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Modeling hydrogen production using *green algae Chlorella vulgaris* utilizing Neural Networks

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Abstract : *The production of hydrogen via biophotolysis using algal strain Chlorella vulgaris within an anaerobic batch reactor has been studied.This paper presents the development of a model used to predict the production of hydrogen as function of time with Artificial Neural Network (ANN). The model reported is based on a multi-layer perceptron function neural network (MLP-NN) with a configuration of 3-6-4-1 combined with sigmoid transfer functions tansig,tansig, purline and trainlm respectively. The architecture of the model has been designed in order to mimic the inter-relationship between three input parameters: substrate concentration, medium pH and the media contents of nitrogen and phosphate. The ANN model was refined and tested with the use of 48 experiments. The correlation coefficient between the experimental data and the model prediction was* R^2*= 0.985 for training and testing. The results showed that the ANN model successfully predicted the production of hydrogen from Chlorella vulgarisalgal strain and provided a high level of accuracy for the training and testing stages with a maximum error of 6% and 2% respectively.*

Keywords*: Hydrogen production;green microalgae; bioprocess modeling, neural network model.*

I. INTRODUCTION

Hydrogen is considered as a key alternative fuel which can help to meet futureenvironmental and energy challenges for the planet. One noted advantage of using hydrogen as a source of fuelis that it is completely free of carbon dioxide emissions as compared to conventional fossil fuels. Hydrogen has been proven to be used as a clean transportation fuel and for production of electricity via fuel cell [1]. Hydrogen gas can be obtainedvia chemical processes, but the use of anaerobic microorganisms to produce hydrogen from biomass has been declared as an innovative and promising biotechnology [2]. The bioproduction of fuels from renewable feed-stocks has become a global priority owing to a limited resource of petroleum oil, increased environmental concerns and awareness of global warming[3]. One way to produce hydrogen biologically is by using microalgae exposed to anaerobic conditions [4,5]. Biohydrogenprocess modeling became necessary in order to provide information based on the different factors affecting the process of hydrogen production.

Optimization of experimental methods such as “One-factor-at-a-time”were proven to be ineffective, time and resource consuming; these methods donot take into consideration the interaction between these factors. Recently, studies investigating the combination of two or moreenvironmental variables for the biohydrogen production process were carried which included,pH,substrate concentrations,temperature, pressure and other variables [6-9].The ANN modelis suitable for developing bioprocess models without prior understanding of the kinetics of the metabolic fluxes within the cell and the cultural environment. Artificial neural networks are densely interconnected processing units that use parallel computation algorithms.ANNsare also recognized for connectionism, parallel distributed processing, neuron-computing, natural intelligent systems and machine learning algorithms. One of the advantages of using theANN model is their capacity in learning from representative examples without providing any special programming modules to simulate any special patterns withinthe data set.Thisallows ANN to learn and adapt to a continuously changing environment[10].

The ANN models are exclusively data-based and the most widely utilized ANN architecture is the multi layered perceptron (MLP-NN) that approximates non-linear relationships existing between multiple causal (input) process variables and the corresponding dependent (output) variables[11,12].Literature review showed that a limited number of articlesare published with use of ANN models for biohydrogen production [10,13], especially those dealing with studies of biohydrogen production using green algae such as *Chlorella vulgaris*.The objective of this research therefore was to construct a suitable model of biohydrogen production by monitoring variables, such as glucose concentration, pH andmedia contents of nitrogen and phosphate (referred as N-p).

II. MATERIALS AND METHODS

II.1. Algal strain, culture media and growth conditions

Chlorella vulgaris stored on agar was obtained from Carolina Biological Supply (Burlington, North Carolina, Catalogue No. 15-2075) and grown on Bold’s Basal Medium [14] having the following composition in mgL−1 of deionized water: 75 K_2HPO_4, 175 KH_2PO_4, 75 $MgSO_4.7H_2O$, 250 $NaNO_3$, 25 $CaCl_2.2H_2O$, 25 NaCl, 50 EDTA Na_4, 31 KOH, 5

$FeSO_4.7H_2O$, 11.4 H_3BO_3, 1.4 $ZnSO_4.7H_2O$, 0.24 $MnCl_2.4H_2O$, 0.25 $CuSO_4.5H_2O$, and 0.2 $Na_2MoO_4.2H_2O$. After stirring, the pH of the medium is measured and it was 6.9±0.1.

