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Scaled Conjugate Back-Propagation Algorithm for Prediction of Phenol Adsorption Characteristics

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Abstract*: *In the present investigation the adsorption characteristics of phenol on the surface of chemically modified natural clay was predicted by using three-layer artificial neural network. The effect of various operational parameters on the adsorption process was determined by using scaled conjugate back-propagation algorithm. For this purpose, a feed forward network (5 - 11 - 1) with a learning rate of 0.02 was constructed. Various transfer functions such as, tangent sigmoid, saturated linear and positive linear were applied to hidden layer whereas pure linear transfer function was used in the output layer. The network performance was defined in terms of mean squared error (MSE) and validation error (VDE). The optimum number of neurons in the hidden layer was found to be 11 with "poselin" and "purelin" transfer functions in the hidden layer and output layer respectively. The MSE and VDE in this case were 2×10^{-5} and 5×10^{-5} respectively.

Index Terms*: *Adsorption, ANN, MSE, VDE.

I. INTRODUCTION

Inspired by biological neural system, an artificial network is constructed to simulate a given physical process. This network is called an artificial neural network (ANN). The inherent characteristics of solving complex nonlinear equations irrespective of any prior assumptions, recognizes ANN as a versatile mathematical tool of computer aided simulation of a given system [1]. The artificial neural network enables to predict the behavior of a process at an unknown experimental condition without actually performing any practical experiments. The physical aspects of mathematical modeling extends the creation of a nonlinear relationship between the input and output variables of a given physical process such as adsorption in order to prognosticate the removal efficiency [2]. Adsorption is one of such prevailing removal techniques which can be adopted for removal of wide variety of hazardous pollutants such as phenol even if it is present at a very lower concentration [3]. The presence of phenolic compounds inflates the immanent toxicity of the aquatic environment as it is carcinogenic and mutagenic in nature [4]. The minimum tolerance limit for phenol in drinking water is set aside by US Environmental Protection Agency (USEPA) and the Central Pollution Control Board (CPCB). In India the value is 0.5 mg/L [5]. Therefore, it has become very essential to remove phenol from aquatic environment by an efficient removal technique such as adsorption. Several efforts have been made so far to remove phenol by adsorption and to predict the adsorption characteristics through various mathematical modeling approaches [6–7]. However, very little or no effort was made to remove phenol by chemically modified natural clay. Therefore, in the present investigation the phenol removal characteristics on the surface of chemically treated natural clay was studied and the adsorption process was modeled by ANN.

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II. EXPERIMENTAL

A. Preparation of adsorbent

The adsorbent was prepared through chemical modification of natural clay collected from local Ganga basin by using zinc acetate dihydrate (98% pure) for 12 hours and subsequent washing with distilled water until the pH reached 7. The prepared adsorbent was then dried in an air oven at 105 °C for 30 mins. The procedure was elaborately described in previous study by Bhar et al. (2017).

B. Construction of ANN

The ANN helps to create an empirical relationship between the input and output variables of a physical process based on existing experimental data. The successful simulation of a given physical process is found to be dependent on several factors including number of neurons in the hidden layer, transfer function, training algorithm, momentum factor and training rate etc. The basic architecture of ANN mainly comprises of an input layer, a hidden layer and an output layer [9]. The input layer generally consists of input vectors which are nothing but various input parameters. The hidden layer is composed of vectors of N number of neurons which are functions of various factors such as network structure, number of iterations, training algorithm, transfer function, learning rate etc. ANN can be simulated using various algorithms such as Levenberg–Marquardt back-propagation (trainlm), resilient back-propagation (trainrp), scaled conjugate gradient (trainscg), Polak-Ribiére update (traincgp) and gradient.

descent back-propagation with various transfer fucnctions namely tangent sigmoid ("tansig"), saturated linear ("satlin") and positive linear ("poselin") and pure linear ("purelin").

