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Research Article

Modeling of Ion Effect on Fermentation for Bioethanol Production using Artificial Neural Network (ANN)

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Abstract

The object of this study is modeling the effect of the interaction of Na, Ca and Mg ions on the ethanol fermentation process by using Artificial Neural Network (ANN). The obtained model results were compared with the optimised results by The Response Surface Method (RSM) and the experimental laboratory data obtained before. Model success criteria was measured via the parameters of Mean Squared Error (MSE) and the correlation coefficient (R). ANN model input variables were the concentration of ions Na, Ca and Mg (Ca: 69-2961 g/L, Na: 209-3621 g/L, Mg: 4-253 g/L) and output was percent ethanol yield. ANN training was done with the Levenberg–Marquardt feed forward algorithm and the data was categorised as 75% training, 15% validation and 15% testing. The maximum epoch value was determined as 14 iterations. R^2 values of the system were determined as 99% for education, 99% for validation and 99% for the whole biosorption system. MSE value was 0.0004 for education, 0.00381 for validation and 0.0285 for testing. Different activation functions such as logsig, tansig, purelin and different transfer training algorithm such as trainrp, trainbfg, trainlm and others were tried, tansig and trainlm gave the best results with higher R^2 value.

Keywords

Bioethanol, Artificial Neural Network, Modeling, Fermentation

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1. INTRODUCTION

In all of the world because of increasing technology and fast life, the need of energy also sustainable energy has become more important. Burning fossil fuels such as natural gas, oil and coal has significant importance for producing energy. Using fossil fuels as the main energy resources brings environmental pollution and global warming. Green house effect and catastrophic changes in the climate are main problems. Continued use of fossil fuels means that the world will face many problems related to the lack of primal materials and environmental pollution. All of these improvements say us it is necessary to find environmentally, friendly, renewable and sustainable energy by the government, industry and energy sector. Alternative fuels such as bio-diesel, bio-alcohol (methanol,ethanol, butane) are lower air pollutant and have more economic profits compare to fossil fuels [1].

Alternative fuels comes from natural resources but fossil fuels from petroleum. One of these alternative biofuels is bioethanol (ethylic alcohol or ethanol) which is high octane number and produces from fermentation of corn, potatoes, sugar cane, grains and etc. Ethanol is producted by fermentation process by different microorganisms such as bacteria, fungi and yeasts like *S. cerevisiae* [2].

Modeling studies of biofuels production process will increase the understanding the process dynamics and improve the ethanol production yield [3]. Biofuels are producted by fermentation and fermentation process systems include biological and chemical parts together. Fermentation process are difficult to model due to have both nonlinear and dynamic properties of microorganism metabolic process. Fermentation process runs take place in a quite short and large differences exist between different runs [4].

Most simple mathematical models are unable to describe the behaviour of the fermentation process well and researchers get attention on intelligent computation systems such as neural network, fuzzy, anfis and other algorithms [5]. One of these methods, ANN, as one of the modern modeling methods in recent years, has received considerable interest in modeling chemical and biochemical processes with complex input-output relationships [6].

In literatüre, Betiku and Taiwo applied ANN and RSM for investigating the optimization of fermentation parameters. Feedforward multilayer network structure with hyperbolic tangent function was used, R^2 value was found 1 for ANN, 0.99 for RSM [7]. Ahmadian-Moghadam et al. examined bioethanol production from sugar beet with *S. cerevisiae* microorganism in a laboratory environment. Live and dead form of cell and sugar concentration were chosen as an input variable for ANN to create a precise model that would benefit during alcohol production. With the value of 0.92 R^2, they concluded that the ANN modeled the system quite well [8]. Rahman et al. investigated the bioethanol production by using Jatropha curcas. Production parameters were chosen as input variable and the glucose and the bioethanol concentration were in the output layer. ANN with feedback with the Tansig transfer function was used and results showed that ANN was found to be very successful with a small error value of 0.0390 [9]. Nagata and Chu optimised the fermentation medium for the production of the enzyme hydantoinase by *Agrobacterium radiobacter* by ANN and genetic algorithms (GA). ANN model inputs were optimised by GA to find the maximum enzyme and cell production [10]. Zentou et al. used Andrews and Monod models for molasses fermentation [11].

Ion effects for improving the bioethanol product efficiency has been studied by researchers for along time. Yeast cell physiology effects the fermentation process efficiency directly and some metal ions such as K, Mg, Ca and Zn are very important for this physiology. Yeast needs metals ion in fermentation process for cell-cell interactions, gene expression, cell growth and division. Literature studies showed that cationic nutrients such as K, Mg, Ca and Zn effect the fermentation process for *S. cerevisiae* [12].

