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Multi Linear Regression and Artificial Neural Network Modeling Performance for Predicting Coating Rate: Nano-Graphene Coated Cotton as a Case Study

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Abstract

To critique the proficiency of multilinear regression (MLR) and artificial neural network (ANN) models for predicting coating process is the major subject of this paper. The efficiency of coating nano-graphene particles on surface cotton as a case study was analyzed. Taguchi L27 orthogonal array was elected as experimental design. The Taguchi results were tested using both S/N (signal to noise) ratios and ANOVA (analysis of variance). The outcome of Taguchi design is labeled as the input for each of MLR and ANN models. The parameters for the MLR model and network architecture for the ANN model were amended. Comparing MLR performance with ANN method, ANOVA test and data analysis showed that ANN is at 99.9% confidence level to predict the process of covering graphene surface on cotton better than MLR model.

Keywords: Artificial neural network • Cotton • Graphene • Multi Linear Regression • Network architecture

Introduction

Graphene has a variety of applications when coatings on different materials, such as fibers [1], metal meshes [2], textiles [3], membranes [4], foams [5] and gauze [6]. Fibers have the maximum flexibility and minimum cost related to the rest. Cotton is a suitable selection to switch for graphene to a 3D framework [7]. Cotton fibers are non-toxic, lightweight and eco-friendly [8]. Pretreatment of fibers helps with the easy penetration of the nanoparticles into the surface. NaOH treatment of kapok/cotton fabric improves adhesion characteristics by creating surface roughness [9]. The experimentation has been effected on concentrations of NaOH solution on cellulose in fibers and wood [10-13]. Reduction agent helps to process of coating of cotton by graphene. Naturally, there are several kinds of the reducing agent such as HI, hydrazine derivate, Al, vitamin C in this case [1]. Also, the catalyst helps to accelerate reducing ability of GO. For example, $AlCl_3$ and $CaCl_2$ were used as catalysts [14,15].

Optimizing the factors affecting on coating cotton by graphene can carry out by a successful statistical method for analyzing and predicting chemical data. The chemometric is a way that widely applied in modeling of different science. To achieve sufficient input data for the appropriate model, experimental design Taguchi output had been used. Taguchi is considered an important role in designing methodology [16,17]. A good prediction model can be very powerful in providing a low-cost way to predict the rate and quality of the coating. To effectuate this, the MLR and ANN are the statistical tools are compared. In two options receive inputs (measured data), transmit and produce an output (response variable) [18,19].

The main intention of this study is to compare the abilities of MLR and ANN models predictive models that yield actual results. An adapted prediction model can be very successful in providing an inexpensive way to predict the rate of the coating.

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Materials and Methods

Chemicals and software

The natural cotton was obtained from a regional store. All of the chemical materials obtained from Merck, Germany. GO was processed in hummers procedure [20]. The MINITAB has been applied to create the Taguchi design and MLR model. ANN calculus was handled using the MATLAB software.

Procedure

A piece of cotton (about 1gr) was first soaked in 4% NaOH solution for one hour. Next, it was washed with 10% acetic acid solution and distilled water (up to pH=7). The resulting cotton was placed in a dispersion GO solution, $NaHB_4$ as reducer agent and $CaCl_2$ as a catalyst. Then, the mixture was kept stirring at room temperature for one hour to obtain RGO. Finally, the obtained graphene coated on cotton (GCC) was rinsed with distilled water and dried at 50-60°C [9,14,21].

Graphene oxide concentration, reducing reagent, catalyst and contact time is used for experimental tests. Table 1 enlisted the results of experiments designed by the Taguchi method. Table 2 shows 27 experiments obtained from Taguchi method instead of 1594323 experiments (3)13 that were required for one factor at a time method. Table 3 appears the ranging of the factors set upon by delta values (decrement between higher and lower S/N ratio). For S/N ratio analysis, choosing the "larger- the- better", because the goal of our experiment is enlarged the response. Table 4 shows, the GO concentration with 34.657% of contribution and time with 32.859% of the contribution, have the greatest effect among the factors.

