www.dergipark.gov.tr
ISSN:2148-3736

El-Cezerî Journal of Science and Engineering
Vol: 10, No: 1, 2023 (137-146)
DOI :10.31202/ecjse.1172965

ECJSE

Research Paper

Modeling of Artificial Neural Networks for Hydrogen Production via Water Electrolysis

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Received: 11.09.2022 **Accepted:** 11.01.2023

Abstract: Artificial neural networks (ANN) have emerged as a promising tool for estimating hydrogen production process variables for reaction condition optimization. The objective of the study was to predict complex nonlinear systems using ANN for modeling hydrogen production by water electrolysis and to evaluate the common challenges encountered. To estimate the effect of different electrolyzer systems input parameters such as electrolyte material, electrolyte type, supplied power (voltage and current), temperature, and time on hydrogen production, a predictive model was developed. The percentage contributions of the input parameters to hydrogen production and the best network architecture to minimize computation time and maximize network accuracy were shown. The results show that the hydrogen production parameters from electrolysis and the predicted safety explosive limit are 7% of the average Root Mean Square Error (RMSE). Furthermore, the coefficient of determination value was found 0.93. This predicted value is very close to the observed values. The neural network algorithm developed in this study could be used to make critical decisions in the electrolysis process for parameters affecting hydrogen production.

Keywords: Artificial Neural Networks, Hydrogen Production, Water electrolysis

1. Introduction

Hydrogen production has become more and more important to meet the increasing demand for renewable energy. Hydrogen is a non-toxic fuel that fuel cells can easily convert into electricity. When compared to conventional fuels, hydrogen has the highest energy content per unit mass and can be used in place of hydrocarbons [1]. Hydrogen has an energy density of 140 MJ/kg, which is 2.75 times that of hydrocarbon fuels (50 MJ/kg) [2]. The combustion process is non-polluting to the environment and can be used in fuel cells to generate both electricity and valuable heat. In nature, hydrogen does not exist as a single element but must be synthesized from the compounds that make it up. Hydrocarbon pyrolysis, hydrocarbon reforming, biomass processing, and water splitting are the four primary methods for producing hydrogen [3].

One of the most appealing features of hydrogen is its ease of production from water, which is abundant in nature. For hydrogen production from water splitting, there are water electrolysis (WE) processes available, including alkaline WE, proton exchange membrane WE, solid oxide WE, and alkaline anion exchange membrane WE [4]. Typically hydrogen production via WE is the process of converting water into hydrogen and oxygen by passing a direct current from the cathode and anode electrodes in the electrolyte to each other [4,5,6,7].

How to cite this article
Bilgiç, G., Öztürk, B., "Modeling of Artificial Neural Networks for Hydrogen Production via Water Electrolysis", El-Cezerî Journal of Science and Engineering, 2023, 10 (1); 137-146.
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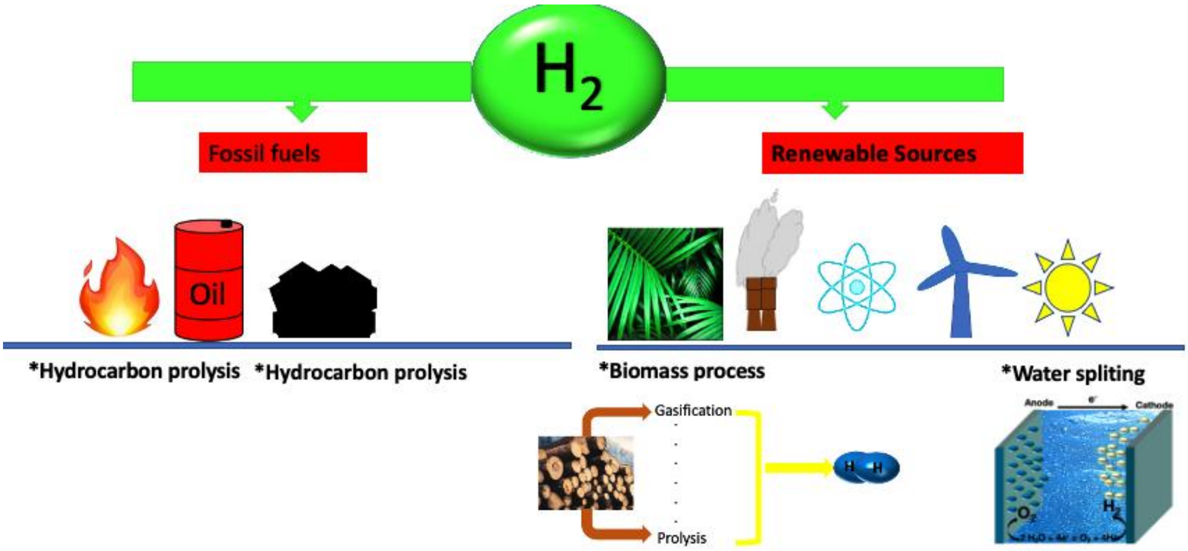