II.2.Experimental set- up

After filtration the microalgae were transferred to the anaerobic process using sulfur-deficient medium [7,8]. A Duran bottle was used as bioreactor,having a nitrogen gas inlet for flushing in order to insure an anaerobic process,and an outlet collecting the gas produce by the culture. The hydrogen was produced by the degradation of stored organic compounds (glucose) by algae inthe bioreactor. The evolved gas passed through a 5M KOH solutiontoremove thecarbon dioxide and was then sent to thegas chromatography (GC)for analysis [15].The growth experiment was performed at room temperature using a one liter Erlenmeyer flasks containing 500 ml of Bold's Basal Medium (BBM)[16-18]. Eight fluorescent lamps of 20 W were utilized to reproduce natural lightening to help the growth of the algae.

II.3. Analysis methods

The composition of the evolved gas was analyzed using gas chromatography (GC-17A, Shimazdu) with argon as carrier gas. The GC was equipped with a 5A molecular sieve column (Alltech)coupled with a thermal conductivity detector (TCD) for the analysis. The packed column was maintained at 80°C and the thermal conductivity detector was set at 120°C. The biomass cell concentration at the start and the end of the experiment wasdetermined by measuring the optical density (O.D) at the 600 nm wavelength using a UV- visible spectrophotometer (Biomate 3S) .The concentration of glucose in the medium during the experiment was determined by blood- glucose analyzerby(ACUU-CHECK ACTIVE, Roche Diagnostics Corporation)[19].

II.4. Experimental data and ANN structure

In this study MLP-NN was considered to predict hydrogen production with time and the selectedthree input parameters were:media concentration (N-p)in the culture, substrate concentration and pHof the medium.In this study,the collected experimental were used to establish the model.The subsequent effects of concentrations of glucose as the substrate were studied atdifferentconcentrations between 5 to 40 g/l.Media concentration (N-p) content of the culturewas increased by mole (10%, 20% and 30%)and the range of the medium pH was varied from 6.0±0.2 to 9.0±0.2. The data used in establishing the ANN model are shown in Table1. Input and output variables were normalized in the range of (-1, +1) to avoid any numerical over flow prior to training, as well as reducing any errors and overall training time [10,22-25]. The normalization process was made according to Equations 1and2for both input and output variables, respectively.

Table 1: Range for input and output parameters used in ANN model.

Variables	minimum	maximum	unit
Totalcontent (N-p)	10	30	% mole
initial substrate concentration	5	40	g/l
initial pH	6	9	–

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

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

Where$X_n$is the normalized input, Xisthe input variable, $Y_n$isthe normalized output, and Yisthe output variable. The scaled data was then used to train the ANN model utilizing training and testing stages respectively.In order to accelerate the training procedure and to achieve minimum mean square estimation error, the inflow data was normalized. Different MLP-NN architectures (while keeping three neurons in the input layer and only one neuron in the output layer) were used to examine the best performance. The choice of the number of hidden layers and thenumber of neurons in each layer was based on two performance indices The mean square error (MSE) between the experimental and predicted data calculated gave the number of neurons in the hidden layers [10, 26-29]. Therefore, this study presented some equations 3,4 and5for investigating model performance. These included: mean absolute relative error (MARE), mean absolute error (MAE) andmean sum of squares (MSE) and evaluated models by the following:

$$\mathrm{MARE} = \frac{1}{N}\sum\frac{|y-y'|}{y} * 100 \quad (3)$$

$$\mathrm{MAE} = \frac{1}{N}\frac{\sum|y-y'|}{N} * 100 \quad (4)$$

$$\mathrm{MSE} = \frac{\sum(y-y')^2}{N} * 100 \quad (5)$$

Where, y is the experimental Hydrogen production,y' predicated Hydrogen production by the model and N is the total number of data.Correlation coefficientwas obtained by linear correlation between actual and simulated data. The ANN was trained using a Matlab platform (7.10.R2010a)to provide the hydrogen yield as a response with different variables and wastested with sigmoid transfer function.