Table 1. Levels for the various parameters studied to the coating rate.

Process parameter	GO (gr/l) concentration	Reagent reduction amount (gr)	Catalyst amount (gr)	Contact time (min)
Level 1 (L1)	0.025	0.500	0.01	30
Level 2 (L2)	0.050	0.570	0.02	60
Level 3 (L3)	0.075	0.687	0.03	90

Table 2. L_{27} orthogonal array design matrix along with the mean conversion values and the S/N ratios.

Run No.	GO (gr/l) concentration	Reagent reduction Amount (gr)	Catalyst amount (gr)	Contact Time (min)	Coating (%)	S/N ratio
1	0.025	0.500	0.01	0.3	94.20	39.48
2	0.050	0.570	0.01	60	59.50	35.49
3	0.075	0.687	0.01	90	97.50	39.78
4	0.025	0.570	0.02	90	77.60	37.79
5	0.050	0.687	0.02	30	82.50	38.33
6	0.075	0.500	0.02	60	89.20	39.00
7	0.025	0.687	0.03	60	80.10	38.07
8	0.050	0.500	0.03	90	91.90	39.26
9	0.075	0.570	0.03	30	98.10	39.83
10	0.025	0.500	0.01	30	94.20	39.48
11	0.050	0.570	0.01	60	59.50	35.49
12	0.075	0.687	0.01	90	97.50	39.78
13	0.025	0.570	0.02	90	77.60	37.79
14	0.050	0.687	0.02	30	82.50	38.33
15	0.075	0.500	0.02	60	89.20	39.00
16	0.025	0.687	0.03	60	80.10	38.07
17	0.050	0.500	0.03	90	91.90	39.26
18	0.075	0.570	0.03	30	98.10	39.83
19	0.025	0.500	0.01	30	94.20	39.48
20	0.050	0.570	0.01	60	59.50	35.49
21	0.075	0.687	0.01	90	97.50	39.78
22	0.025	0.570	0.02	90	77.60	37.79
23	0.050	0.687	0.02	30	82.50	38.33
24	0.075	0.500	0.02	60	89.20	39.00
25	0.025	0.687	0.03	60	80.10	38.07
26	0.050	0.500	0.03	90	91.90	39.26
27	0.075	0.570	0.03	30	98.10	39.83

Table 3. Response table for S/N ratio.

Level	GO (gr/l)	NaBH4 (gr)	CaCl2 (gr)	Time (h)
1	38.25	38.45	39.25	39.21
2	38.37	37.69	37.70	37.52
3	39.05	39.54	38.72	38.94
Delta	0.80	1.85	1.55	1.69
Rank	4	1	3	2

Table 4. Analysis of variance (ANOVA) results of Taguchi design for coating yield.

Factor	DOF (f)	Sum of Sqrs. (S)	Variance (V)	F-ratio (F)	Pure Sum (S2)	Contribution C (%)
Catalyst (gr)	2	1.124	0.562	1.74	1.124	7.473
GO (g/l)	2	5.214	2.607	0.88	5.214	34.657
Reagent reduction (gr)	2	3.763	1.881	0.24	3.763	25.009
Contact time	2	4.944	2.472	1.50	4.944	32.859

MLR modeling

Including mathematical models is based on least squares is MLR. It is easy to use. A multiple linear regression equation shows linear relevance between a response variable (Y), two or more predictorsvariable (X_1, X_2, ..., X_K), estimated value of Y-intercept (b_0) and coefficient variable (b_1, b_2, ..., b_K) [22-24]. So the MLR equation is equal to:

$\hat{Y} = b_0 + b_1 X_1 + b_2 X_2 + ... + b_k X_k$ (1)

The multiple linear regression model used in this study,

$\hat{Y} = b_0 + b_1 [GO] + b_2 [NaHB_4] + b_3 [CaCl_2] + b_4 \Delta t$ (2)

ANN modeling

ANN is similar to biological neurons that consist of a set of neurons connects with each other by axon connection. Every neuron includes weights associated with many inputs and only one output. Naturally, except inputs and output layers, ANN also consists of hidden layers, where the communication among the inputs and output are specific by synaptic weights. ANNs are the strongest implements that can be used to predict system identification [25-28]. ANNs are efficient to achieve linear and nonlinear functions. Feedforward backpropagation (FFBP) and Radial basis function (RBF) are examples of network types [29].