Figure 1. Production process of hydrogen

Water is the reactant in the WE process, and under the influence of a direct current, it is dissociated into hydrogen and oxygen. During alkaline WE, the anode releases oxygen, and the cathode emits hydrogen [8]. The following reaction couples are listed;

Cathodic reaction: $2H_2O+2e^-= H_2+2OH^-$ (1)

Anodic reaction: $2OH= {}^1/_2\, O_2^- + H_2O+2e^-$ (2)

Overall reaction: $H_2O= H_2+ {}^1/_2\, O_2$ (3)

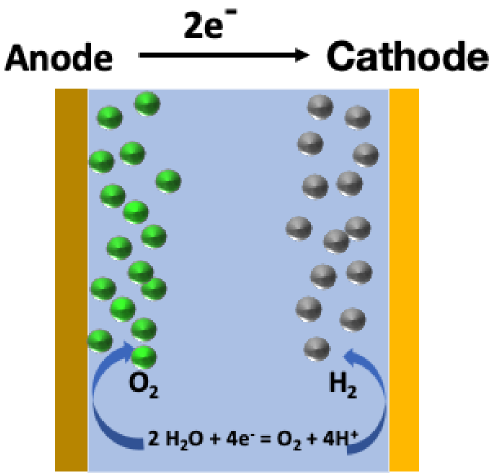

Figure 2. Systematic view of the water electrolysis process

Water is basically broken down into hydrogen and hydroxyl ions (H+ and OH-). By picking up electrons and forming hydrogen molecules, hydrogen ions migrate towards the cathode, the negative electrode. Water electrolysis is a great and practical way to get high-purity hydrogen. WE-generated hydrogen has a high purity (99.9%) and can be used as a reactant in a variety of industrial processes [9]. WE, on the other hand, is not widely used due to its low efficiency in comparison to fossil fuel reforming [3].

ANN systems are increasingly being used in fields that require output prediction based on input parameter specifications that are limited or incomplete. ANN is a modeling system that simulates the human brain's learning process by mathematically modeling the network structure of interconnected nerve cells [10]. ANNs are data-driven systems that have no prior knowledge of the events that govern the process. These data-driven systems examine existing relationships between input and output parameters in an attempt to identify the influences governing process output. An input layer, one or more hidden layers, and an output layer are the three layers that make them up [11]. The hidden layer neurons aid the network in creating the complex connections between the parameters of input and output. [12]. ANNs are a nonlinear statistical model and an effective tool for representing complex nonlinear systems, as opposed to traditional modeling tools [10, 11].

In recent years, ANN has received much attention for predicting hydrogen production because it has several advantages like efficiency, generalization, and simplicity [13]. The papers are separated into four groups: studies on the applications of ANN to modeling the hydrogen generation process, evaluation of ANNs in comparison to other modeling approaches, consideration of hybrid ANN-optimization approaches, and lastly hardware-implemented ANN models [14]. The fundamental benefit of utilizing ANNs in the production of hydrogen is that they are composed of numerous processing components connected by multiple weighted couplings. There are many neurons carrying a specific piece of information in these connections, which are scattered representations of input and output data from hydrogen synthesis. These neurons are able to handle and correct data with great computational power due to their batch behaviour.

