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Noha Nasr, *Western University*
Hisham Hafez, *Western University*
M. Hesham El Naggar, *Western University*
George Nakhla, *Western University*

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Application of artificial neural networks for modeling of biohydrogen production

Noha Nasr [a], Hisham Hafez [b,*], M. Hesham El Naggar [a], George Nakhla [a,c]

[a] Department of Civil Engineering, The University of Western Ontario, London, Ontario N6A 5B9, Canada
[b] GreenField Ethanol Inc., Chatham, Ontario N7M 5J4, Canada
[c] Department of Chemical and Biochemical Engineering, The University of Western Ontario, London, Ontario N6A 5B9, Canada

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ABSTRACT

In this study, an artificial neural network (ANN) model was developed to estimate the hydrogen production profile with time in batch studies. A back propagation artificial neural network ANN configuration of 5–6–4–1 layers was developed. The ANN inputs were the initial pH, initial substrate and biomass concentrations, temperature, and time. The model training was done using 313 data points from 26 published experiments. The correlation coefficient between the experimental and estimated hydrogen production was 0.989 for training, validating, and testing the model. Results showed that the trained ANN successfully predicted the hydrogen production profile with time for new data with a correlation coefficient of 0.976.

1. Introduction

Dark fermentation is a promising method for biohydrogen production since it has higher production rates than other processes, and can utilize a wide range of renewable feedstocks [1]. Many factors can influence the fermentative process such as the inoculum type and concentration, substrate type and concentration, reactor configuration, temperature, and pH because they affect the activity and type of the hydrogen producing bacteria [2].

To date, hydrogen is not commercialized as an energy source but it is widely used as a chemical reactant in the production of fertilizers, diesel refining, and industrial synthesis of ammonia [3]. It has been well documented that modeling fermentative hydrogen production process is one of the most critical requirements for improving our ability to predict the biohydrogen yield [4]. Modeling the biohydrogen process is very important so as to provide information on the different factors affecting the production processes.

Experimental optimization methods such as the "One-factor-at-a-time" are ineffective, time and materials consuming, and they do not take into consideration the interaction between these factors. Some studies investigated the combined effect of two variables such as pH and substrate concentrations [5,6], temperature and pressure release methods [7], and pH and sulfate concentration [8] on the biohydrogen production process. Ginkel and Sung [5] tested the effect of varying pH (4.5–7.5) and substrate concentration (1.5–44.8 g COD/L) and

Abbreviations: ADM1, anaerobic digestion model No. 1; ADS, anaerobic digester sludge; ANN, artificial neural network; APE, average percentage error; COD, chemical oxygen demand; HRT, hydraulic retention time; MAE, mean absolute error; MSE, mean square error; UASB, upflow anaerobic sludge blanket.

* *Corresponding author*. Tel.: +1 519 784 6230; fax: +1 519 352 9559.
E-mail addresses: h.hafez@greenfieldethanol.com, hishambahaa@gmail.com (H. Hafez).

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their interaction on hydrogen production in batch tests using compost as the seed microflora and sucrose as the substrate. The aforementioned authors achieved maximum hydrogen production of 74.7 mL/L-h at pH 5.5 and substrate concentration of 7.5 g COD/L. These findings were consistent with Li et al. [6] who observed optimum conditions of pH 6.0 and substrate concentration of 8 g COD/L to achieve a hydrogen yield of 1.83 mol/mol$_{glucose}$ using seed sludge from a riverbed and glucose as the substrate. The effects of varying sulfate concentration (0–20 g/L) with pH (5.5–6.2) on continuous fermentative hydrogen production were investigated using anaerobic digester sludge (ADS) growing on glucose in a chemostat reactor [8]. The aforementioned authors found optimum conditions of pH 5.5 and sulfate concentration of 3 g/L to produce maximum hydrogen production rate of 2.8 L/d.

Several mathematical techniques were employed to investigate biohydrogen production. Empirical models, such as the modified Gompertz equation, have been widely used for batch fermentative biohydrogen production [9,10]. The modified Gompertz equation includes three parameters that are used to fit the equation; lag time, hydrogen production potential, and hydrogen production rate. Due to the empirical nature of the model, it does not take into consideration the effect of many important parameters such as the substrate concentration, pH, and temperature.

