PREDICTION OF HYDROGEN PRODUCTION USING ARTIFICIAL NEURAL NETWORK

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ABSTRACT

Biohydrogen production from starch wastewater industry via up-flow anaerobic staged reactor (UASR) was investigated. The reactor was operated at a hydraulic retention time (HRT) of 0.28 d, and different food to micro-organisms ratios (F/M) of 0.5, 0.9, 1.4, 1.9 and 2.8 g-COD/g-VSS.d. Peak hydrogen production rate (HPR) of 246 mmol-H2/L.d was observed at F/M of 1.4 g-COD/g-VSS.d. Artificial Neural Network (ANN) with a three layers feed-forward back-propagation (3-8-4-1) was developed to predict the fermentation of biohydrogen production. The network used the default Levenberg-Marquardt algorithm for training. Network inputs were organic loading rate (OLR) (g-COD/L.d), pH and volatile suspended solids (VSS) yield (mg-VSS/g-starch). Network output was HPR (mmol-H2/L.d). It is observed that, the output tracks the targets very well for training (R2-value= 0.945), validation (R2-value=0.652) and testing (R2-value=0.791). These values can be equivalent to a total response of R2-value= 0.849. In this case, the network response is acceptable, and simulation can be used for entering new inputs.

Keywords: Artificial neural network, Biohydrogen production, Food to micro-organisms ratio, Starch wastewater, Up-flow anaerobic staged reactor

1 INTRODUCTION

Starch processing industry consumes a lot of water resulting in huge amounts of industrial wastewater. This wastewater is mainly discharged into sewerage network without any treatment, which negatively affects the wastewater treatment plants (WWTP) of the cities. Fortunately, starch wastewater contains high percentage of carbohydrates, cellulose, protein and nutrients, representing an important energy-rich source, which can be potentially converted to a wide variety of useful products.
Dark fermentation of starch wastewater industry is a promising method for biohydrogen production. Many factors are influencing the fermentative process; the inoculum type and concentration, substrate type and concentration, reactor configuration, temperature, and pH (Wang et al. [1]).

Modeling of fermentative hydrogen production process is a critical requirement for improving the ability to simulate, control and predict the biohydrogen yield (Prakasham et al. [2]). Moreover, modeling the biohydrogen process is very important so as to provide information on the different factors affecting the production processes.

Previous researches investigated the effect of two variables such as pH and substrate concentrations (Ginkel et al. [3], Li et al. [4]), temperature and pressure release methods (Gadhamshetty et al. [5]), and pH and sulfate concentration (Hwang et al. [6]) on the biohydrogen production process.

Various mathematical equations were used to investigate biohydrogen production. Empirical models, such as the modified Gompertz equation, have been widely used for batch fermentative biohydrogen production (Elbeshbishy et al. [7]; Gadhamshetty et al. [8]). The modified Gompertz equation (Zwietering et al. [9]) is used to determine the effect of time (h) on hydrogen potential, P (mL-H2), maximum hydrogen production rate, Rm (mL-H2/h), and duration of the lag phase, λ (h). However, it does not take into consideration the effect of many important parameters such as the substrate concentration, pH, and temperature.

Anaerobic digestion model no.1 (ADM1) has been employed for modeling the anaerobic digestion process (Batstone et al. [10]) as well as for modeling biohydrogen production. But still the ADM1 mathematical complexity limits its wide application.

Another method used to model and simulate the fermentative hydrogen production is Artificial Neural Network (ANN). ANN is an information processing system that is inspired by the way such as biological nervous systems e.g. brain. The objective of a neural network is to compute output values from input values by some internal calculations (Delgrange et al. [11]). ANN is trained to perform a particular function by adjusting the values of the connections (weights) between elements (based on a comparison of the output and the target) until the network output matches the target, so that the network can predict the correct outputs for a given set of inputs. There are many different types of training algorithms. One of the most common classes is called a back propagation (BP) ANN (Demuth et al. [12]).

This study investigated the application of ANN to model the biohydrogen production in a continuous fermenter reactor as a function of organic loading rate (OLR) (g-COD/L.d), pH and volatile suspended solids (VSS) yield (mg-VSS/g-starch). The database used for training, validating, and testing was measured for a period of 6 months.