In literature for metal ions effect studies, Nabais et al. found that the addition of Ca^{2+} ion at optimum concentration 0.025 mM caused higher concentrations of ethanol by *S. cerevisiae*, S. bayanus, and Kluyveromyces marxianus [13]. Fakruddin et al. studied effect of adding Ca, Mg, Cr and Na to the fermentation medium and found that Cr had positive effect on ethanol production [14]. Xu et al. used Ca to see the ion effect on fermentation process they found that high calcium concentration improve the ethanol production rate [15]. Palukurty et al. found optimum metal ion concentration $FeSO_4$. $7H_2O$ 0.0036g/L, $MgSO_4.7H_2O$ 0.0033 g/L, $MnCl_2$. $4H_2O$ 0.0017 g/L and $ZnSO_4.7H_2O$ 0.0026 g/L to get maximum bioethanol production rate by Lackett-Burman and Box-Behnken design method. The ethanol yield has increased to 94.8 from 75.4 g/L [16]. Soyuduru et al. investigated Ca, Na, and Mg ion effects on bioethanol production by *S. cerevisiae*. They used RSM experimental design method and compare the modeling results with experimental results. The maximum ethanol concentration of 3.73% (v/v) was obtained at Ca, Na, and Mg concentration were 1.515, 930, and 128 mg/L, respectively [17].

In this study, as a continuation of the study by Soyuduru et al., the ethanol yield values obtained by ANN and results were compared. Due to dynamic, complex and unsteady status of the fermentation process, modeling is important to know effect of different parameters on ethanol production efficiency without spending time and cost. Also this study will contribute to the literature since there are very few studies on the modeling of bioethanol fermentation processes.

2. MATERIALS AND METHODS

2.1. Model Theory

The first ANN model was carried out by a neuroscientist Walter Pitts and a mathematician Warren McCulloch in 1943 [18]. Neurons are basic processing element of the central nervous system about 10 billion in the human brain. Neuron consist of 3 component; cell body, dendrites and axons [19]. ANN is a mathematical system and consist of many mathematical processing units together. Human brain acquired by living learns through experiences. Artificial neural networks similar to the human brain unlike mathematical methods by training the relationship between input and output data.

Generally in ANN three layers are available as input, hidden and output layer. A certain number of neurons are linked to neurons in other layers. One the signal from the neuron to the other neuron is reaches the other neuron after it is multiplied by the signal number. These weights are updated to achieve a more suitable result.

Data is first enter into layer, then hidden layer and exit respectively and output data is obtained as shown at Figure 1.

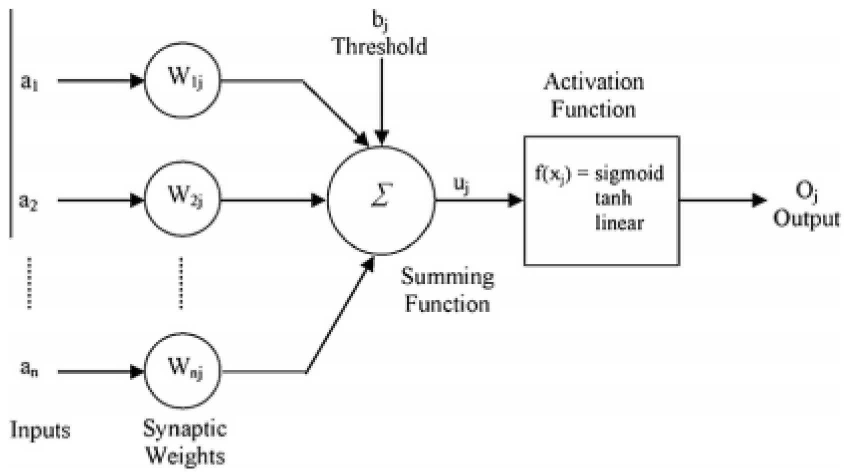

Figure 1. Working principle of an artificial neuron

Numeric input values a_1, a_2,….a_n is multiplied by weight numbers W_{1j}, W_{2j}, and W_{nj} and net input is created. Net input is converted into output with the help of an transfer function. Bias b_j, is other input for the system.

$$u_{j=} \sum_{i=1}^{n}(W_{ij} * a_i) + b_j \quad (1)$$

Transfer function calculates the net input to a neuron by converting the value it gets into a real output with an algorithm. Depending on the transfer function used, the output value is usually between [-1,1] or [0,1]. Transfer function is generally a nonlinear function which allows artificial neural networks to be complex and very different problems.