The Feedforward (FF) neural network is an uncomplicated architecture, and the backpropagation (BP) is an interest form of ANN. The rigidity of the network depends on the weights of the concrete neurons what are improved for training via backpropagation construction. By exhibit the network algorithm to a special complex of data, the weights and biases are corrected to generate the tendency output [27,30]. Four types of algorithms are used in this study, which is: Levenberg-Marquardt backpropagation (LM), scaled conjugate gradient backpropagation (SCG), gradient descent with momentum backpropagation (GDM), Resilient back-propagation (RP) [31]. Results of statistical data for the coating rate using these four learning algorithms are showed in Table 5. LM learning algorithm has been the best and fastest.

Trial and error is the basis of activation function and architecture of the network figure out. Table 6 is attended the suitable architecture (4-6-1-1) for this model. Figure 1 exact refers to the network model. That's mean, the network architecture consists four neurons (GO concentration, reagent reduction amount, catalyst dosage and contact time) in the input layer, six neurons in the hidden layer, one neuron in each of the outer and final layers, That's a corrected response (coating rate). The input layer is triggered using the sigmoid activation function whereas the second and third layers are the hidden layer and the output layer, respectively. Figure 2 shows that the network consists of two transfer function, tansig and purelin [32]. The equation for the ANN model is:

ANN output = $\hat{Y}_{ANN}$ = Purelin [w2 × tansig (w1 × {x (1); x (2); x (3); x (4)} + b1) + b2] (3)

Where, w1 and b1 are the weight and bias of output layers, while the x (1), x (2), … x (3) represent the inputs.

Results and Discussion

To study the optimization of MLR and ANN models of experimental data and for best results, the Taguchi design outputs act as inputs. From experimental data in Table 7 the MLR estimation equation was calculated:

$\hat{Y}_{MLR}$ =80.9 + 219 [GO] - 17 [$NaHB_4$] + 315 [$CaCl_2$] – 2.6Δt (4)

The following equation indicates ANN model used in this study:

$\hat{Y}_{ANN}$ = Purelin [w2 × tansig (w1 × { [GO]; [$NaHB_4$]; [$CaCl_2$]; Δt} + b1) + b2] (5)

Table 8 shows, the amount of weight and bias for each layer that completed the best ANN structure.

Table 9 the results of ANN predicted are revealed. According to this Table, the recoveries are entirely gratifying. By collation the result of Tables 7 and 9, the ANN technique can be suggested for predicting of coating rate.

Table 5. Statistical data for the coating rate using four learning algorithms.