Mechanistic models such as the anaerobic digestion model no.1 (ADM1) have been used for modeling the whole anaerobic digestion process [11] as well as for modeling biohydrogen production [10]. The major limitation of the ADM1 model is its mathematical complexity, as it consists of more than 20 biochemical reactions and more than 30 kinetic parameters, and the extreme analytical difficulty of measuring these parameters.

Artificial Neural Network (ANN) is a mathematical representation of the neurological functioning of a brain. It simulates the brain's learning process by mathematically modeling the network structure of interconnected nerve cells [12]. ANN is a powerful modeling tool for problems where the parameters that govern the results are either not defined properly or too complex [13]. ANN is able to describe the interactive effects among these different parameters in a complicated bioprocess [14]. ANN is capable of modeling the complex relationships between input and output parameters without requiring a detailed mechanistic description of the phenomena that is governing the process [15].

A typical neural network has an input layer, one or more hidden layers, and an output layer. The neurons in the hidden layer, which are linked to the neurons in the input and output layers by adjustable weights, enable the network to compute complex associations between the input and output variables [12]. Training the model is the process of determining the adjustable weights and it is similar to the process of determining the coefficients of a polynomial by regression. The weights are initially selected randomly and an iterative algorithm is then used to find the weights that minimize the differences between the model-calculated and the actual outputs.

The most commonly used algorithm in ANN is the back propagation neural network [12]. In this training algorithm, the error between the model results of the output neurons and the actual outputs is calculated and propagated backward through the network. The algorithm adjusts the weights in each successive layer to reduce the error. This procedure is repeated until the error between the actual experimental and network-calculated outputs satisfies a pre-specified error criterion [12].

Few studies in the literature investigated the modeling of biohydrogen production in batch studies using ANN. Table 1 shows a summary of the different biohydrogen production studies that used ANN as a modeling tool. Wang and Wan [14] studied the effects of temperature, initial pH, and glucose concentration on fermentative hydrogen production by mixed cultures in batch tests. The ANN model successfully described the effects of these parameters on the substrate degradation efficiency, hydrogen yield, and average hydrogen production rate.

Shi et al. [15] presented a back propagation ANN model that accurately predicted the steady-state performance of bioreactors for the biohydrogen production process using sugar refinery wastewater in an integrative biological reactor comprising a continuous stirred tank reactor and an upflow anaerobic sludge blanket reactor (UASB). Another continuous flow system performance was simulated using ANN by Mu and Yu [16]. A model was designed, trained, and validated to predict the steady-state performance of a laboratory-scale granular-based hydrogen-producing UASB reactor treating sucrose-rich synthetic wastewater. Organic loading rate, hydraulic retention time (HRT), and influent bicarbonate alkalinity were the model inputs, while the output variables were either hydrogen concentration, hydrogen production rate, hydrogen yield, effluent total organic carbon, or effluent aqueous products including acetate, propionate, butyrate, valerate, and caporate. The model effectively described the daily variations of the UASB reactor performance and predicted the steady-state performance at various substrate concentrations and HRTs.

Although ANN models may be successfully applied in biohydrogen production systems and can capture effectively the nonlinear relationships existing between variables in complex systems like fermentative biohydrogen production, one of the main limitations of ANN is the uncertainty of outputs prediction outside the data range, used in establishing the model [17,18].

It is apparent from the literature survey that there is no explicit agreement on the specific input parameters for ANN modeling of biohydrogen systems. In addition, most of these studies focused only on the prediction of the ultimate hydrogen production and hydrogen yield [2,4,15]. However, the prediction of hydrogen production profile with time is crucial for better understanding the process and in evaluating the kinetics of the process. Therefore, the main objective of this study is to use ANN to predict the temporal variation of hydrogen production in batch reactors as a function of initial pH, initial substrate and biomass concentrations, temperature, and time. A database for the hydrogen production tests was established from the literature and used for training, validating, and testing the ANN model.

2. Methodology

2.1. *Analytical approach*

An analytical approach was tested to model hydrogen production in batch experiments using the ADM1, which has

Table 1 – Experimental data used for BPNN model.