2 MATERIALS AND METHODS

2.1 Experimental procedure

Up-flow anaerobic staged reactor (UASR) was fed continuously with starch wastewater. The working volume of the UASR is 28 L. Sludge was thermal pre-heated at 90°C for 30 minutes to inactivate non spore forming methanogens (Hafez et al. [13]). The heated sludge’s pH and VSS concentration were 7.4 and 38 g/L, respectively. Steady-state conditions reached when the product concentrations such as hydrogen gas content, digestion gas volume, and effluent volatile fatty acid (VFA) concentration were stable (less than 10% variation). Continuous experiments were conducted at different F/M ratios of 0.5, 0.9, 1.4, 1.9 and 2.8 (g-COD/g-VSS.d).

2.2 Artificial neural network structure

To predict hydrogen production with time, a feed forward back propagation ANN was considered and the chosen input parameters (as shown in Table 1) were; organic loading rate (OLR) (g-COD/L.d), pH and volatile suspended solids (VSS) yield (mg-VSS/g-starch).

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

F/M (g-COD/g-VSS.d)	Input						Output	
	OLR (g-COD/L.d)		pH		VSS yield (mg-VSS/g-starch)		HPR (mmol-H_2/L.d)	
	min	max	min	max	min	max	min	max
0.5	16.11	19.88	5.18	6.81	235.83	270.35	68.28	91.30
0.9	34.13	37.91	5.11	6.90	244.63	291.43	137.42	178.83
1.4	50.03	57.97	5.16	6.76	272.33	323.26	237.10	254.69
1.9	70.10	73.87	5.26	6.73	205.91	253.07	187.68	215.02
2.8	100.80	117.47	5.33	6.78	112.07	126.62	100.02	159.88

All neurons in the hidden layers were non-linear with a sigmoid transfer function. The ANN was trained on MATLAB software R2009 (MathWorks, Inc., Natick, MA, USA) that offers a platform for the simulation application. MATLAB Toolbox opens the network/data manager window, which allows the user to import, create, use, and export neural networks and data. A feed forward neural network with back propagation algorithm was used in this study.

Error between the experimental data and the corresponding predicted data mean square error (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. This procedure is repeated, frequently, until the error between the experimental and predicted data satisfies certain error criterion.

Figure 1 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.