C. Scaled Conjugate Gradient (trainscg)

The scaled conjugate gradient algorithm (SCG) was developed to save the computation time by avoiding line search at each iteration. In this algorithm a model-trust region approach is coupled up with the conjugate gradient approach [10]. For this purpose, reinitialization of weights and biases is done followed by retaining, using the scaled conjugate gradient algorithm. The change in weights for the second derivative are designated by a function sigma whereas, other parameter lamda defines indefiniteness of the Hessian matrix. Various parameters used in the training process in this algorithm are epochs, goal, time, min-grad, max-fail, sigma, lambda etc. The salient feature of scaled conjugate gradient algorithm (SCG) is the reduction of computation time and hence improving the system performance although it requires more iteration.

D. Different transfer functions

There are various transfer functions which are generally used for neural network training such as hyperbolic tangent transfer function ("tansig"), saturating linear transfer function ("satlin"), positive linear transfer function ("poselin") and pure linear transfer function ("purelin"). The "tansig" transfer function generates the output from the given input which lies in the range of -1 to +1. This function is equivalent to tangent hyperbolic function tanh(n) but it helps to produce more faster convergence than tanh [11]. Some physical models are seen to have approximately linear input-output characteristics where "purelin" transfer function is suitably applicable [12]. The saturating linear transfer function actually helps to determine the system output of a two-dimensional input matrix of the input elements by varying the value of the output parameter between 0 to +1. The positive linear transfer function also produces the system output in the same way as "satlin" transfer function but the only difference is in this case the output varies between 0 to ∞. The linear transfer function calculates a system output from its input variables and the output variables are varied between +1 to -1.

E. ANN for adsorptive removal

The experimental data are divided as 3:1:1 for training, test and validation purpose [13]. In the present study, scaled conjugate gradient ("trainscg") with positive linear transfer function ("poselin") in the hidden layer and pure linear transfer function in the output layer was used to train the network. The respective ranges of the input variables are shown in Table I. The performance of the developed model was judged by mean squared error and validation error. In the present study, ANN (MATLAB 7.6.0, R2008a) mathematical software is used to predict the phenol adsorption capacity of treated natural clay where a feed forward network has been taken into consideration.

Table I: The Range of Input Variables

Input parameters	Range
Initial pH	2 – 8
Initial concentration (mg/L)	60 – 120
Adsorbent dose (g/L)	1 – 3
Contact time (min)	5 – 120
Temperature (°C)	30 - 50

III. Results and Discussion

A. ANN modeling

The chances of over-training can be avoided through proper selection of hidden layer neurons for a given network. Therefore, the network performance is inherently improved by selection of optimum number of neuron in the hidden layer. The network performance is generally characterized by average deviation. In this study, the performance of the developed network was judged in terms of mean squared error (MSE) and validation error (VDE). Different numbers of neurons along with various transfer functions were used in the hidden layer to predict the phenol adsorption characteristics. For the present study "tansig", "satlin" and "poselin" transfer functions were applied to hidden layer with varying number of neurons from 5 – 11. The result is tabulated in Table II. As it is shown in Table II, the "satlin" and "poselin" transfer functions have similar correlation coefficient values which are close to 0.998 but their performance varies in terms of MSE and VDE. Therefore, by considering these errors "poselin" transfer function exhibits a better performance than "satlin" transfer function. The "purelin" transfer function was applied in the output layer which successfully predicts the process performance. Similar kind of behavior was also observed in the previous literature [14].

Table II: The comparison of various transfer functions

t_f	N	MSE	VDE	LR	R^2
"tansig"	5	0.00120	0.00079	0.02	0.998
	7	0.00110	0.00053	0.02	0.998
	9	0.00026	0.00070	0.02	0.999
	1	0.00095	0.00290	0.02	0.998
"satlin"	5	0.00200	0.00340	0.02	0.995
	7	0.00190	0.00170	0.02	0.996
	9	0.00110	0.00063	0.02	0.998
	1	0.00060	0.00025	0.02	0.999
"poselin"	5	0.00008	0.00006	0.02	0.999
	7	0.00006	0.00006	0.02	0.999
	9	0.00003	0.00001	0.02	0.999
	1	0.00002	0.00005	0.02	0.999

t_f = transfer function, N = number of neurons, LR = Learning rate

It can be seen from Table II that 11 numbers of neuron in the hidden layer produces mean squared error (2×10^{-5}) and validation error (5×10^{-5}). In the present investigation, the training, validation, and test errors as a function of the number of iterations taken were studied. The simulation result is shown in Fig. 1. It can be seen from Fig. 1 that the best validation resulted at 56 epochs.

