Data Analysis of Photochemical Reactions using ANN

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ABSTRACT
Degradation of organic compounds using light energy is a kind of photochemical reactions. Large amount of data especially when multidimensional pose a difficulty in meaningful interpretation. Conventional methods are used to interpret data for such reactions. In recent times, various computational data analysis techniques like Artificial Neural Networks have been developed to solve the problems associated with a set of data. This paper examines analogies employed in computational data analysis technique and its comparison with conventional analytical technique for photochemical reaction under study.

Keywords
Photochemical reactions, Artificial Neural Networks, data analysis technique

1. INTRODUCTION
A photoreaction when accelerated by a catalyst is known as photocatalysis. Interests in recent years, has been focused on the use of photocatalysis for the degradation of organic species from aqueous phase. Photocatalysis has served for clean energy generation and several promising environmental applications. However, the current problem relates to the complexity of reactions and kinetics of photocatalytic degradation process. Recently, the availability of the computational support has involved assembling large amount of data which is beneficial for testing empirical claims. Artificial Neural Network is one of them being robust and reliable is capable to capture the non-linear relationship between variables in complex systems.

The Artificial Neural Network (ANN) is a tool used in simulation, prediction and modeling of processes in many areas of science and engineering [1].Bodaghi and Moradi, 2014 studied the photocatalytic degradation of Acid Red14 dye in aqueous solutions by uv/ nano TiO_2using ANN [2]. Abdolahi et. al. reported ANN modeling of p-cresol photodegradation [3]. ANN has been used to study many environmental organic pollutants such as ethylene- diamine tetra acetic acid [4], nitrilotriacetic acid [5], 2,4-dihidroxy benzoic acid [6] and decolorization of Cl Acid Blue 9 [7]. Khatee and Kasiri reported ANN modeling of contaminated water treatment processes by homogeneous and heterogeneous nanocatalysis [8] whereas, the application of ANN for modeling of the treatment of waste water contaminated with methyl tert-butyl ether (MTBE) by uv/ H_2O_2process has been observed by Salari et. al.[9]

In the present study, an artificial neural network was applied for modeling the CdS sensitized photocatalytic degradation of benzoic acid, an organic compound of industrial importance.

2. EXPERIMENT BY ANALYTICAL TECHNIQUE
0.1526 g of benzoic acid was dissolved in 250ml of doubly distilled water to prepare $5.0x10^{-3}$M stock solution. Photocatalytic degradation of benzoic acid was observed by preparing different concentration of benzoic acid solution and different amount of of CdS was added to it. This solution was exposed to varying light intensity from a 200 Watt tungsten lamp. At regular time interval an aliquot of 2.0 ml was taken out from the reaction mixture, to which 0.1 ml of blue litmus solution was added to develop a red colour. The optical density of this red solution was measured with the help of spectrophotometer (λmax = 530 nm).

3. EXPERIMENTAL DESIGN FOR ANN

3.1 ANN: A Description
In general, ANN's are mathematical models, inspired from the biology of the human brain, which has interconnected neurons responsible to process various complex information. Accordingly, a computational neural network has neuron (nodes) as a simple processing unit. Each network comprises of artificial neurons which are grouped into layers and related to each other by parallel connections. The weight associated with them is a direct measure of the strength exhibited by these interconnections. For every ANN, the first layer is input layer (independent variables) which via weights send data to the nodes of second layer (hidden layer) and then eventually to the third layer or output layer (dependent variable)[10]. The weighted sum of all the inputs of preceding layer is used to calculate the input to hidden and output layers. The weighted sum of the inputs transferred to hidden neurons is transformed using an activation function, which for input and hidden layer is sigmoid transfer function.

$$f(x) = \frac{1}{1+e^{-x}} \quad (1)$$

Whereas, the linear activation function is used as an output layer activation function.

$$f(x) = x \quad (2)$$

3.2 ANN modeling
The modeling of the photocatalytic degradation was carried out by MATLAB 2010 b(7.10.0.499) version. Experiments were designed by selecting pH, concentration of benzoic acid, light intensity, amount of photocatalyst, as independent variables (inputs), whereas, rate of reaction was selected as dependent variable i.e. output. It is evident in Figure 1. The experiment after being held by conventional technique in the lab, values obtained were used for ANN modeling. Training and Testing set of data are evident in Table 1. These data have been used to compute and confirm robustness of the network parameters respectively.