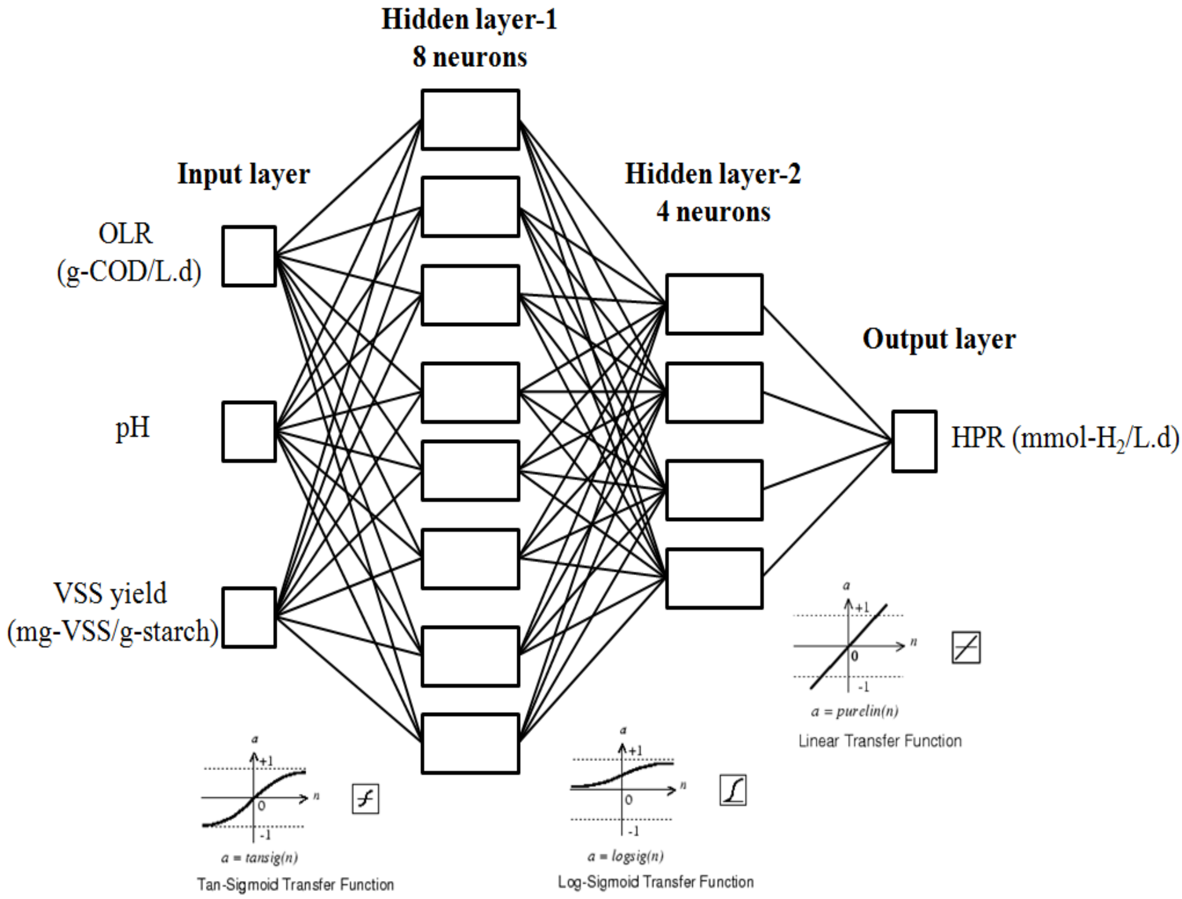

Figure 1: Artificial neural network (ANN) configuration

3 RESULTS AND DISCUSSION

3.1 Hydrogen production rates

The results presented in Figure 2 shows the effect of F/M ratio on the performance of UASR treating starch wastewater. The results revealed that, an increase in the volumetric HPR from 80±8.12 to 246±6.03 mmol-H2/L.d was associated by an increase in the F/M from 0.5 to 1.4 g-COD/g-VSS.d. However, further increase of F/M ratio to a value of 2.8 g-COD/g-VSS.d decreased the volumetric HPR to 125±17.88 mmol-H2/L.d. It is observed that, maximum HPR of 246±6.03 mmol-H2/L.d is higher than 155 mmol-H2/L.d achieved by Sen et al. [14], but lower than another study by Lee et al. [15] who showed HPR of 1198 mmol-H2/L.d.

It is also found that, F/M ratio of 0.5-1.4 g-COD/g-VSS.d attained better substrate utilization efficiency (44-46.7%) and cell yield (256-303 mg-VSS/g-starch) than those for F/M of 1.9-2.8 g-COD/g-VSS.d (40-26.7%, and 235-118 mg-VSS/g-starch, respectively) suggesting that the F/M range (0.5-1.4 g-COD/g-VSS.d) was better condition for the cells to utilize starch for growth.

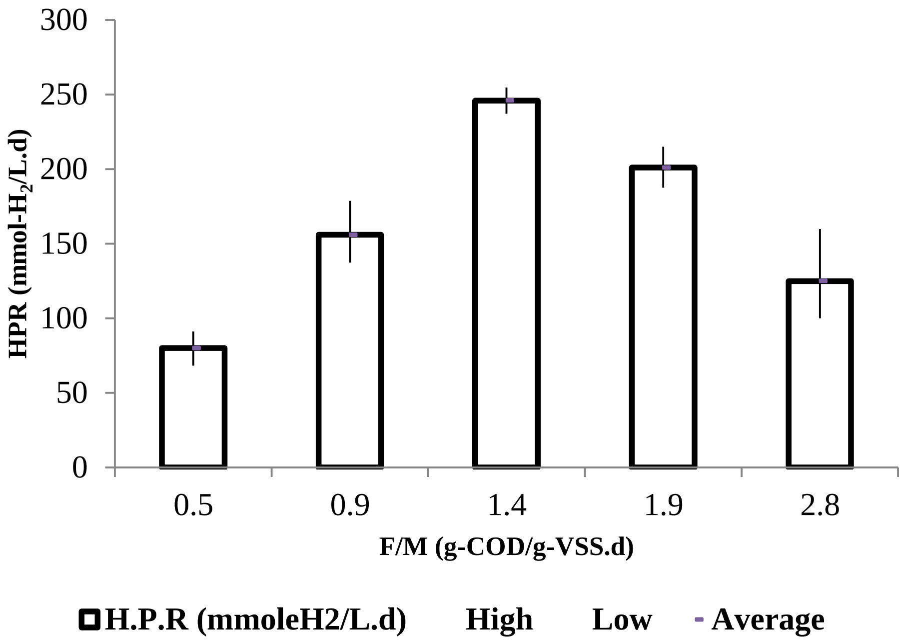

Figure 2: Steady state hydrogen production rates from starch processing wastewater at different F/M ratios