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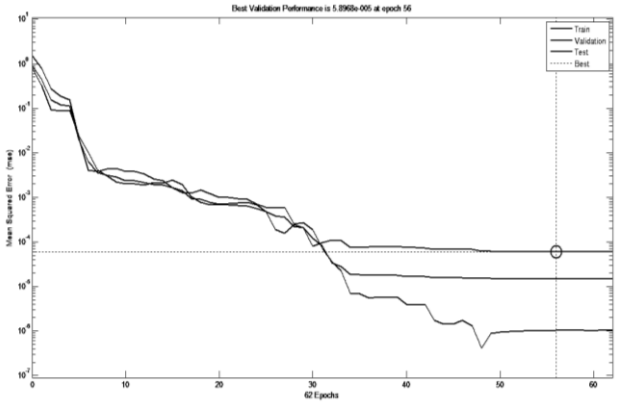

Fig. 1: Expression of various errors as a function of epochs

The rate of change of gradient was also determined as a function of epochs as shown in Fig. 2.

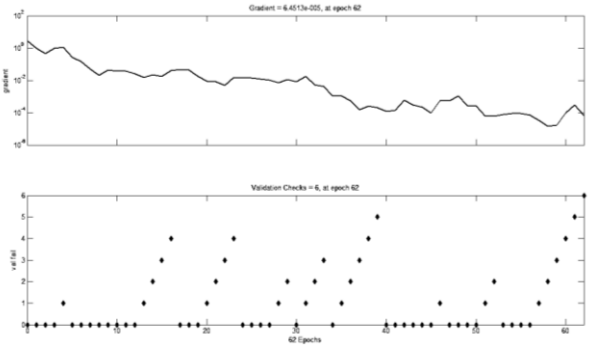

Fig. 2: Change in gradient as a function of epochs

It is evident from Fig. 2 that the rate of change of gradient has become 6×10^{-5} at 62^{th} epoch. The experimental values were also compared with the predictive values for training, test and validation steps. The comparison is shown in Fig. 3 and it can be seen from Fig 3 that both the values are in well agreement with each other for each cases. The values of regression coefficients (R^2) are also indicated in this figure.

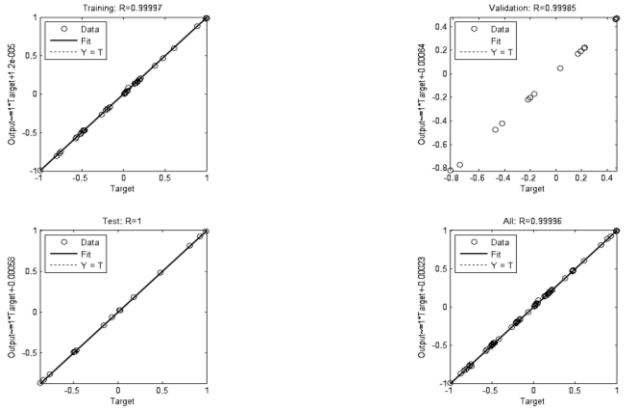

Fig. 3: Comparison of experimental and predicted values

IV. CONCLUSION

In the present work, chemically treated natural clay was employed to remove phenol from its aqueous solution and the adsorption characteristics of phenol were predicted by a three-layer artificial neural network. Scaled conjugate back-propagation algorithm with various transfer function in the hidden layer was applied to determine the optimum number of neurons in the hidden layer. The optimum number of neuron was found to be 11 with "poselin" and purelin transfer functions in the hidden and output layers respectively. The process performance was designated in terms of MSE (2×10^{-5}) and VDE (5×10^{-5}) respectively.

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