Commonly used transfer functions are as follows [20]:

Sigmoid transfer function:

$$f(x) = \frac{1}{1+e^{-x}} \qquad 0 \le f(x) \le 1 \tag{2}$$

Hyperbolic tangent transfer function

$$f(x) = \tanh(x) = \frac{e^{z}-e^{-x}}{e^{z}+e^{-x}} \quad -1 \le f(x) \le 1 \tag{3}$$

Linear transfer function

$$\mathrm{f}(x) = \mathrm{x} \qquad -\infty \le f(x) \le +\infty \tag{4}$$

The success of the training set is determined with the values of the differences between the desired output values and the values produced by the network The weight values of the connections are changed using this information. Typical main error fuction MSE is as shown Equation 5. Correlation coefficient R^2 can be used along with R to analyse network performance as shown Equation 6.

MSE and R^2 shows the prediction performance of the network. Generally a R^2 value grater than 0.9 indicates a very satisfactory model performance while a R^2 value in the range 0.8-0.9 signifies a good performance, and the value less than 0.8 indicates a rather unsatisfactory model performance [21].

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(Y_{observed} - Y_{predicted}) \tag{5}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(Y_{observed}-Y_{predicted})^2}{\sum_{i=1}^{n}(Y_{observed}-Y_{mean})^2} \tag{6}$$

2.2. Tuning Parameters of ANN

ANN network architecture is very important to get best modeling result. Architectures of ANN effects the results directly and it depends on the problem type and the way you choose the parameters.

Input and Output: number of input can change according to problem but if they haven't much more effect on results increasing input number only change time to train. Output was chosen to which value wanted to be predicted and maximised [22].

Dataset: ANN use dataset for predicting the output. Data set is cathegorised such as training, validation and test data sets. A training dataset is a dataset of examples used for learning, test data set is used to test training results until the results are good training will continue. Validation dataset is used to make sure that training and test data sets are working on the way. There are any rules to determine the number of data in each data sets. Division can be done 75:15:15, 60:20:20,…etc. Generally from the literature it can be observed that if data set is large any division is suitable but if data set is small generally 75:15:15 ratio is used [23, 24].

Number of hidden layers: for complex nonlinear system single hidden layer is suitable [25]. More hidden layer number brings overfitting problem also too few hidden layer number can bring a problem that in model the interactions between inputs are not fully developed [26].

Number of hidden layer in neurons: the problem that finding the suitable number of the number of neurons in hidden layer is an unknown issue and there is no systematic way to consider this number and it can be found by trial and error method. At this trial and error stage the main objective is to find the neuron number that produce the lowest error values and higher R^2 value.

Transfer Function: selecting the transfer function is also important for ANN. The transfer function is necessary for converting the input signals to output signals and introduce non-linearity into the network. Different studies showed that for the complex and nonlinear biological and chemical systems the advantages of tansig become more apparent [27].

Training Function: training function such as trainrp, traincgp, trainbfg, trainlm, traingdm, trainr and traingdx must be selected to minimise the differency between the predicted value and target value also error of prediction [28].Trainlm is generally the fastest backpropagation algorithm than others and is highly recommended. The Levenberg-Marquardt algorithm uses the steepest descent method and the Gauss-Newton algorithm together and it provides high speed and stability [29].

3. RESULTS AND DISCUSSION

In this study, the effect of the interaction of Na, Ca and Mg ions on the ethanol fermentation process was investigated by ANN. For ANN application Neural Fitting toolbox, Matlab R2017a was used. Three different metal ions concentration was chosen as an input for this study and output was % ethanol yield which was wanted to be predicted and maximised. In this study data set was small with 20 experimental point and divided into 75% training, 15% validation and 15% testing (75:15:15). The maximum epoch value was determined as 14 iterations as shown Figure 2. The Levenberg-Marquardt algorithm with the feed forward algorithm was used. Fermentation process is highly nonlinear and unsteady process so for this study one single hidden layer was suitable. Tangent sigmoid (tansig) was used in the hidden layer as a transfer function because of nonlineaity and complexity of the bioethanol process. Number of neurons in the hidden layer were by trial and error varying from 1 to 10 and results were given at Table 1. Optimum number of hidden neuron was found 4 with R^2 0.99.