Input	Output	Reactor	Substrate	Inoculum	ANN structure[a]	Number of data points	Ref.
ORP, pH, dissolved CO_2	HP with time	Batch	Cheese whey	*E. coli*	–	102	[19]
HRT, S_o, X_o, ethanol, organic acids conc., ORP, pH, recycle ratio, alkalinity	HPR	CSTR	Sucrose	Sewage sludge	12–20–1	–	[20]
OLR, ORP, pH, alkalinity	HP	CSTR	Kitchen wastes	Anaerobic activated sludge	4–3–1	–	[15]
OLR, HRT, influent alkalinity	H_2%, HPR, HY, TOC_{eff}, products conc.	UASB	Sucrose	ADS	–	140	[16]
pH, glucose: xylose, inoculum size, inoculum age	Cumulative H_2	Batch	Glucose + xylose	Compost	4–10–1	16	[4]
T°C, pH_i, S_o	HY	Batch	Glucose	ADS	3–4–1	20	[2]
T°C, pH_i, S_o	Substrate degradation efficiency %, HPR, HY	Batch	Glucose	ADS	3–5–1	29	[14]

ORP: Oxidation reduction potential, HP: Hydrogen production, HRT: Hydraulic retention time, S_o: initial substrate concentration, X_o: initial biomass concentration, HPR: Hydrogen production rate, CSTR: Continuous stirred tank reactor, OLR: Organic loading rate, HY: Hydrogen yield, TOC_{eff}: Effluent total organic carbons, UASB: Upflow anaerobic sludge blanket.
a ANN structure: no. of input parameters-no. of neurons in hidden layer-no. of output parameters.

been used for modeling the whole anaerobic digestion process for methane production. Hydrogen was set as the end product from sugar degradation, and methane production pathways from either acetate utilization or hydrogen consumption were neglected. The main equations for modeling the hydrogen production process were the substrate uptake (Equation (1)), biomass growth (Equation (2)), and products formation (Equations (3)–(6)) [11]. For simplicity, in order to solve these equations, the biomass decay and inhibition effects were neglected, and only one culture was assumed for substrate degradation and products formation.

$$-\frac{dS_{su}}{dt} = k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X \tag{1}$$

$$\frac{dX}{dt} = Y_{su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X + Y_{bu}k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}}X + Y_{pr}k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}X \tag{2}$$

$$\frac{dS_{bu}}{dt} = (1-Y_{su})f_{bu,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X - k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}}X \tag{3}$$

$$\frac{dS_{pr}}{dt} = (1-Y_{su})f_{pr,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X - k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}X \tag{4}$$

$$\frac{dS_{ac}}{dt} = (1-Y_{su})f_{ac,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X + (1-Y_{bu})*0.8k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}}X + (1-Y_{pr})*0.57k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}X \tag{5}$$

$$\frac{dS_{H_2}}{dt} = (1-Y_{su})f_{H_2,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X + (1-Y_{bu})*0.2k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}}X + (1-Y_{pr})*0.43k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}X \tag{6}$$

where S_{bu}, S_{pr}, S_{ac}, and S_{H_2}, are the butyrate, propionate, acetate, and hydrogen concentrations (g COD/L), Y_{su}, Y_{bu}, and Y_{ac}, are the biomass yields for sugars, butyrate, and acetate degradation (g $COD_{biomass}$/g $COD_{substrate}$), $f_{bu,su}$, $f_{pr,su}$, $f_{ac,su}$, and $f_{H_2,su}$, are the butyrate, propionate, acetate, and hydrogen yields on sugars (g COD/g COD_{su}), $k_{m,su}$, $k_{m,bu}$, and $k_{m,pr}$, are the maximum rates of sugar, butyrate, and propionate utilization (d^{-1}), and $k_{s,su}$, $k_{s,bu}$, and $k_{s,pr}$ are the sugar, butyrate, and propionate uptake affinity constants (g COD/L). Trying to solve these equations lead to three difficult differential equations that could not be solved analytically (Equations (7)–(9)). Therefore, a numerical approach using ANN was investigated.

