Simulation of the biodegradation of petroleum hydrocarbons utilizing Artificial Neural Networks

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Abstract - Prediction of the biodegradation of petroleum hydrocarbons, under any experimental approach is considered as a highly stochastic process. This paper presents the development of an artificial neural network (ANN) model to predict the biodegradation of petroleum hydrocarbon by Pseudomonas alkanolytica via rotating biological contractor reactor (RBC). Experimental data were collected and analyzed to predict the biodegradation of hydrocarbon under different parameters. The model structure is based on varying three input variables, such as initial biomass, hydrocarbon source and the number of rotating. The results obtained show that the proposed ANN model with a nonlinear architecture could provide significant level of prediction for the biodegradation of hydrocarbons and provided a high level of accuracy for the training and testing stages with a maximum error of 10 % and 2% respectively.

Key words - biological treatment; hydrocarbon dodecane; Pseudomonas alkanolytica; rotating biological Contractor (RBC).

I. INTRODUCTION

During petroleum and gas industry process huge amount of waste stream is produced. This stream is usually contaminated with pollutants, such as heavy metals, organic compounds, and dissolved/suspended solids [1, 2]. The environmental impacts of petroleum are often negative because they are toxic to almost all life styles. There, for various operational problems are faced during biodegradation of hydrocarbon-rich industrial in bioreactors using heterotrophic microorganisms. An ecological way to remove these contaminants is to use biodegradation process using microorganisms as reported by [3, 4, 5]. Petroleum hydrocarbons are accounted as one of the major pollutants found during most of industrial processes.

Alternatively hydrocarbons can be treated by chemical process but the use of biological treatment using biomass microorganism/microalgae has been declared as promising biotechnology [6]. The treating of oily wastewaters is very widespread in the entire oil industry, in petroleum refining, in oil storage, in petroleum transportation, and in the petrochemical industry [7]. Biological treatment is an effective and economical approach that can be used in oil de-emulsification and wastewater treatment. The biological wastewater treatment of hydrocarbons using mixed or pure bacterial cultures has attracted substantial interest recently due to its high conversion and non-polluting nature and these methods have little impact on the environment as reported by [8, 9]. Artificial neural networks (ANN) is an information processing system that is inspired by the way such as biological nervous systems similar to brain. It can be defined as a mathematical representation of the neurological functioning of a brain. Therefore, it has the capability to simulate the brain's learning process through a mathematically modeling the network structure of interconnected nerve cells and that is a substantiality advantage [10].

ANNs are densely interconnected processing units that utilize parallel computation algorithms. Numerous studies have reported the use of ANN models in other fields of environmental engineering applications and have been successfully applied as reported by [10, 11,12]. Prediction of the biodegradation of hydrocarbons rates within bioreactors is a key step for the design, monitoring and management of biodegradation.

ANN model is a significant progress in the field of nonlinear pattern recognition and system control theory. Therefore, ANN has the ability to predict the biodegradation of hydrocarbon in RBC reactor. The main goal of this study is to utilize the ANN technique as a prediction model for biodegradation hydrocarbons, especially from *Pseudomonas alkanolytica* (ATCC 13564). The model architecture is based on varying variables, such as initial biomass, hydrocarbon source as substrate concentration and number of rotating.

II. MATERIALS AND METHODS

Experimental set up and data collection

Pseudomonas alkanolytica culture stock was obtained from a culture collection maintained at the Chemical and Material Engineering Department King Abdulaziz University, KSA and reported previously by [3]. In this work marmul+ was used as a medium, this medium is a synthetic produced water similar to the water produced from one of the wells in the Middle East as reported by [13]. This medium was incubated aerobically in distillate water under mixing. Mineral medium salt containing: 3.15g Na_2HPO_4, 1.75g KH_2PO_4, 0.2g $MgSO_4.7H_2O$, 2g $(NH_4)SO_4$, 0.05g $CaCl_2$, 0.001g $FeSO_4.7H_2O$, 0.01g H_3BO_3, 0.01g $MnSO_4.7H_2O$, 0.07g $ZnSO_4$. $7H_2O$, 0.01g $(NH4)_6$ $Mo7O_4$. $4H_2O$, 0.05g $CuSO_4.5H_2O$ per liter of distilled water. The concentration of glucose will be fixed 5g/l for growth. During the experiments the pH solution medium was adjusted at 7± 0.2 with a solution of NaOH (1N). In this project the dodecane was used as a source of hydrocarbon with low solubility in water (0.0037 mg/l at 25°C) and rotating biological contactor RBC as reactor was used to treat the produced water continuously at laboratory scale.

