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Comparison of RSM and ANN Optimization Methods in Determining Antibacterial Properties of Cotton against *E. coli*

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In this paper, antibacterial properties of cotton fabric samples treated with nano titanium dioxide (NTO) and butane tetra carboxylic acid (BTCA) under different curing conditions (UV, High temp and UV-Temp) are compared. Response surface methodology (RSM) and artificial neural network (ANN) optimization methods are used to determine the antibacterial properties of samples and results of the two methods are compared with each other. The comparison between these two model optimization procedures shows clearly that ANN procedure can maximize *E. coli* reduction by 5 units more than that of RSM procedure.

Keywords: ANN, antibacterial, BTCA, NTO, RSM, UV.

In recent years, NTO attracts much attention because of their photo catalytic activity and ability to absorb ultra-violet irradiation[1]. In addition, the deposition of NTO particles on fabrics used to obtain different characteristics such as: self-cleaning[2], waste material and pollutants decomposition[3], harmful bacteria growth prevention[4], crease recovery angle improvement[5] and UV-protection[6].

TiO_2 has been attended more than other kind of nano particles, because of its chemical durability, reasonable cost, availability, non-poisoning, and optical properties[7]. When UV rays (λ< 388 nm), irradiate to TiO_2, an electron from the valence band exited to the conduction band, creating pairs of negative electrons (e^-) and positive holes (h^+)[8]. The construction of efficient species such as OH° has much activity for materials oxidation, organic pollutions and microorganism deactivation[9].

Over the past decade, multifunctional carboxylic acids have been used as non-formaldehyde durable press and cross linking agents for cotton[10]. Among the different investigated poly carboxylic acids, BTCA is the most effective cross linking agent for cotton[11]. Several studies have been conducted to use the NTO and BTCA in order to improve crease recovery angle[12].

In this paper Response Surface Methodology (RSM) and Artificial neural network (ANN) have been used to evaluate the effective parameters and create models for selecting optimum conditions of variables for a desirable response, Antibacterial Properties of Cotton Fabric against *E. coli* (Bacteria Reduction).

In statistics, response surface methodology (RSM) explores the relationships between several explanatory variables and one or more response variables. The method was introduced by G. E. P. Box and K. B. Wilson in 1951.

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The main idea of RSM is to use a sequence of designed experiments to obtain an optimal response. Box and Wilson suggest using a second-degree polynomial model to do this. They acknowledge that this model is only an approximation, but use it because such a model is easy to estimate and apply, even when little is known about the process. An easy way to estimate a first-degree polynomial model is to use a factorial experiment or a fractional factorial design. This is sufficient to determine which explanatory variables have an impact on the response variable(s) of interest. Once it is suspected that only significant explanatory variables are left, then a more complicated design, such as a central composite design can be implemented to estimate a second-degree polynomial model, which is still only an approximation at best. However, the second-degree model can be used to optimize (maximize, minimize, or attain a specific target for).

On the other hand, Artificial Neural Networks (ANNs) are arithmetical models inspired from the human brain. The main characteristic of this technique is ability of learning using experimental data. This model can predict patterns and behaviors from a finite set of experimental data, that called the "training set" of the ANN[13]. The structure of ANN typically consists of three layers including input, hidden and output layers. First primary data is collected in the input layer, and then send to the hidden layer of the networks[14]. The structure of a neuron consists of weight vectors and activation function is shown in Fig 1.

According to the inputs as shown the total input of the neuron is sum of all input values that each is multiplied by its weight and a bias term. Activation function receives an argument **n** and generates an output **a**. Many activation functions are used in ANN model such as: triangular basis, pure line, soft max, log sigmoid, tan sigmoid and hard limit. The ANN is trained to minimize the error between ANN output and experimental data, to achieve an acceptable predict.

METHOD

The samples of cotton fabric were prepared in14×5 cm^2 swatches. Bleaching treatment of cotton fiber was performed using 3.5% hydrogen peroxide and 2% sodium hydroxide (based on weight of fabric: o.w.f) at a liquor ratio of 8:1 under the boiling condition for 90 min. The dispersion of aqueous finishing was prepared with mixture of BTCA, SHP (60% of BTCA) and NTO with required distilled water in ultrasound bath for 30 min. The cotton fabrics were padded with 95% wet pick-up using freshly prepared aqueous solutions and dried at 65°C for 3 min followed by curing with different conditions: 15 min under UVA (UV), 180°C for 2 min (Temp) and UV-Temp. Then, the finished samples were washed at 75°C for 20 min with 1.5 g/L Na_2CO_3 and 1 g/L non-ionic detergent (Rucogen DEN), and finally dried at room temperature. One pathogenic microorganisms including *Escherichia coli* (*E.coli)* as Gram-negative was tested using AATCC 100-2004 test method. In this method, treated samples were placed adjacent to the bacteria suspension and exposed to (UV-C) irradiation for 30 min and then incubated for 24 h. The number of viable bacteria was colonies on the agar plate before and after NTO/BTCA treatment was counted and the results reported as percentages of bacteria reduction according to Eq. (1).