$$k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}dX = \left[Y_{su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}} + Y_{bu}k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}} + Y_{pr}k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}\right]dS_{su} \tag{7}$$

$$k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}dS_{ac} = \left[(1-Y_{su})f_{ac,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}} + 0.8(1-Y_{bu})k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}} + 0.57(1-Y_{pr})k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}\right]dS_{su} \tag{8}$$

$$k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}dS_{H_2} = \left[(1-Y_{su})f_{H_2,su}k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}} + 0.2(1-Y_{bu})k_{m,bu}\frac{S_{bu}}{k_{s,bu}+S_{bu}} + 0.43(1-Y_{pr})k_{m,pr}\frac{S_{pr}}{k_{s,pr}+S_{pr}}\right]dS_{su} \tag{9}$$

2.2. *Experimental data and ANN structure*

To predict hydrogen production with time, a back propagation ANN was considered and the chosen input parameters were initial pH, initial substrate concentration (S_o), initial biomass concentration (X_o), temperature (T), and time (t).

Experimental data was collected from the published literature in order to establish the model. The limitation in number of studies used was due to choosing the studies that only provided data covering the input and output parameters under the same experimental conditions. Table 2 shows the experimental data sources, as well as the minimum and maximum values for the input and output parameters.

Initial pH ranged from 5.5 to 7.5, initial substrate concentration ranged from 0.3 to 58.6 g COD/L, initial biomass concentration ranged from 0.9 to 17.6 g COD/L, temperature ranged from 20 to 55 °C (mesophilic and thermophilic conditions), maximum fermentation time for batches was 97 h, and maximum volumetric hydrogen production was 382 mL. All experiments were batch studies and used glucose, sucrose, or real wastes as the substrate and mixed cultures as the seed microflora. Three hundred and thirteen data points from 26 different batch experiments were collected from 7 different studies as shown in Table 2. Ranges for the input and output data used in establishing the ANN model are shown in Table 3. Input and output variables were normalized in the range of (−1, 1) to avoid any numerical overflow prior to training, as well as reducing the errors and decreasing the training time [27]. The normalization process was according to Equations (10) and (11) for both input and output variables, respectively.

$$X_n = 2 \times \frac{(X - X_{min})}{(X_{max} - X_{min})} - 1 \quad (10)$$

$$Y_n = 2 \times \frac{(Y - Y_{min})}{(Y_{max} - Y_{min})} - 1 \quad (11)$$

where X_n is the normalized input, X is the input variable, Y_n is the normalized output, and Y is the output variable. The scaled data was then used to train the ANN by randomly utilizing 60%, 20%, and 20% of the data for training, validation, and testing, respectively. The output data from the model should then be processed to convert the data back into the unnormalized values to get the actual output data according to Equation (12).

$$Y = 0.5 \times (Y_n + 1)(Y_{max} - Y_{min}) + Y_{min} \quad (12)$$

The input layer consisted of five neurons (pH, S_o, X_o, T, t), while the output layer had one neuron which is the hydrogen production with time. A single hidden layer configuration with different numbers of neurons was tested but showed high errors. Therefore, a double layer configuration was selected for the hidden layer. In order to determine the number of neurons in the hidden layers, different trials were investigated. Fig. 1 shows the mean square error (MSE) between the experimental and predicted data calculated by the following equation for different number of neurons in both hidden layers.

Table 3 – Range for input and output parameters used in BPNN model.

Parameter	Minimum	Maximum	Unit
pH_i	5.5	7.5	–
S_o	0.3	58.6	g COD/L
X_o	0.9	17.6	g COD/L
T	20	55	°C
t	0	97	h
H_2	0	382	mL

X_o: biomass initial concentration, T: temperature, t: time.
pH_i: initial pH, S_o: substrate initial concentration.
H_2: volumetric hydrogen production.

$$MSE = \frac{\sum_{i=1}^{n}(Y_{i,e} - Y_{i,p})^2}{n} \quad (13)$$

where $Y_{i,e}$ is the experimental data, $Y_{i,p}$ is the corresponding predicted data output, and n is the number of experimental data points.

Fig. 1 indicates that the minimum MSE occurred at 6 neurons and 4 neurons in the first and second hidden layers, respectively. It has been reported that when the number of neurons in the hidden layer is higher than the optimum, the neural network becomes very complex and will take longer time to train [14].