Experimental data and ANN structure

The target of ANN is compute output values from input values by some internal calculations. Therefore, the main approach of ANN model is important modeling tool for learning from delegated examples without providing special programming modules to simulate special patterns in the data set problems [14]. There are many different types of training algorithms, the most commonly used algorithm in ANN is the backpropagation (Bp) neural network [15]. Figure 1 shows that the algorithms can predict the correct outputs for a given set of inputs as presented in Fig. 1.

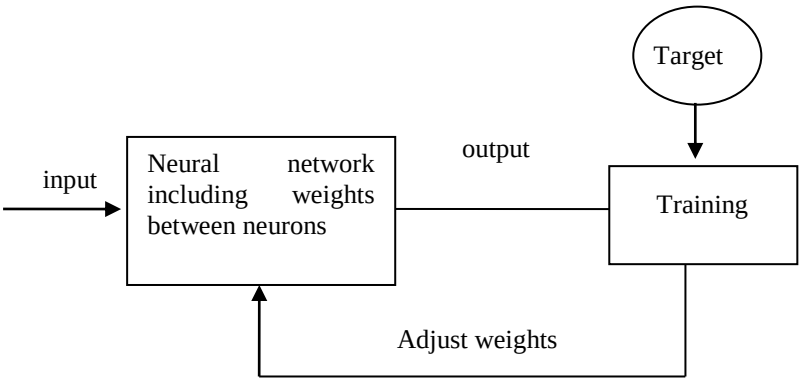

Fig.1: training stage structure in neural network.

In this paper, ANN was considered and chosen the input parameters were initial substrate concentration (So), initial biomass concentration (Xo), and number of rotating (N) to predict the biodegradation of hydrocarbons with time. The main principle approach in this training (Bp) algorithm is calculated the error between the model results of the output neurons and the actual outputs as called mean square error (MSE), the mean absolute error (MAE) with correlation coefficient used to evaluate the model. However,(MSEreg) is called the regularization technique includes modifying the performance function which is normally chosen to be the sum of squares of the network errors on the training set, α is the performance ratio that takes values between 0 and 1. The mean squares of the network weights and biases can be evaluated by equation (3) [16]. Randomly the weights are initially selected and then an iterative algorithm is used to find the weights that minimize the differences between the model-calculated and the actual outputs. MSW is mean squares of the network weights and biases, where n is the number of weights utilized inside the network structure and w is weight matrix of the network. The algorithm adjusts the weights in each successive layer to reduce the error.

$$MSE = \frac{\sum_{i=1}^{n}(Y-Y^{-})^2}{n} \quad (1)$$

$$MAR = \frac{\sum|Y-Y^{-}|}{N} * 100 \quad (2)$$

$$MSE_{reg} = \alpha * MSE + (1- \alpha) * MSW \quad (3)$$

$$\text{MSW} = \frac{1}{n}\sum_{j=1}^{n=1} w^2{}_j \quad (4)$$

Where Y is the experimental data, Y^- is the predicted data and n is the number of experimental data.

Model performance

Figure 2 shows the pathway of the single node of a neural network during hidden layers, various data points with replicates were collected and the ranges for the input and output variables were normalized in the range of (+1,-1). The data points randomly divides as 85% are used for training; 15% are used for testing processes. Numerous trials were tested to estimate number of neurons in the hidden layers. The transfer function can be used to estimate an output signal by multiplied the corresponding weight factor with the input parameters. Equation (4) can be used to determine the neuron output Uj.

$$U_{j=\sum_{i=1}^{n}\left(W_{ij*X_i}\right)+ b_j} \quad (5)$$

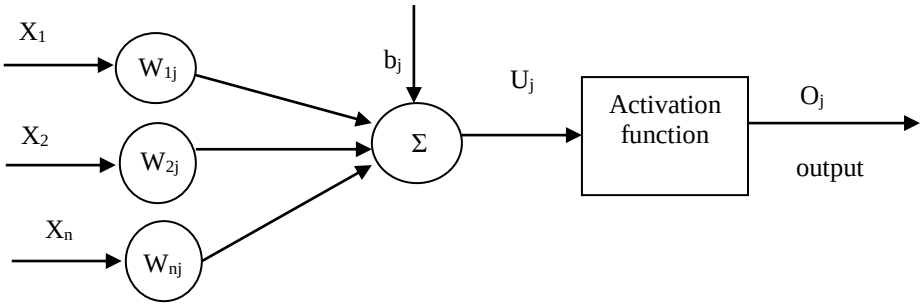

Fig. 2: Single node pathway of the neural network during hidden layers

Where: X_1, X_2 and X_n are represented the inputs parameters, W_1j, W_2j, and W_3j, are weight factors associated with the inputs to the node. Oj is the output and bj, is the bias.