Zamaniyan et al. [15] created a three-layer ANN to model an industrial hydrogen production plant. The researchers created a network of four input neurons and three output neurons for the plant's production. Input parameters of this network; were temperature, pressure, steam-carbon ratio, and carbon dioxide-methane ratio, while output parameters were temperature, hydrogen mole fraction, and the carbon monoxide mole fraction of hydrogen product. The proposed neural network by the researchers was trained using gradient descent algorithm and in the hidden and output layers, the tangential sigmoid transfer function was used. While determining the appropriate number of neurons in the hidden layer, the Mean Square Error (MSE) value was taken into account and it was chosen as 5 because it gives the lowest calculated MSE value of 0.00045.

In a continuous fermenter reactor, Nasr et al. [16] constructed an ANN with a three-layer feed-forward back-propagation for the production of biohydrogen from the starch wastewater industry. Organic loading rate (OLR), pH, and volatile suspended solids (VSS) yield were the network inputs. The hydrogen production rate (HPR) was the network output. Using empirical data gathered during a six-month period when starch wastewater was utilized to power an up-flow anaerobic staged reactor, the model was trained, validated, and tested (UASR). The Levenberg-Marquardt algorithm with a 3-8-4-1 network structure was used to train the model. The weights between neurons were then changed at each cycle by backpropagating across the network after calculating the MSE between the experimental data and the corresponding predicted data. This cycle was repeated until the error between experimental and predicted data was minimized. The transfer functions between input and hidden layer-1, between hidden layer-1 and hidden layer-2, and between hidden layer-2 and output layer were linear, tan-sigmoid, and log-sigmoid, respectively. An average R^2 of 0.945, 0.652, and 0.791 was obtained for the train, validation, and test data points, respectively. The researchers claim that it is possible to predict the complex nonlinear forms of HPR using the well-established model ANN.

Nasr et al [17], established a ANN to forecast the temporal variation of hydrogen generation profile in batch reactors. A feed-forward neural network with backpropagation algorithm model was consisted of 5-6-4-1. 313 data points from 26 published experiments were used to train the model.

The initial pH, initial biomass concentration (X_o), initial substrate concentration (S_o), time (t).and temperature (T) were the ANN inputs. Hydrogen production is an output parameter. The log-sigmoid transfer function was used between the input and hidden layer 1 and hidden layer 1, linear transfer function was used between hidden layer 2 and the output layer. For the training, validating, and testing data points, respectively, correlation coefficients of 0.988, 0.987, and 0.996 were obtained, as well as MAEs of 1.89 mL, 6.16 mL, and 4.89 mL. With a R^2 of 0.976, the results demonstrated that the trained ANN was successful in predicting the hydrogen production profile over time for new data.

Karaci et al. [18], developed a back propagation neural network (BPNN) to predict the hydrogen gas production from waste pyrolysis. Three different wastes were studied by the researchers: tea trash, olive husks, and cotton cocoon shells. Additionally, they investigated the impacts of several catalysts, such as $ZnCl_2$, $NaCO_3$, and K_2CO_3. The network input parameters were product type, catalyst type, catalyst amount, and future. The rate of creation of hydrogen-rich gas was the only output of the network. The researchers determined that 13 neurons were the appropriate number for the hidden layer based on the MSE results. They used 102 experimental data points to train the network, 33 for testing, and 33 more for validation. For the training, validating, and testing phases, their model achieved R_2 values of 0.975, 0.955, and 0.905, respectively. These findings show a strong correlation between the model's anticipated values and the values attained through experimentation.

Whatever method is used, some production environment parameters must be determined in order to maximize the hydrogen production rate. Artificial intelligence methods, particularly ANN, have gained attention for this purpose due to their ability to deal with unknown conditions. However, most ANN studies on hydrogen production in the literature focus on hydrocarbon-based hydrogen production. There is a significant gap in ANN research on hydrogen production via water electrolysis. With the motivation from this gap in the literature, in this study, hydrogen production prediction was made by ANN in water electrolysis. Electrolyte material, electrolyte type, time, surface area, temperature, and supplied power, were used as input parameters and hydrogen production was used as the only output. Results, the error rate and coefficient of determination (R^2) were determined, and it was seen that the actual data and the estimated values matched very well with R^2=0.93. It represents the initial stage of water electrolysis and provides a good idea of the enormous potential of such models in this area. However, more experimental data to increase the database will be helpful for ANN training in the future and for enhancing the created models. This research will make a substantial contribution to the study of hybrid solutions. Finally, the process can be optimized and controlled using the proposed ANN models.