Table 1. R^2 values for different neuron number

Neuron number	R^2	Neuron number	R^2
1	0.73	6	0.89
2	0.94	7	0.62
3	0.74	8	0.68
4	**0.99**	9	0.82
5	0.91	10	0.77

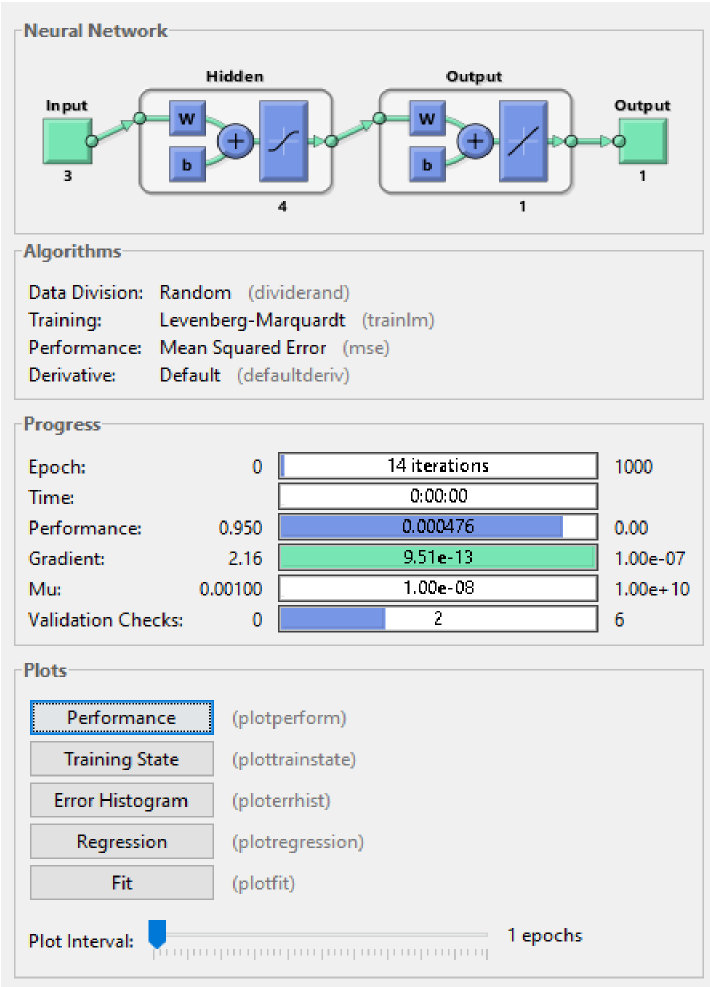

Figure 2. ANN topology image

Different transfer functions ‘‘logsig” and “purelin” were tested as transfer function and R^2 values of the system determined 0.57 with logsis and 0.67 with purelin transfer function as seen from Figure 3.