III. RESULTS AND DISCUSSION

Hydrogen production prediction using ANN

Fig. 1 shows the structure of the ANN and the type of transfer functions between the input,the hidden layers and the output.In this study the feed forward used was a neural network with a multi-layer perceptronmodel (MLP-NN) with a configuration of 3-6-4-1 was tested combined with sigmoid transfer functions tansig, tansig, purline and trainlm respectively. The sigmoid transfer functions were selected as showing the more accurate estimation byadjusted the weights in each layer to reduce inaccuracybased on a trial and error.

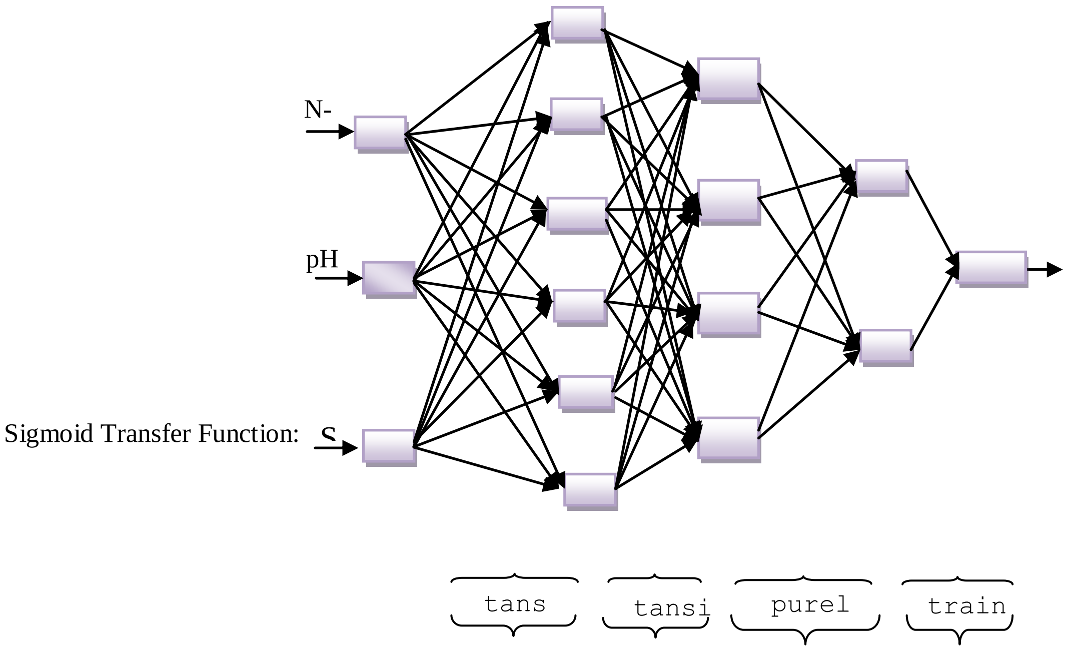

Figure 1: Artificial neural network (ANN) configuration.

The model was examined utilizing 48 records with replicates were collected for hydrogen yield from experiments associated with three variables such as media concentration (N-p) in the culture, medium pH and glucose concentration to achieve the Mean Square Error (MSE) target successfully. The model architecture was re-arranged to consider a total of 48 records of hydrogen yield experiments, out of which 30 records were fixed as the training session and the last 10 records utilized for the testing session. The training process with convergence to the target (MSE) of 0.0001 after 252 iterations. In fact, it is of high significance to evaluate the performance of the prediction model considering a wide range of the stochastic pattern of the hydrogen production. The ANN techniques based on (MLP-NN) proved to have the ability to predict any records data experiment [10,33].