2. Materials Methods

2.1. Experimental Data Collection

The 104 data extracted from collected literature were used to develop the ANN model [19]. While preparing the data set, studies that produce hydrogen using the alkaline water electrolysis method were selected. The different inputs were selected for single output to obtain the best fit model and so reduce the high complexity of the model. In this work, selected independent parameters for the models are electrolyte material, electrolyte type, time, temperature, surface area, and supplied power, while the output data was total hydrogen production flow (mL/min). An ANN with an 6-8-12-1 configuration was used as the model. The model had six input neurons and a single output neuron that represented the single outcome, the rate of hydrogen production. The model had two hidden layers.

2.2. Methodology of ANN architecture

The Python program was used to create the ANN and train it in this case. Designing ANN models using Python software generally follows five steps: 1. collecting data, 2. preprocessing data randomizing data into training, 3. building the network, 4. training, and 5. testing the model. The testing, and training of ANN were executed as an electrolyte material, electrolyte type, time, surface area, temperature, and supplied power given to the model as inputs, and the H_2 value was taken as output.

In this model ANN, the following data were used: the 104 experimental data for the training and 20 experimental data, which the network has never seen before, for the tests. The training set was used to calculate the gradient and update the network weights and biases while the test set was used to evaluate the model's suitability [20]. These data were distributed at random using a Python program. The number of neurons in the output layer should match the findings of the experiments. As a result, the constructed ANN model outputs the H_2 ratio and has one neuron in the output layer. Data is always routed from the input layer to the output layer. As a result, interconnected sets of ANN were created using the same input data sets but mapping to different output data [21].