2.3. *ANN model training*

All the neurons in the hidden layer were non-linear with a sigmoid transfer function. Fig. 2 shows the structure of the ANN and the type of transfer functions between the input and hidden layer 1, hidden layer 1 and hidden layer 2, and that between hidden layer 2 and the output layer. The ANN was trained on a Matlab platform R2009 (MathWorks, Inc., Natick, MA, USA).

A feed forward neural network with back propagation algorithm was used in this study. In the ANN training process,

Table 2 – Database sources and experimental conditions.

Carbon source	No. of batches	No. of data points	pH_i	T°C	S_o g COD/L	X_o g COD/L	Source
Glucose	8	72	7	20–55	10.7	1.68	[21]
Glucose	1	6	6	37	10.7	3.12	[22]
Glucose	1	6	6.7	37	10.7	2.84	[23]
Glucose	1	9	6.5	37	8.6	2.27	[9]
Sucrose	6	56	5.5	36	0.3–9.0	1.15–0.87	[24]
Glucose	2	10	5.5	25	3.0	2.84	[25]
Thin stillage[a]	7	154	5.5	37	4.4–58.6	9.74–17.62	[26]

pH_i: initial pH, T: temperature, S_o: substrate initial concentration, X_o: biomass initial concentration.
a Thin stillage: from corn processing bioethanol plant.

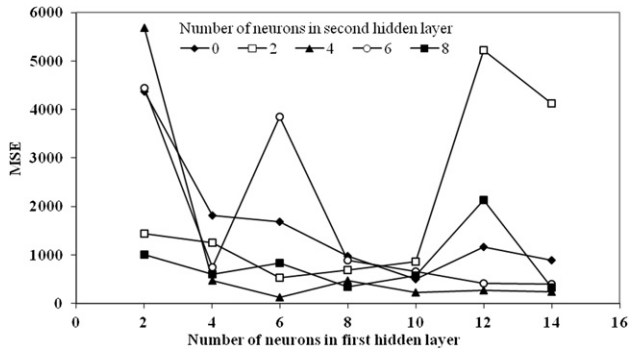

Fig. 1 – Error calculated at different number of neurons in first and second hidden layers.

the error between the experimental data and the corresponding predicted data MSE was calculated and then propagated backward through the network in each cycle. The algorithm adjusts the weights between the input, hidden layers, and output neurons in order to reduce the error and the procedure is repeated until the error between the experimental and predicted data satisfies certain error criterion.

The weight and bias matrices obtained after the training phase of the ANN model are:

$$W_1 = \begin{bmatrix} 2.7604 & -1.4851 & 1.4963 & 1.3453 & 1.4764 \\ -0.3414 & 1.1921 & -1.4907 & 2.3011 & 2.6455 \\ -2.0486 & 1.1434 & 2.7576 & 0.7630 & 1.5372 \\ 1.9923 & -1.8804 & 1.6281 & 0.3726 & -2.3998 \\ 2.7125 & -0.9574 & -1.1360 & -1.7970 & 1.8054 \\ 3.4058 & -2.0009 & -0.0187 & -0.3880 & -0.5475 \end{bmatrix},$$

$$B_1 = \begin{bmatrix} -4.0067 \\ 2.4040 \\ 0.8013 \\ 0.8013 \\ 2.4040 \\ 4.0067 \end{bmatrix}$$

$$W_2 = \begin{bmatrix} -0.7755 & -3.1651 & 0.7723 & 1.9648 & 4.1392 & -4.1919 \\ -3.6428 & -1.4961 & -0.9910 & 4.2892 & -3.4782 & -1.6720 \\ 3.4811 & -1.3751 & -1.1269 & 2.4597 & -4.8622 & -2.1933 \\ -1.8333 & 0.4873 & 0.1609 & -1.0459 & -4.3517 & -5.1113 \end{bmatrix},$$