Learning algorithm	Number of neurons	Training data		Testing data	
		R2	MSE	R2	MSE
LM	1	0.81975	0.002747	0.97178	0.007428
LM	2	0.98828	0.000431	0.97859	0.001309
LM	3	0.95122	0.000046	0.92059	0.003086
LM	4	0.97549	0.000064	0.92745	0.002218
LM	5	0.99801	0.000016	0.99998	0.000015
LM	6	1	0.000003	1	0.000003
LM	7	0.79234	0.003545	1	0.000991
SCG	1	0.85457	0.007567	0.99993	0.04802
SCG	2	0.91824	0.003868	0.82094	0.001058
SCG	3	0.94835	0.003029	0.60908	0.01164
SCG	4	0.96592	0.003187	0.91385	0.002366
SCG	5	0.99738	0.003438	0.98414	0.007274
SCG	6	0.95234	0.003402	0.97123	0.008501
SCG	7	0.99872	0.001678	0.99991	0.003804
SCG	8	1	0.0002975	1	0.0003658
SCG	9	1	0.001525	1	0.001525
SCG	10	0.96556	0.005002	0.86025	0.003658
RP	1	0.84605	0.004304	0.94882	0.01384
RP	2	0.98185	0.01018	0.8454	0.002079
RP	3	0.97057	0.003616	0.99751	0.004348
RP	4	0.94445	0.001244	0.98089	0.000358
RP	5	0.99838	0.004373	0.98212	0.003575
RP	6	1	0.002666	1	0.002666
RP	7	0.99924	0.002224	0.96972	0.006697
GDM	1	0.46625	0.0115	0.93695	0.03062
GDM	2	0.27910	0.03542	0.98011	0.06121
GDM	3	-0.032757	0.06208	0.029816	0.04931
GDM	4	-0.31799	0.1227	-0.82368	0.05235
GDM	5	0.53999	0.03063	-0.66922	0.05697
GDM	6	0.87229	0.0609	0.98804	0.02774
GDM	7	0.69184	0.05538	0.86077	0.05538

Table 6. The best results for four different learning algorithms.

Learning algorithm	Network architecture	Training set		Testing set	
		R2	MSE	R2	MSE
LM	4-6-1-1	1	0.000003	1	0.000003
SCG	4-8-1-1	1	0.0002975	1	0.0003658
RP	4-6-1-1	1	0.002666	1	0.002666
GDM	4-6-1-1	0.87229	0.0609	0.98804	0.02774

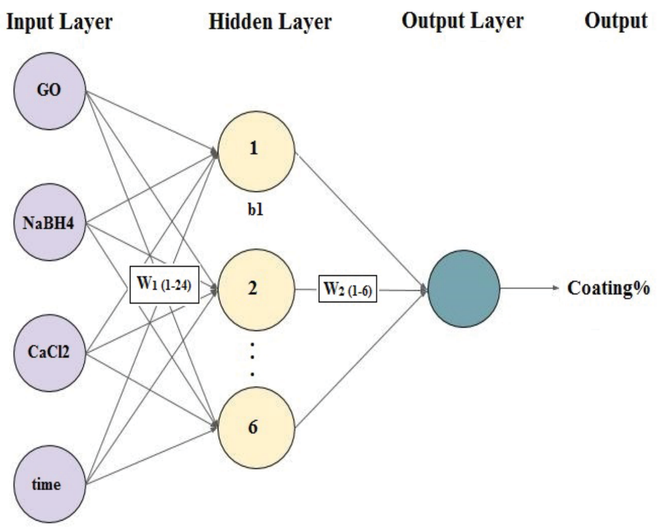

Figure 1. ANN architecture with a single hidden layer used in this work.

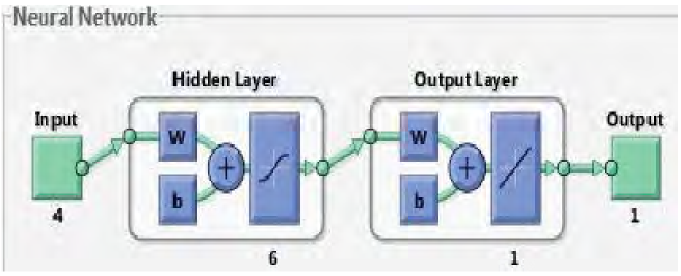

Figure 2. Screen shots of modified software used in this work.

Table 7. MLR prediction and recovery (%) for coating yield.