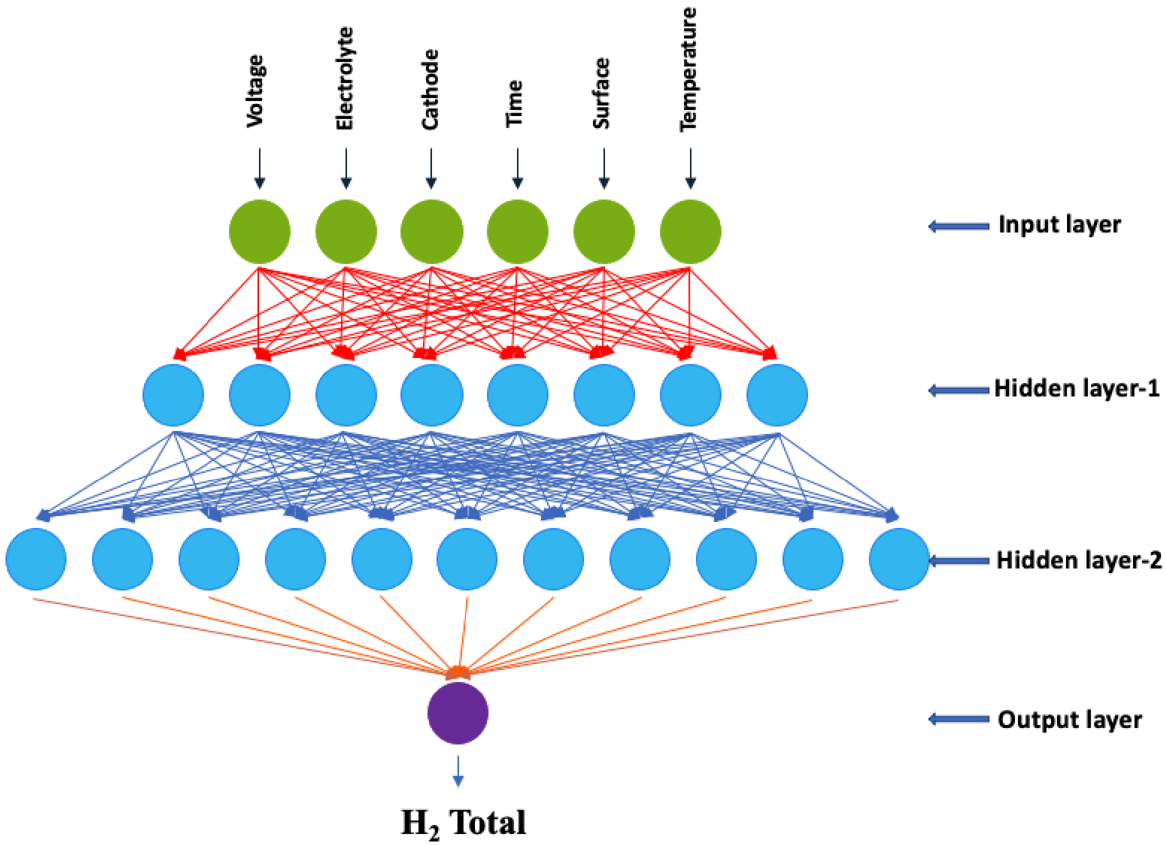

Figure 3. Schematic representation of the general topology of a multilayer structure of an ANN

Figure 3 shows the ANN structure used in the model, the hidden layers, and the neurons in the layers. Shown are the six input variables with their neurons, were interlinked from each input to all hidden layer neurons along with the calculated weightings. The weighted outputs were then merged and fed into the output neuron to form the output values. ReLU transfer functions are used in both hidden layers. The purelin (linear) activation function is used in the output layer. While the number of epochs is 117 in the ANN model, the batch size is 5. To test the robustness and predictability of the models, the data sets in the ANN model were randomly divided into training (80%) and test (20%) subsets from the available database [15]. Because the database was small, the validation and test sets were the same. The outputs of each ANN were compared to experimental data targets reported by references. The performance of the various ANNs was statistically measured using the regression coefficient (R^2) and the experimental values and network predictions.

3. Results and Discussion

3.1. Performance Analysis of ANN Models

Figures 4 show the performance of the 6-8-12-1 Adam (learning rate=1e-3) regularization trained networks in terms of predicting hydrogen production from water electrolysis. The observed hydrogen yield for each of the experimental runs, as shown in Figure 4, is close to the predicted values, as indicated by the regression plot. This means that the 6-8-12-1 trained ANN model is capable of learning the non-linear relationship between the input and output parameters of the water electrolysis reaction, resulting in a well-generalized prediction.

The performance of neural network models was evaluated using mean absolute percentage error (MAPE), root mean square error (RMSE), coefficient of correlation (R^2), and mean square error (MSE). RMSE measures prediction error and provides a summary of overall model performance, whereas r is a commonly used model goodness of fit criterion. Lower RMSE values indicate that the model is working properly. A well-trained model should have an R^2 value close to one and as little error as possible [22]. Table 1 shows the performance metrics of the ANN model. RMSE value is 0.077 in the model.

Table 1. Performance Metrics

R^2 SCORE	0.9361
MSE	0.0060
RMSE	0.0774
MAE	0.05631
MAPE	0.6627

Coefficient of determination (R^2)

A figure of merit that measures how well the model fits the data is the coefficient of determination. [23]. Eq. (4) provides the mathematical formula for the coefficient of determination:

$$R^2=1-\frac{\sum_{i=1}^{N}\left(Y_{measured,\,i}-Y_{predicted,i}\right)^2}{\sum_{i=1}^{N}\left(Y_{measured,\,i}-\overline{Y_{measured,i}}\right)^2} \tag{4}$$

where N is the number of features, $Y_{measured,i}$ is the actual measured value for feature i, $\overline{Y_{measured,i}}$ is the average of all measured values $Y_{predicted,i}$ is the predicted value for feature i.
Here R^2 is a used criterion for the goodness of fit for the model. A well-trained model should have an R^2 value close to one and as little error as possible. The regression plot (R^2) is depicted in Figure 4. The data points in the graph from observed and predicted hydrogen production revealed that they

were closely related. A high R^2 of 0.936 indicates that the Adam (learning rate=1e^{-3}) regularization-trained multilayer perceptron ANN model can learn and generalize 93 percent of datasets. The performance of a training algorithm is largely determined by how well it can learn and train the input model and the targeted parameters. According to the graph, the actual and estimated hydrogen yields are very close. This demonstrated that ANN is a reliable technique for modeling a process with a nonlinear relationship. To estimate the hydrogen yield, a near-perfect R^2 of 0.9361 was obtained (see Figure 4).