$$B_2 = \begin{bmatrix} 4.1559 \\ 4.6714 \\ 2.9843 \\ 2.3192 \end{bmatrix}$$

$$W_3 = [-0.0798 \quad -0.8093 \quad 0.7070 \quad 0.2623], \; B_3 = [0.7186]$$

where W_1 is the matrix representing connection weights between input and first hidden layer neurons, W_2 is the matrix representing connection weights between first and second hidden layer neurons, W_3 is the matrix representing connection weights between second and output layer neurons, B_1 is the bias matrix for the first hidden layer neurons, B_2 is the bias matrix for the second hidden layer neurons, and B_3 is the bias matrix for the output layer neurons. The ANN model described can be used to predict hydrogen production with time after normalizing the input data as in Equation (10). The normalized Y_n for hydrogen production can be calculated as follows:

$$Y_n = W_3 \times (\text{logsig}(W_2 \times (\text{logsig}(W_1 \times X_n + B_1)) + B_2)) + B_3 \quad (14)$$

$$\text{logsig}(x) = \frac{1}{1 + \exp(-x)} \quad (15)$$

3. Results and discussion

3.1. Hydrogen production prediction using ANN

In order to evaluate the ANN modeling ability, experimental data were compared to the predicted data. The correlation coefficient and the mean absolute error (MAE) were used to assess model predictability

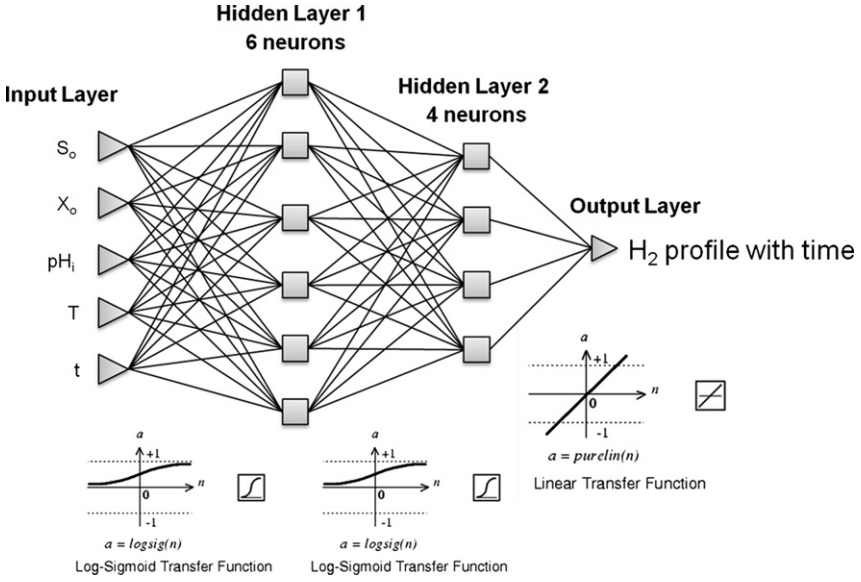

Fig. 2 – Artificial neural network (ANN) configuration.

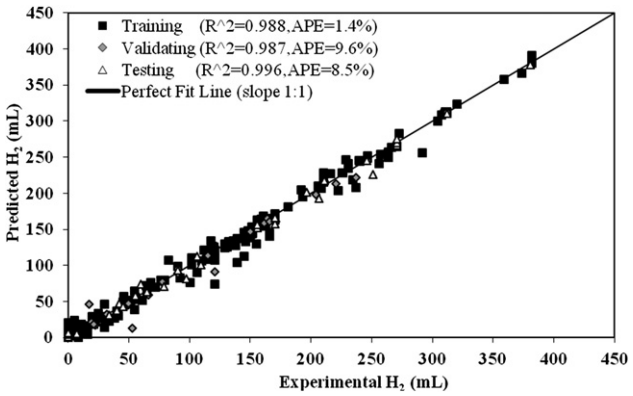

Fig. 3 – Correlation between experimental and predicted data used in ANN model.