$$R(\%) = 100(A-B)/A \quad ...(1)$$

where (A) and (B) are the numbers of bacteria colonies recovered from the untreated and the treated cotton samples respectively after inoculation and (R) is the reduction percentage of bacteria colonies.

Experimental Design

The central composite design was used for experimental plan with three variables. These variables were amounts of BTCA, NTO and different curing conditions. The ranges of these variables were: BTCA (50.96-99.04 g/L), NTO (0.12-5.02%) and curing method (UV, High temp, UV-Temp). Details of the design for cotton fabric samples with BTCA in the presence of NTO are given in Table 4 (Run 1-39). Also, influence of the

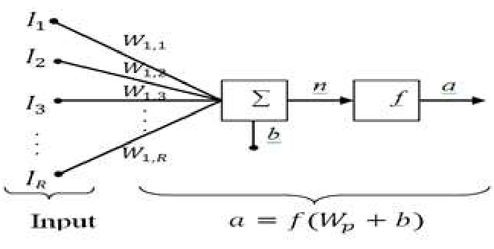

Fig. 1. A neuron structure

variables on the results Y (reduction of *E. Coli*) was adjusted using the following second order polynomial function:

$Y = b_0 + \Sigma b_i X_i + \Sigma b_{ij} X_i X_j + \Sigma c_i X_i^2$ i≥j i,j=1,2,3 ...(1)

In this equation, b_0 is an independent term according to the mean value of the experimental plan, b_i are regression coefficients that explain the influence of the variables in their linear form, b_{ij} are regression coefficients of the interaction terms between variables, and c_i are the coefficients of quadratic form of variables. The analysis of variance (ANOVA) is given in Table 1. According to the experimental design, the result was analyzed and approximating function of reduction of *E. coli* were obtained in below, respectively.

Reduction of *E. coli* = +84.02+5.39×BTCA + 5.66×NTO -9.65× C[1]+0.038×C[2]-2.80×AB-6.40×B^2 (2)

Therefore, maximizing the response variable (reduction of *E. coli*), the optimal values of input factors (BTCA, NTO and Curing) and predicted *E.Coli* reduction are 92.00, 2.96, UV-Temp and 99.34, respectively.

Modeling Approach in ANN

An ANN is based on the operation of biological neural networks. An artificial neuron is the fundamental processing unit of the ANN[15]. MLP networks are the most widely used ANNs[16]. The simplified overview of the proposed MLP model is shown in Fig.2, where the inputs are BTCA, NTO and the situation (UV-Temp-UV&Temp) and the output is the value of *E.coli* reduction.

Table 1. ANOVA for *E. coli*

Source	Sum of squares	Df	Mean Square	F Value	p-valueProb>F
Model	4841.91	6	806.98	108.97	<0.0001 signifcant
A [BTCA]	698.32	1	698.32	94.30	<0.0001
B [NTO]	768.22	1	768.22	103.73	<0.0001
C [Curing]	2411.38	2	1205.69	162.81	<0.0001
AB	94.08	1	94.08	12.70	0.0012
B^2	869.91	1	869.91	117.46	<0.0001
Residual	236.98	32	7.41		
Cor Total	5078.89	38			

Reduction of *E. coli* = +84.02+5.39×BTCA + 5.66×NTO -9.65× C[1]+0.038×C[2]-2.80×AB-6.40×B^2 (2)

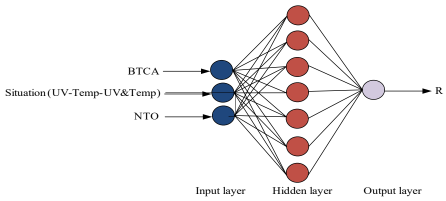

Fig. 2. Architecture for the proposed MLP model

The input to the node *t* in the first hidden layer can be written as

$$\eta_t = \sum_{u=1}^{2} (X_u W_{ut}) + \theta_t \quad t=1, 2, \ldots, 7 \qquad ...(1)$$