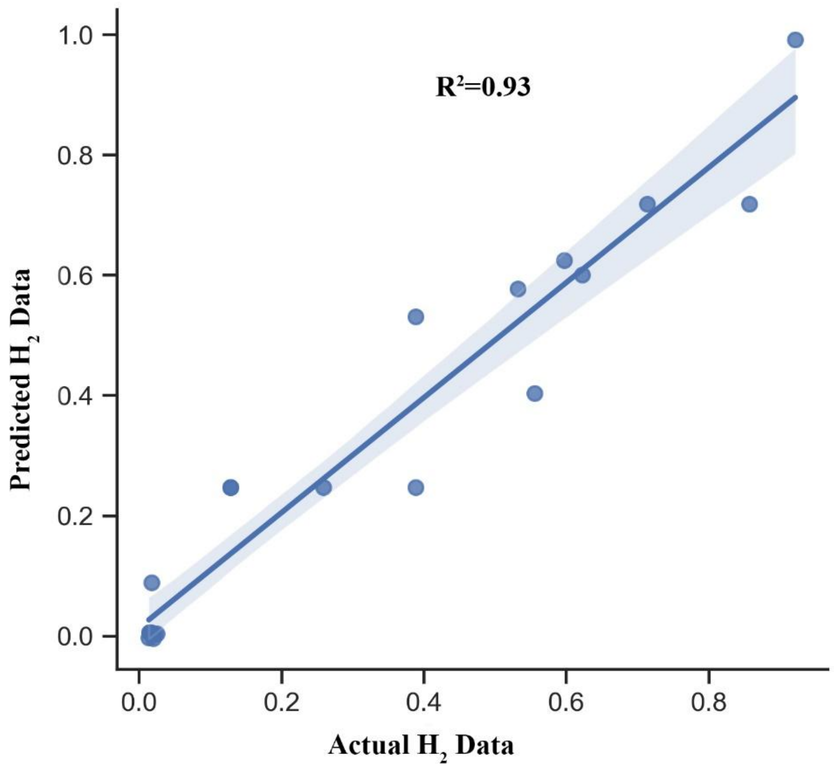

Figure 4. Comparison of the experimental results and predicted results derived from the ANN model

3.2. Kernel Density Estimation (KDE)

A non-parametric technique for estimating the probability density function of a variable is called kernel density estimation (KDE) [24]. The density plot depicts how data are distributed across an ongoing period of time. The kernel smoothing method is used in this graph, which is a variation on the histogram. By removing unnecessary clutter from value projections, it enables, smoother transitions. The intensity graph's peaks identify the areas of concentration for the values over the given period of time. The density plot has one advantage over the histogram: it exhibits the distribution's shape more accurately. The number of columns used has no bearing on it, unlike the histogram, which uses one column to represent a set of data. The discrete histogram of the distribution of hydrogen generation parameters was replaced with KDE. It is crucial to take the rectangle's width and height into account while interpreting this histogram. K is often a symme trical oriented unimodal density function. The kernel estimate is obtained by applying a kernel function to each sample point. The total of the y coordinates (coordinates) of the n nuclei located at a given place x determines the value of the kernel function estimate for that location. For instance, the kernel estimate at x will be relatively high with many sample points and lower with fewer sample points [24]. Figure 5 shows the KDE graph. Bandwidth on the x-axis is between -0.5 and 1.5, while on the y-axis it is between 0.7 and 0.6. As a result, the kernel estimate is relatively high.

From this point of view, we can say that the bandwidth and the number of sample points are important factors in the kernel density estimation method.