Fig. 2 presents the prediction of hydrogen yield by ANN with experimental hydrogen yield. It was found that the correlation between the experimental hydrogen production data and the hydrogen production as predicted by the ANN model for data points. The correlation coefficient was 0.985 that subsequently seen the experimental data with model prediction was noted linear and high significant. Results demonstrated that the ANN model ismuch more accurate and highlyefficient in achieving prediction errors lower than that obtained from central composite design which is in agreement with reference[33,34], who reported that root mean square error and the standard error of prediction for the neural network model were much smaller than those for the response surface methodology mode.

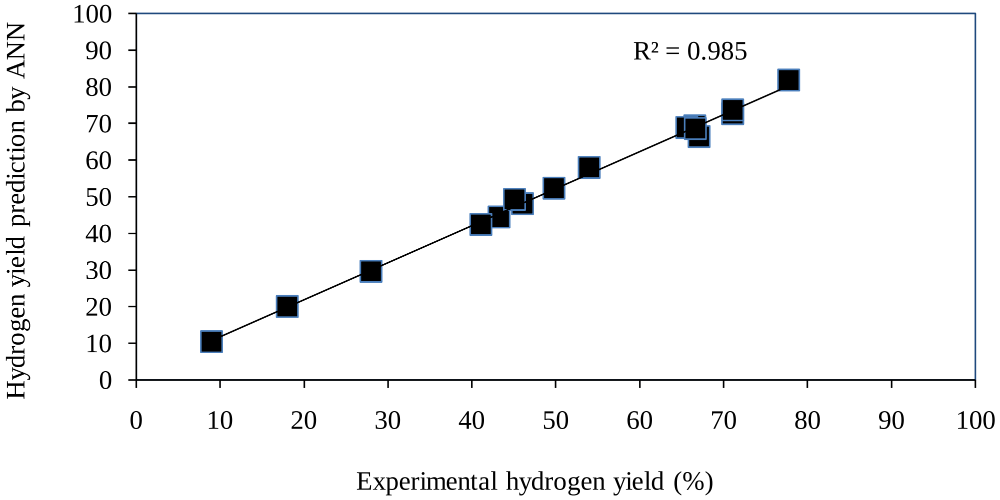

Figure 2: Hydrogen yield (%) predicted by ANN

In this studythe mean absolute error (MAE), mean square error (MSE) and mean absolute relative error were used toassess model predictability utilizing equations (8, 9 and 10) respectively. The result was in the same line that literature [10,30, 31- 36], who investigated the effect of temperature, initial pH and glucose concentration on fermentative for hydrogen production (by mixed and pure cultures in batch test).The literature found the neural network model much higher compared with a traditional approach design statistically. They also estimated the temporal hydrogen evolution for three new sets of data and investigated biohydrogen production from glucose within the specified batch studies by varying temperatures as well as different initial pH during dark fermentation. This indicated that the neural network model had a much higher modelling ability than the response surface methodology model [36].
In this work the measured hydrogen with its associated variables over data experiments were used to train the specified ANN model both within the training and testing stages. Fig.3 illustrates that the proposed ANN model could provide hydrogen yield prediction within error less than 6% during training stage. This model was able to reduce the error in predicting hydrogen yield to be less than the ± 5% as shown in Fig.4.On the other hand, during the testing session, the ANN model achieve a prediction error lower than 2%. Fig. 6 shows the error in testing stage was more accurate noted at 2% inclusively. Results based on the ANN model obtained a higher level of accuracy and efficiency in order to achieve the prediction error that was agreed to [36], who reported that root MSE and the standard error of prediction for the neural network model were much smaller than those for the response surface methodology mode. This also can be explained by the highly stochastic pattern experienced.Therefore, the neural networks model with a sigmoid transfer function and linear output layer were capable of approximating any function with a finite number of discontinuities [10].
Therefore, this result showed that this model could successfully describe the effects of media concentration (N-P), medium pH and glucose concentration on the hydrogen yield.