The output of the second hidden layer, from t^{th} neuron is given by:

Table 2. Specification of proposed ANN model

Neural network	MLP
Number of neurons in the input layer	3
Number of neurons in the hidden layer	7
Number of neurons in the output layer	1
Number of epochs	1750
Activation function	Tansig

Table 3. Obtained errors for training and testing results of the proposed ANN model

Test	Train	Error
0.0536	0.0066	MRE%
0.8935	0.6491	RMSE

$$O_t = f(\eta_t) \qquad ...(2)$$

where X is the input variables, θ is the bias term, W is the weighting factor and f represents the activation function of the hidden layer. The output of the neuron in the output layer can be shown as:

$$Y = \sum_{u=1}^{6}(O_u W_u) + b \qquad ...(3)$$

Levenberg-Marquardt (LM) algorithm is used to train the presented MLP network. In this method, first derivative and second derivative (hessian) matrices are used for network weight

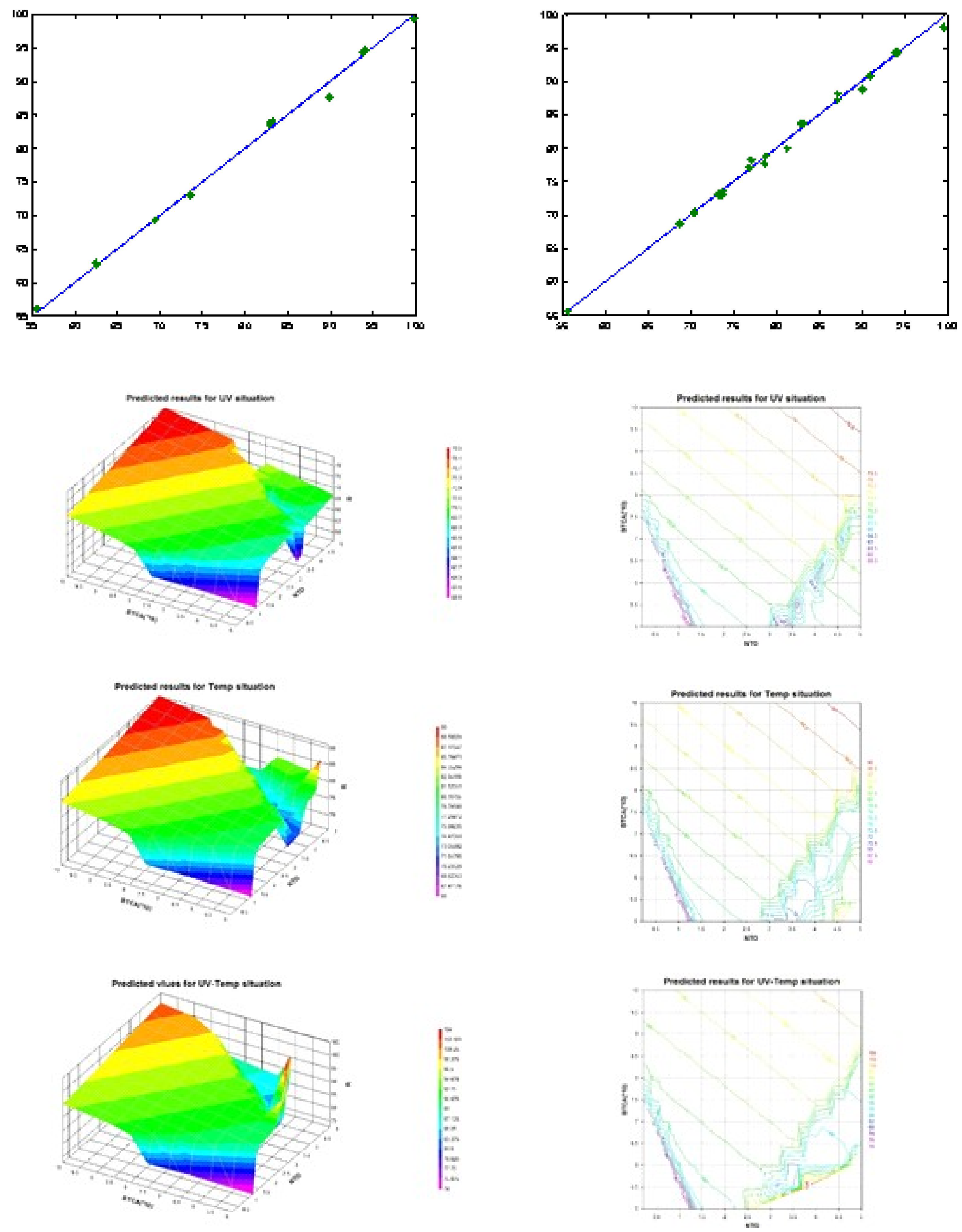

Fig. 3. Experimental and predicted results of the proposed ANN model for training and testing data

