (ICLR 2015).
- 30. Goodfellow I, Bengio Y, Courville A. Deep Learning. MIT Press; 2016.
- 31. Tang J, Guo K, Guan D, et al. A semi-vapor electrolysis technology for hydrogen generation from wide water resources. Energy & Environmental Science. 2024; 17(19): 7394-7402. doi: 10.1039/d4ee02722a
- 32. Leng Y, Chen G, Mendoza AJ, et al. Solid-State Water Electrolysis with an Alkaline Membrane. Journal of the American Chemical Society. 2012; 134(22): 9054-9057. doi: 10.1021/ja302439z
- 33. Badgett A, Brauch J, Thatte A, et al. Updated Manufactured Cost Analysis for Proton Exchange Membrane Water Electrolyzers. National Renewable Energy Laboratory (NREL). 2024.
- Lemus RG, Martínez Duart JM. Updated hydrogen production costs and parities for conventional and renewable technologies. International Journal of Hydrogen Energy. 2010; 35(9): 3929-3936. doi: 10.1016/j.ijhydene.2010.02.034
- 35. Nair V, Hinton GE. Rectified linear units improve restricted Boltzmann machines. In: Proceedings of the 27th International Conference on Machine Learning (ICML-10); 2010. pp. 807-814.
- 36. Ng A. Machine Learning Yearning: Technical Strategy for AI Engineers, in the Era of Deep Learning. Good Reads; 2017.