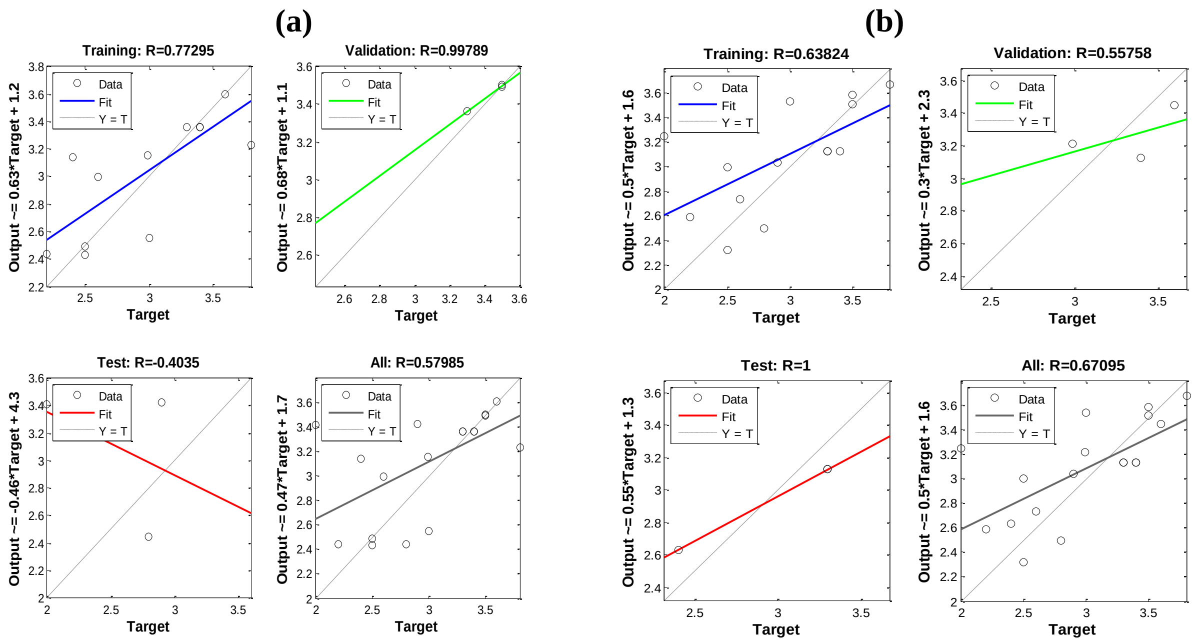

Figure 3. Network regression for different transfer functions **(a)** Logsis **(b)** Purelin

The effect of learning algorithm function on ANN was studied by using 7 different learning algorithm function (Table 2) and results showed trainlm gave the best result with higher R^2 value.

Table 2. Performance of training functions

	Transfer Function	$\mathbf{R^2}$
trainrp	RPROP backpropagation	0.92
traincgp	Conjugate gradient backpropagation with Polak-Ribiere updates	0.41
trainbfg	BFGS quasi-Newton backpropagation	0.76
trainlm	**Levenberg-Marquardt backpropagation**	**0.99**
traingdm	Gradient descent with momentum	0.82
trainr	Random order incremental training w/learning functions	0.88
traingdx	Gradient descent w/momentum & adaptive lr backpropagation	0.44

R^2 values of the system were determined as 99% for education, 99% for validation and 99% for the whole biosorption system as shown Figure 4. MSE value was 0.0004 for education, 0.00381 for validation and 0.0285 for testing.

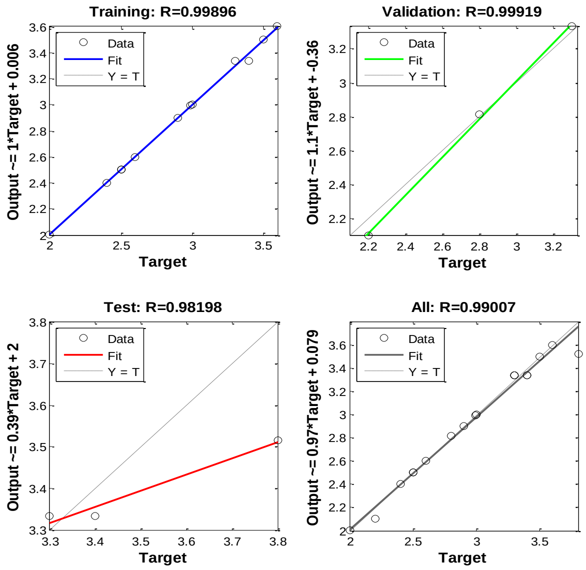

Figure 4. Network regression

When Figure 4 is examined, the graphs consist of three indicators, Data, Fit and Y = T. While the experimental data used in network education is included in the X axis, the estimated values 200Bare located in the Y axis. The fit line represented the relationship between the input and the estimated value. Y=T line is the targeted line where the real value and the estimated value are equal. Data are model estimation values obtained by ANN. The high correlation coefficient values obtained and the ANN can learn the difficult relationship between the input and output data in the best way and will give the closest output to the desired values and it turns out that the output variable ispredicted with high accuracy.

Soyuduru et al. used RSM for modeling studies and they found the maximum ethanol yield 3.73 % with R^2=0.91. In this study modeling study was done by ANN for same experimental results and maximum ethanol yield was found 4.02 % with R^2= 0.99. Similar the literature, this study showed that well trained ANN showed better predictability and gave better result than RSM with high ethanol yield and R^2 [30-32].

4. CONCLUSIONS

Modeling of the bioethanol production process is difficult due to its non-linear and complex structure. Modeling studies reduce the power consumption and increase the production rate. In this study the effect of the interaction of Na, Ca and Mg ions on the ethanol fermentation process was investigated by Artificial Neural Network (ANN). The model results obtained with ANN were compared with the experimental data and RSM model outputs. It showed that RSM and ANN modeling tools gave good results but ANN gave good predictions with high R^2 (0.99) and low MSE values than RSM with R^2 0.91. The ANN model is superior for both data fitting and prediction capabilities in comparison to the RSM model.

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