The substrate balance model developed by Borja et al. [16] defines the total chemical oxygen demand (TCOD) balance of the reactor based on two hypotheses: (i) the anaerobic reactor is operated under steady state at all the F/M ratios; and (ii) the suspended solids in the feeding are readily biodegradable and the volatile suspended solids in the effluent corresponds to the biomass generated (Wang et al. [17]). The COD mass balance for the UASR (as shown in Table 2) was computed considering all the metabolites products, the hydrogen gas produced and the equivalent COD for the biomass produced. Due to neglecting the fraction of TCOD-in consumed for cell maintenance, COD mass balance was in range of 75-79%.

Table 2: Total COD mass balance for UASR fed with starch processing wastewater

	F/M: 0.5	F/M: 0.9	F/M: 1.4	F/M: 1.9	F/M: 2.8
%H2/TCOD	7.2	7	7.3	4.5	1.9
%VSS-out/TCOD	14.2	14.2	17	11.4	3.8
% sCOD-eff./TCOD	54	56	53.3	60	73.3
TCOD balance	75.4	77.2	77.7	75.9	79

3.2 Hydrogen production prediction using artificial neural network (ANN)

The weight and bias matrices obtained after the training phase of the ANN model are (Considering F/M of 1.4 g-COD/g-VSS.d as an example):

w{1,1}-Weight to layer 1 from input 1

$$\begin{bmatrix} 0.084001 & 0.65162 & -3.7756 \\ -1.6458 & -2.4141 & -2.8493 \\ -2.4894 & -3.5307 & 1.4129 \\ -2.1641 & -0.40942 & -2.0165 \\ 1.5707 & -1.5567 & -2.6117 \\ 2.2163 & 0.35595 & -1.213 \\ 0.22762 & -1.2276 & -1.629 \\ -1.5982 & -2.1243 & 1.3171 \end{bmatrix}$$

w{2,1}-Weight to layer

$$\begin{bmatrix} 2.4439 & -1.0558 & -3.1638 & -1.5342 & -3.2593 & 0.37915 & -1.8359 & 0.9042 \\ -1.7234 & -3.5171 & -1.6365 & 2.6055 & -1.2856 & -1.8343 & 0.56262 & -1.0976 \\ 0.86665 & -2.086 & -4.3158 & -0.29104 & -2.1534 & -0.84887 & -0.13629 & 1.3392 \\ -0.7711 & -0.93364 & -1.7908 & 0.46598 & 0.60675 & 0.064624 & 1.9168 & 1.2497 \end{bmatrix}$$

w{3,2}-Weight to layer

$$\begin{bmatrix} 3.9218 & 1.8767 & -2.4566 & -0.46976 \end{bmatrix}$$

b{1}-Bias to layer 1

$$\begin{bmatrix} -2.1442 \\ -1.6322 \\ 0.88322 \\ 0.94842 \\ 2.0791 \\ 1.9504 \\ -2.7322 \\ -1.6713 \end{bmatrix}$$

b{2}-Bias to layer 2

$$\begin{bmatrix} -3.3475 \\ 1.7376 \\ 1.1933 \\ -4.1399 \end{bmatrix}$$

b{3}-Bias to layer 3

$$\begin{bmatrix} -0.85995 \end{bmatrix}$$

Figure 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 3).

It is observed that the output tracks the targets very well for training (R2-value= 0.945), validation (R2-value=0.652), and testing (R2-value=0.791). These values can be equivalent to a total response of R2-value= 0.849. In this case, the network response is satisfactory, and simulation can be used for entering new inputs.