ANN has an input layer, one or more hidden layers, and an output layer. ANN is able to describe the interactive effects among these different parameters in a complicated bioprocess by adjusting the values of the weights between elements (based on a comparison of the output and the target) until the network output matches the target Illustrated in Figure 3. After the training phase the weight and bias were obtained in a matrices. These matrix were between input, hidden layers and output, ANN configuration and the type of transfer functions between the input, hidden layers and output layer. The transfer function can transform the node's net input in a linear or non-linear manner using three different types of transfer functions as: sigmoid transfer, tangent transfer and linear transfer functions.

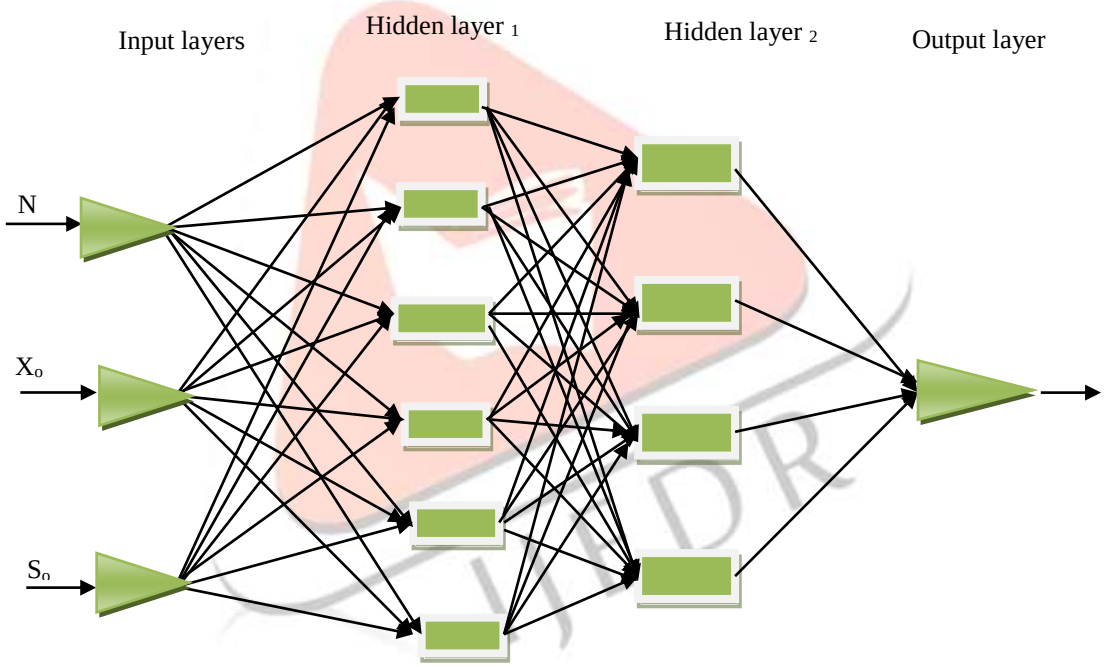

Fig. 3. Artificial neural network (ANN) configuration.

III. RESULTS AND DISCUSSION

Fig. 3 is utilized to provide the prediction of biodegradation hydrocarbon with its related variables such as, initial biomass, hydrocarbon concentration and number of rotating. Algorithm (BP) was used as input vectors and corresponding target vectors to train an ANN. The ANN techniques based on this algorithm proved to have the ability to predict any records data experiment. This algorithm was utilized and tested with a configuration of 3-6-4-1 combined with sigmoid transfer functions sigmoid transfer, tangent transfer and linear transfer respectively. Therefore, all the neurons in the hidden layer were non-linear with a sigmoid transfer function. The neural networks model with a non linear sigmoid transfer function and linear output layer were capable of approximating any function with a finite number of discontinuities. Data points for biodegradation of hydrocarbon with input forward parameters, over 75 % records were fixed as the training session and the last 25% records utilized for the testing session in this work. The correlation coefficient, the mean absolute error, mean square error and regularization mean square error were used to estimate the model prediction utilizing equations (1, 2 and 3). Results shows a high accuracy and efficiency with sigmoid transfer functions were selected due to adjusted the weights in each layer to reduce inaccuracy based on a trial and error. Therefore, It was found the results demonstrated by ANN model was much more accurate and highly efficient. Figure 4 shows a linear regression performs between the network outputs and the corresponding targets, R-value =0.93823 and 0.90317 for training and testing processes respectively.