The performance of the model was further assessed by comparing predicted and observed H_2 production kernel density plots. Overall, the ANN predicted H_2 distribution reproduced the observed H_2 distribution better, both as the median value and as the high-value tail. The linear model's predicted H_2 distribution, on the other hand, was shifted to the right, indicating that the observed H_2 median value was significantly overestimated, while the high values were underpredicted.

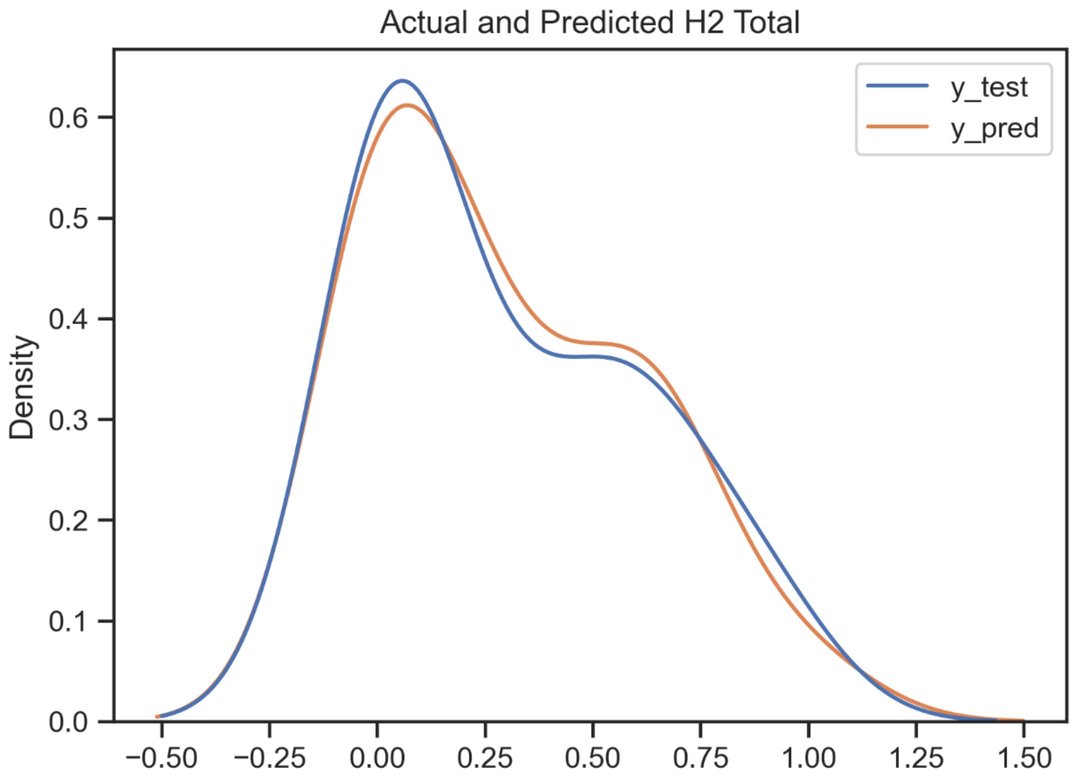

Figure 5. Kernel density plot of hydrogen production rate predicted and observed by the ANN model

4. Conclusions

Water electrolysis is one of the most important methods in hydrogen production with high purity oxygen production and is renewable. This ANN study is the first step in water electrolysis and provides an excellent introduction to the enormous potential of this type of model in this field. The high accuracy of the ANN model for predicting hydrogen production has shown that it can be used in these studies. However, more experimental data to supplement the database would be beneficial for further ANN training and improving the developed models. Finally, the ANN models proposed here can be used to optimize and control the process. Systems that use hydrogen as a fuel with conventional and renewable energy sources will bring hydrogen energy technology one step closer to actual use.

This research will significantly advance the field of hybrid solutions. The importance of these hydrogen generation techniques is further illustrated by the various ANN models of this study and the proposal to develop these models with various optimization algorithms to reveal and optimize the importance of the input parameters, and by comparing them with other prediction models.

Authors' contributions

GB designed the methodology, collected data, organized and wrote paper. BÖ designed the analysis, performed the model, organized and wrote paper. Both authors read and approved the final manuscript.

Competing interests

The authors declare that they have no competing interests.

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