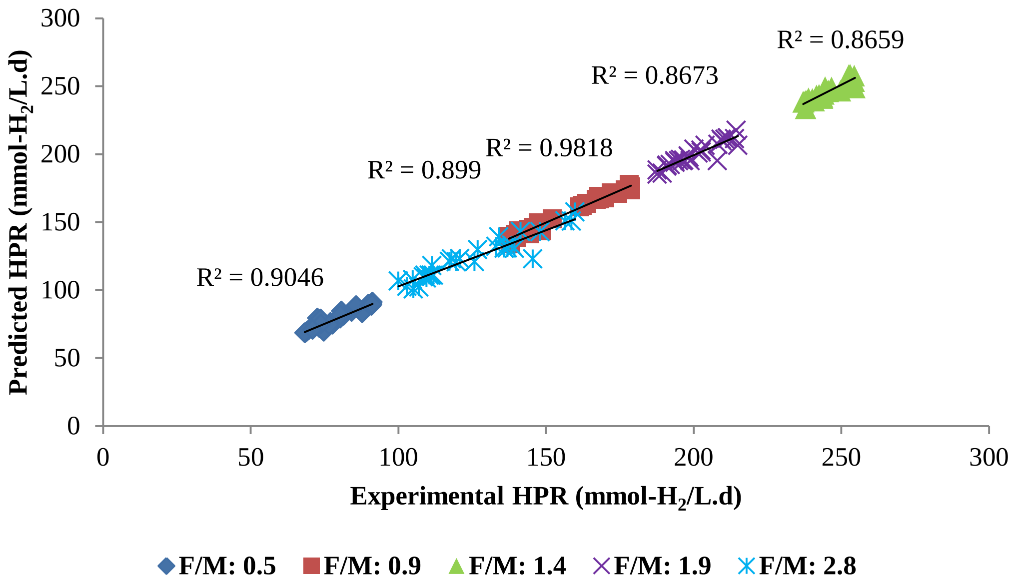

Figure 3: Correlation between experimental and predicted data used in ANN model

Table 3: Regression coefficient R2 of training, validation and testing the ANN

F/M (g-COD/g-VSS.d)	**0.5**	**0.9**	**1.4**	**1.9**	**2.8**	**Average**
Training R2	1.000	0.982	0.958	0.839	0.946	0.945
Validation R2	0.615	0.840	0.637	0.686	0.484	0.652
Testing R2	0.996	0.511	0.913	0.894	0.641	0.791
Overall R2	0.886	0.838	0.845	0.853	0.822	0.849

Previous studies in the literature investigated the modeling of biohydrogen production in batch studies using ANN (Table 4). However, there is no clear agreement on the specific input parameters for ANN modeling of biohydrogen systems.

Table 4: Comparison between this study and previous researches for ANN model

Input	**Output**	**Reactor**	**Substrate**	**Inoculum**	**ANN structure a**	**Data points**	**Reference**

OLR, pH, VSS yield	HPR	UASR	Starch	Thermal preheated sludge	3-8-4-1	30	This study
ORP, pH, dissolved CO2	HP with time	Batch	Cheese whey	E. coli	-	102	Rosales-Colunga et al. [18]
HRT, So, Xo, ethanol, organic acids conc., ORP, pH, recycle ratio, Alkalinity	HPR	CSTR	Sucrose	Sewage sludge	12-20-1	-	Nikhil et al. [19]
OLR, ORP, pH, alkalinity	HP	CSTR	Kitchen wastes	Anaerobic activated sludge	4-3-1	-	Shi et al. [20]
OLR, HRT, influent alkalinity	H2%, HPR, HY, TOCeff, products conc.	UASB	Sucrose	ADS	-	140	Mu et al. [21]
pH, glucose: xylose, inoculum size, inoculum age	Cumulative H2	Batch	Glucose xylose	Compost	4-10-1	16	Prakasham et al. [22]
T°C, pHi, So	HY	Batch	Glucose	ADS	3-4-1	20	Wang et al. [23]
T°C, pHi, So	Substrate degradation efficiency %, HPR, HY	Batch	Glucose	ADS	3-5-1	29	Wang et al. [24]

ORP: Oxidation reduction potential, HP: Hydrogen production, HRT: Hydraulic retention time, So: initial substrate concentration, Xo: initial biomass concentration, HPR: Hydrogen production rate, CSTR: Continuous stirred tank reactor, OLR: Organic loading rate, HY: Hydrogen yield, TOCeff: 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.

4 CONCLUSIONS

This study aimed at demonstrating the possibility of adapting ANN to predict HPR at different F/M ratios of 0.5, 0.9, 1.4, 1.9 and 2.8 g-COD/g-VSS.d. It is concluded that peak HPR of 246 mmol-H2/L.d was observed at F/M of 1.4 g-COD/g-VSS.d. The developed ANN model is a viable method for predicting the complex non-linear forms of HPR. ANN showed good ability to capture the interrelationships between dark fermentation process parameters, confirming its versatility. Average R2 of 0.945, 0.652, and 0.791 were achieved for training, validating, and testing data points, respectively.

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