correcting. The number of samples for training and testing data are 28 (about 71%) and 11 (about 29%) respectively. In this study, for optimizing the ANN configuration many different structures with one, two, three and four hidden layers were tested by applying of different number of neurons in each layer and different epochs. MATLAB 7.0.4 software was used to train the ANN model. Table 2 shows the specification of the proposed ANN model being used in this study.

RESULTS AND DISCUSSION

Table 2 shows the obtained errors for train and test results of the proposed ANN model, where the mean relative error percentage (MRE %) and the roots mean square error (RMSE) are:

$$RMSE = \left[\frac{\sum_{m=1}^{N} (X_m(Exp) - X_m(Pred))^2}{N} \right]^{0.5} \quad ...(4)$$

Table 4. The data that were used for training the network and Predicted *E. coli* reduction

Exxp. Run	BTCA (g/L)	NTO (%)	Situation(UV=1, Temp=2, UV&Temp=3)	*E. coli* reduction	Predicted *E. coli* reduction
1	75	2.57	1	73.4	73.1391
2	58	4.3	2	78.72	78.7199
3	92	0.84	1	73.62	73.5503
4	50.96	2.57	2	81.28	79.9035
5	75	2.57	1	73.32	73.1391
6	75	2.57	3	94.02	94.2619
7	92	4.3	2	90.01	88.7625
8	75	2.57	3	93.91	94.2619
9	75	2.57	2	82.98	83.7501
10	75	2.57	3	94.08	94.2619
11	75	2.57	2	82.89	83.7501
12	75	5.02	3	87.15	88.1355
13	99.04	2.57	3	99.57	98.0595
14	75	5.02	1	70.34	70.3399
15	75	2.57	3	94.17	94.2619
16	75	0.12	3	68.59	68.5899
17	50.96	2.57	3	90.89	90.8899
18	58	4.3	3	87.23	87.2299
19	75	2.57	1	73.23	73.1391
20	75	2.57	2	83.06	83.7501
21	92	4.3	1	77.02	78.1988
22	75	2.57	2	83.15	83.7501
23	58	0.84	1	55.53	55.5299
24	75	2.57	1	73.57	73.1391
25	58	4.3	1	70.42	70.4199
26	99.04	2.57	1	76.81	77.0088
27	75	5.02	2	78.64	77.6543
28	58	0.84	3	68.72	68.7199
29	99.04	2.57	2	89.87	87.5836
30	75	0.12	2	62.38	62.9143
31	75	2.57	3	93.83	94.2619
32	50.96	2.57	1	69.36	69.2563
33	92	4.3	3	99.79	99.2274
34	92	0.84	2	83.19	84.1575
35	75	2.57	2	82.81	83.7501
36	92	0.84	3	94.04	94.6655
37	58	0.84	2	62.55	62.6429
38	75	0.12	1	55.49	56.1318
39	75	2.57	1	73.49	73.1391

$$MRE\,\% = 100 \times \frac{1}{N}\sum_{m=1}^{N}\left|\frac{X_m(Exp) - X_m(\mathrm{Pr}ed)}{X_m(Exp)}\right| \qquad ...(5)$$

where N is the number of the data points and '*X (Exp)*' and '*X* (*Pred)*' represent the experimental and predicted (ANN) values, respectively. Table 3 shows the obtained errors for training and testing results of the proposed ANN model

Fig.3 shows comparison between experimental and predicted results using the proposed ANN model for training and testing data.

Calculation of the above ANN procedure shows that the maximum of *E.coli* reduction will be equal to 105 provided that NTO=3.8 (%), BTCA=55 (g/L) and UV-Temp. However, RSM procedure provides maximum of *E.coli* reduction equal to 99.34 with NTO = 2.96 (%), BTCA = 92.00 (g/L) and UV-Temp. The comparison between these two model optimization procedures shows clearly that ANN procedure can maximize *E.Coli* reduction by 5 unit more than that of RSM procedure.

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