Table 1. ANN Modeling table

Training data

DATA	INPUT				OUTPUT	
Run	pH	Conc. of Benzoic Acid	Light Intensity	Amount of Photocatalyst	*Rate of Reaction*(Sec^{-1})	
					Actual	*Predicted*
1.	2.5	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**1.92 x 10^5**	**1.93 x 10^5**
2.	6.0	0.8 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**3.79 x 10^5**	**3.79 x 10^5**
3.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.06g	**4.44 x 10^5**	**4.44 x 10^5**
4.	6.0	1.6 x 10^{-3}M	40 $mWcm^{-2}$	0.14g	**3.51 x 10^5**	**3.51 x 10^5**
5.	3.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**2.13 x 10^5**	**2.13 x 10^5**
6.	6.0	1.0 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**4.02 x 10^5**	**4.02 x 10^5**
7.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.08g	**4.90 x 10^5**	**4.90 x 10^5**
8.	6.0	1.6 x 10^{-3}M	50 $mWcm^{-2}$	0.14g	**5.07 x 10^5**	**4.37 x 10^5**
9.	3.5	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**2.46 x 10^5**	**2.77 x 10^5**
10.	6.0	1.2 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**4.32 x 10^5**	**5.47 x 10^5**
11.	4.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**2.46 x 10^5**	**2.46 x 10^5**
12.	6.0	1.4 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**5.79 x 10^5**	6.**80 x 10^5**
13.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.10g	**5.31 x 10^5**	**5.73 x 10^5**
14.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.12g	**6.60 x 10^5**	**6.60 x 10^5**
15.	6.0	1.6 x 10^{-3}M	60 $mWcm^{-2}$	0.14g	**6.05 x 10^5**	**6.05 x 10^5**
16.	4.5	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**3.44 x 10^5**	**3.44 x 10^5**
17.	5.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**5.09 x 10^5**	**5.82 x 10^5**
18.	6.0	1.8 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**6.13 x 10^5**	**6.13 x 10^5**
19.	6.0	2.0 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**4.94 x 10^5**	**4.94 x 10^5**
20.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.16g	**7.40 x 10^5**	6.**96 x 10^5**
21.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.18g	**7.41 x 10^5**	6.66 **x 10^5**
22.	5.5	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**6.22 x 10^5**	6.70 **x 10^5**
23.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**7.42 x 10^5**	6.96 **x 10^5**
24.	6.0	2.2 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**4.21 x 10^5**	**4.21 x 10^5**
Testing data						
25.	6.0	2.4 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**3.29 x 10^5**	**3.29 x 10^5**
26.	6.5	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**5.74 x 10^5**	**7.07x 10^5**
27.	7.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**4.18 x 10^5**	4.14 **x 10^5**
28.	6.0	2.6 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**2.85 x 10^5**	**2.36 x 10^5**
29.	6.0	2.8 x 10^{-3}M	70 $mWcm^{-2}$	0.14g	**2.12 x 10^5**	**1.98 x 10^5**
30.	6.0	1.6 x 10^{-3}M	70 $mWcm^{-2}$	0.20g	**7.41 x 10^5**	6.**77 x 10^5**

The ANN was trained using the learning algorithmic program which included Levenberg Marquardt algorithm, Gradient Descent Back-propagation algorithm, Resilient Back-propagation algorithm, BFGS Quasi-Newton algorithm. The multilayer feed-forward perception (MCP) network consists of 4-10-1, 4-8-1, 4-10-1 and 4-10-1 architecture for LM algorithm, Gradient Descent Back-propagation algorithm, Resilient Back-propagation algorithm, BFGS Quasi-Newton algorithms respectively. The results are evident in Table 2 and Figure 2.

Table 2. Algorithm used for ANN

Learning Algorithm	**The architecture**	**RMSE**
Levenberg-Marquardt (LM)	**4-10-1**	**1.3015**
Gradient Descent back-propagation (GD)	4-8-1	1.5350
Resilient back-propagation	4-10-1	1.6315
BFGS quasi-Newton	4-10-1	4.9470

RMSE is based on the difference of actual and predicted values:

$$RMSE = \left(\frac{1}{n}\sum_{i=1}^{n}(y_i - y_{di})^2\right)^{1/2} \quad (3)$$

where, n = no. of point, y_i= predicted value and y_{di} = actual values. The minimum RMSE of the node examined demonstrate the desirable networks.