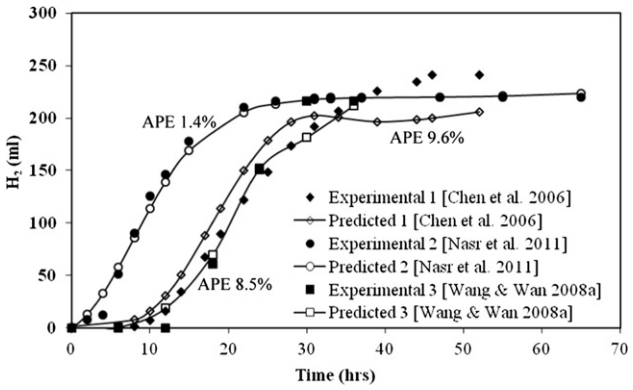

Fig. 5 – Experimental and predicted hydrogen production profile using data from [24,26,28].

$$\mathrm{MAE} = \frac{1}{n}\sum \left| Y_{i,p} - Y_{i,e} \right| \quad (16)$$

where $Y_{i,p}$ is the predicted value, $Y_{i,e}$ is the corresponding experimental value, and n is the number of experimental data points.

Fig. 3 shows the correlation between the experimental hydrogen production data and the hydrogen production predicted by the ANN for data points used for training, validating, and testing the model (Table 2). Correlation coefficients of 0.988, 0.987, and 0.996 and MAE of 1.89 mL, 6.16 mL, and 4.89 mL were achieved for the training, validating, and testing data points, respectively.

The ANN model was then used to estimate the temporal hydrogen evolution for three new data sets adopted from Chen et al. [24], Nasr et al. [26], and Wang and Wan [28] that were not used in the training process. Chen et al. [24] investigated biohydrogen production from sucrose in batch studies using ADS at 36 °C and an initial pH of 5.5. Nasr et al. [26] investigated biohydrogen production from thin stillage as the substrate using ADS as the seed microflora at 37 °C and an initial pH of 5.5. Wang and Wan [28] investigated biohydrogen production from glucose in batch studies at 35 °C using pre-heated ADS at an initial pH of 7. Fig. 4 shows the correlation between the predicted and experimental data points from the aforementioned sets of data, where a correlation coefficient of 0.965 and an MAE of 11.2 mL were obtained. Average percentage error (APE), defined as the summation of the absolute difference between the experimental and predicted values divided by the experimental values, averaged over the number of data points were 1.4%, 9.6%, and 8.5% for the data sets adopted from Nasr et al. [26], Chen et al. [24], and Wang and Wan [28], respectively. Fig. 5 shows the experimental and predicted hydrogen production profile using the three sets of data. Although Nasr et al. [26] used thin stillage from a bioethanol plant as a substrate as opposed to glucose or sucrose that were mostly used in establishing the model, the model was able to predict the hydrogen production profile accurately. The reason is that thin stillage is composed predominantly of carbohydrates. It is evident that ANN accurately predicted the temporal variation of hydrogen production in the three studies, as reflected by APE of 1.4%, 9.6%, and 8.5%.

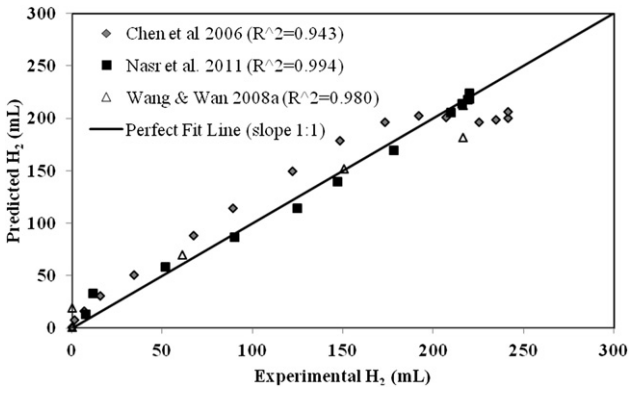

Fig. 4 – Correlation between experimental and predicted data adopted from [24,26,28].

4. Conclusion

Dark fermentative hydrogen production is a highly complex process that is difficult to model mechanistically. This study is aimed at demonstrating the possibility of adapting ANN to predict temporal hydrogen production. The results support these conclusions:

- The developed ANN model is a viable method for predicting temporal hydrogen production from different substrates with excellent ability to capture the interrelationships between process parameters, confirming its versatility.
- R^2 of 0.988, 0.987, and 0.996 were achieved for training, validating, and testing data points, respectively.
- Average R^2 of 0.976 was obtained when testing the proposed model using a new data set.

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