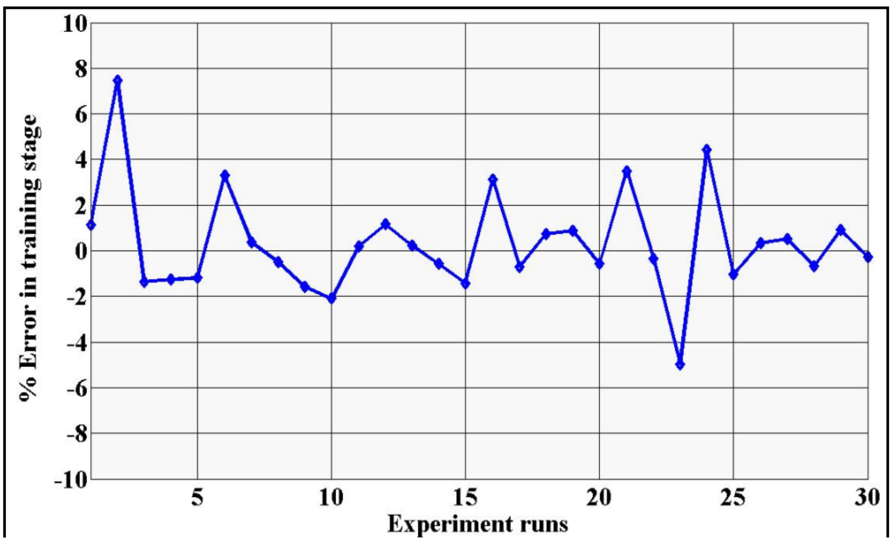

Figure 3: ANN model performance for training process of hydrogen yield using ANN.

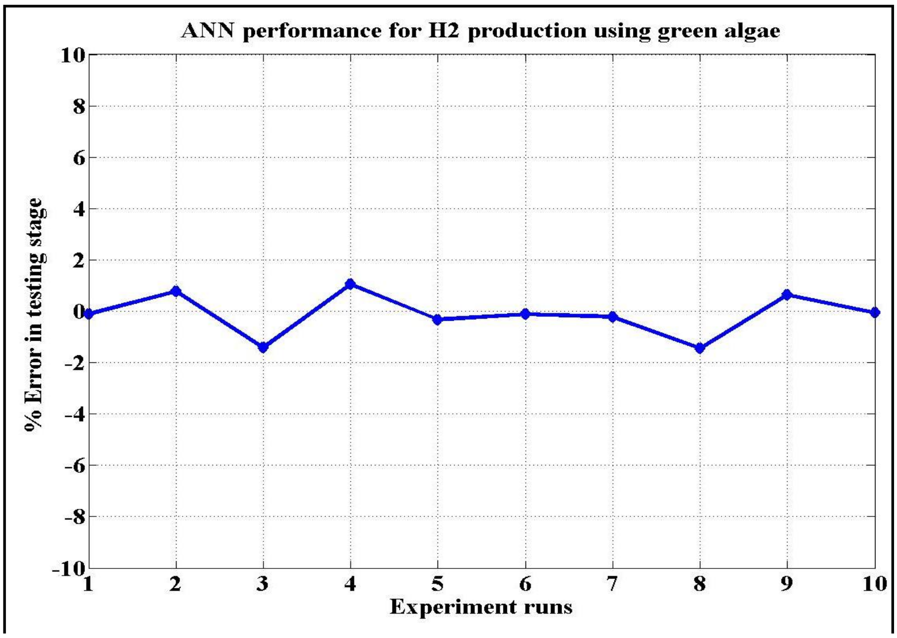

Figure 4: ANN model performance for testing process of hydrogen yield using ANN.

IV. CONCLUSION

This study aimed to demonstrate the possibility of adapting ANN to predict temporal hydrogen production using micro-green algae *Chlorella vulgaris* with three variables: medium pH, media concentration (N-p) in the culture and glucose concentration. ANN model provided significant level of accuracy for prediction with maximum error 6%.Experimental data records have been utilized to develop the ANN model. The results showed that the proposed ANN widens the range of hydrogen yield prediction with consideration of different levels of stochastic patterns of the input of up to 48 records of hydrogen yield experiments, out of which 30 records were fixed as the training session and the last 10 records for the testing session. The results also showed that the proposed ANN model achieved a consistent level of accuracy for hydrogen production, while the training and testing stages for prediction was produced within a maximum error of (6%,2%) respectively.

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