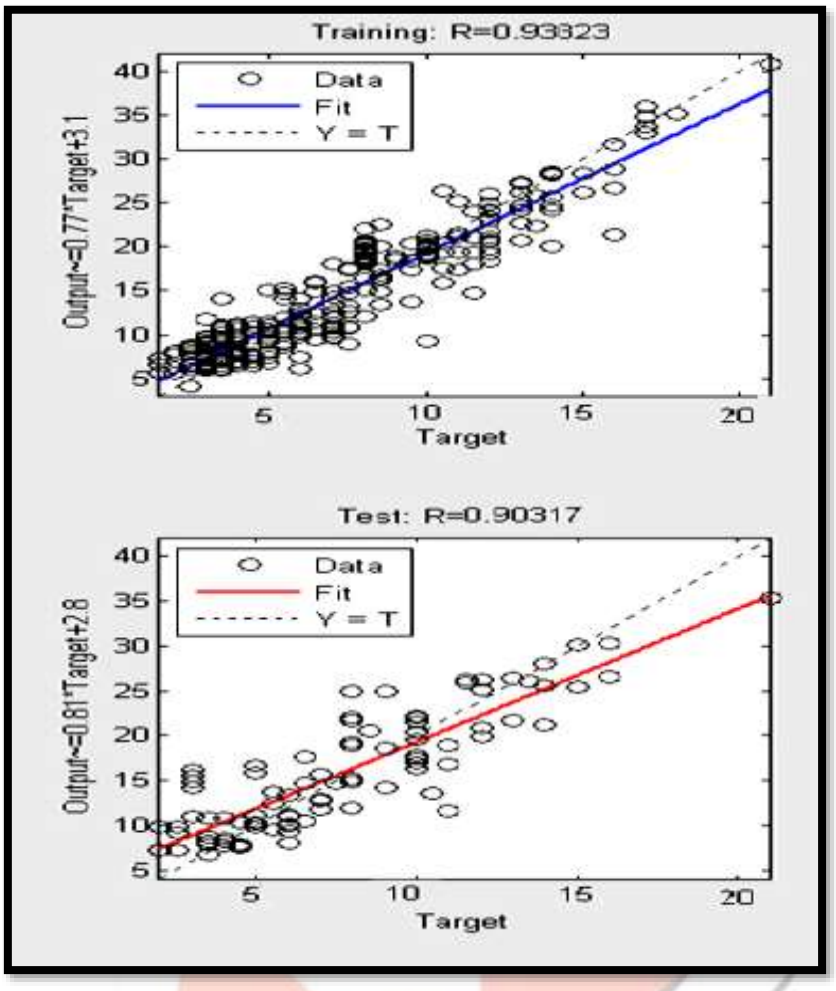

Figure 4. Neural network regression.

In this work the measured biodegradation of hydrocarbon with its associated variables over data experiments were used to train the specified ANN model both within the training and testing stages. Table 1 shows that the proposed ANN model could provide the biodegradation of hydrocarbon within error less than ± 8% during training stage using the prediction error equation the actual and prediction deference . This model was able to reduce the error in predicting biodegradation. On the other hand, during the testing session, that the ANN model achieve a prediction error lower than ± 5%. Table 2 shows the error in testing stage was more accurate noted at 6% inclusively. Results based on the ANN model obtained a higher level of accuracy.

Table 1. Experimental design for constructing ANN models during training stage.

Exp. No	Hydrocarbon consumed (Hc) (%) Experiment	Hc (%) by ANN	Prediction Error (%)
1	28.00	29.60	-2.71
2	54.00	56.81	3.20
3	43.21	44.53	3. 50
4	66.56	69.34	4.25
5	49.80	52.32	-4.10
6	67.08	63.40	5.20
7	65.61	68.90	-4.01
8	77.75	81.86	-5.35
9	41.06	42.52	-3.56
10	66.60	68.67	3.11
11	46.02	48.20	4.74
12	71.07	72.76	-2.38
13	45.09	49.30	-5.34
14	71.07	72.75	2.36
15	71.07	72.75	-2.36
16	53.45	52.22	2.01
17	44.21	42.02	3.05
18	69.55	70.25	-2.12
19	75.05	77.30	-3.95

20	65.60	68.70	-4.01

Table 2. Experimental design for constructing ANN models during testing stage.

Exp. No	Hydrocarbon consumed (Hc) (%) Experiment	Hc (%) by ANN	Error (%)
21	38.00	37.60	1.55
22	59.00	57.81	1.20
23	73.21	74.89	-1.59
24	65.56	66.34	-1.25
25	49.80	48.70	1.10
26	65.08	64.40	1.70
27	44.61	45.90	-1.31
20	55.60	56.70	-1.11

IV. CONCLUSION

The results obtained that the ANN model establish to be successfully used to predict biodegradation of hydrocarbon using *Pseudomonas alkanolytica* with three variables: initial biomass, hydrocarbon source as substrate concentration and number of rotating. Therefore, In this research ANN has been performed and show significant progress for nonlinear pattern. The sigmoid transfer functions were selected give more accurate estimation by adjusted the weights in each layer to reduce inaccuracy based on a trial and error.

V. ACKNOLOGMENT

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