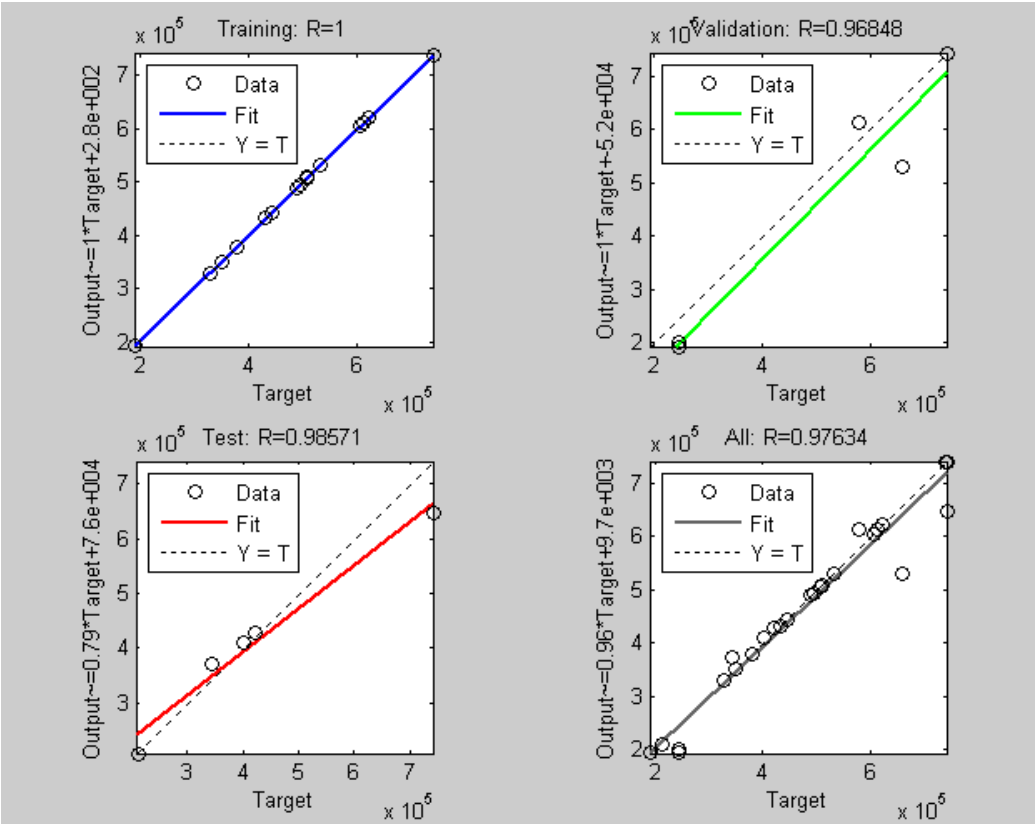

Fig. 1 The scatter plots of ANN predicted photocatalytic degradation of benzoic acid

4. RESULTS AND DISCUSSION

To determine optimum number of neurons in the hidden layer, a series of topologies were examined. Thereafter, RMSE was used as error function. The optimum topologies of the networks were 4-10-1, 4-8-1, 4-10-1 and 4-10-1 for LM algorithm, Gradient Descent Back-propagation algorithm, Resilient Back-propagation algorithm, BFGS Quasi-Newton algorithms respectively. Since LM algorithm has minimum value of RMSE, the performance of this algorithm with 4-10-1 topology was more effective than other studied algorithms.

5. CONCLUSION

The modeling of benzoic acid photocatalytic degradation was carried out by the ANN. The photocatalytic degradation was performed In CdS suspension under light. The model contained input, hidden and output layers. The input included pH, concentration of benzoic acid, light intensity and amount of photocatalyst while the rate of reaction was the output. To obtain optimum model, ANN was trained by LM, GD, and Resilient back-propagation and BFGS Quasi-Newton algorithms. The minimum RMSE values through the repeating data were used as indicator to determine the number of nodes in the hidden layer for each algorithm. RMSE was used as error function to compare optimum topologies. The comparison of the algorithm indicated that the LM algorithm had minimum 1.3015 RMSE which gave the best performance and was selected as the process model. Hence, concluded that the availability of ANN support has enabled a large amount of data to be assembled which benefited to test empirical claim

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