Run No.	GO (gr/L)	NaBH4 (gr)	CaCl2 (gr)	Time (h)	Coating (%)	Predicted MLR Coating (%)	Recovery (%)
1	0.025	0.500	0.01	30	94.20	80.17	85.10
2	0.050	0.570	0.01	60	59.50	83.60	140.5
3	0.075	0.687	0.01	90	97.50	86.20	88.41
4	0.025	0.570	0.02	90	77.60	74.08	95.46
5	0.050	0.687	0.02	30	82.50	85.61	103.7
6	0.075	0.500	0.02	60	89.20	93.41	104.7
7	0.025	0.687	0.03	60	80.10	82.43	102.9
8	0.050	0.500	0.03	90	91.90	90.20	98.15
9	0.075	0.570	0.03	30	98.10	96.23	98.09
10	0.025	0.500	0.01	30	94.20	80.17	85.10
11	0.050	0.570	0.01	60	59.50	83.60	140.5
12	0.075	0.687	0.01	90	97.50	86.20	88.41
13	0.025	0.570	0.02	90	77.60	74.08	95.46
14	0.050	0.687	0.02	30	82.50	85.61	103.7
15	0.075	0.500	0.02	60	89.20	93.41	104.7
16	0.025	0.687	0.03	60	80.10	82.43	102.9
17	0.050	0.500	0.03	90	91.90	90.20	98.15
18	0.075	0.570	0.03	30	98.10	96.23	98.09
19	0.025	0.500	0.01	30	94.20	80.17	85.10
20	0.050	0.570	0.01	60	59.50	83.60	140.5
21	0.075	0.687	0.01	90	97.50	86.20	88.41
22	0.025	0.570	0.02	90	77.60	74.08	95.46
23	0.050	0.687	0.02	30	82.50	85.61	103.7
24	0.075	0.500	0.02	60	89.20	93.41	104.7
25	0.025	0.687	0.03	60	80.10	82.43	102.9
26	0.050	0.500	0.03	90	91.90	90.20	98.15
27	0.075	0.570	0.03	30	98.10	96.23	98.09

With the aid of ANOVA, the MLR and ANN techniques are examined to each other in Table 10. This Table illustrated the ANN model has the higher F-value, sum squares, mean squares and conversely with lower P-value. So this model is deeply near to fact.

Also, R_2 in Figures 3 and 4 was 0.217 for MLR model and 0.999 for the ANN model. Therefore, the MLR method acts poor in predicting the coating rate. It definitely is said; inputs and output are not linearly relevance. The amount of data and linear or nonlinear behavior between variables can control factors of this result. Maybe a small amount of data could be one of the MLR model errors. Therefore, it is concluded that ANN model showed greater prefer in predicting coating rate.

Table 8. The weight and bias of trained ANN for predicting coating rate.

W_1				W_2	b_1	b_2
-1.858	-1.2662	1.4782	0.11853	0.77531	1.721	
0.54837	0.13659	-2.1059	-0.75015	0.61603	-1.2553	
1.2546	0.049105	-0.55372	1.6996	0.20246	-0.48479	0.32841
-0.1225	1.3527	1.4856	-0.99204	0.40083	-0.35942	
-1.2561	0.77923	1.457	0.79404	-0.218110	-1.309	
-0.67795	0.045473	1.7403	1.0508	0.52528	-2.3733	

Table 9. ANN prediction and recovery (%) for coating yield.

Run No.	GO (gr/L)	NaBH4 (gr)	CaCl2 (gr)	Time (h)	Coating (%)	Predicted ANN Coating (%)	Recovery (%)
1	0.025	0.500	0.01	30	94.20	94.20	100
2	0.050	0.570	0.01	60	59.50	59.50	100
3	0.075	0.687	0.01	90	97.50	97.50	100
4	0.025	0.570	0.02	90	77.60	77.60	100
5	0.050	0.687	0.02	30	82.50	82.50	100
6	0.075	0.500	0.02	60	89.20	90.27	101
7	0.025	0.687	0.03	60	80.10	80.10	100
8	0.050	0.500	0.03	90	91.90	91.33	99.38
9	0.075	0.570	0.03	30	98.10	98.10	100
10	0.025	0.500	0.01	30	94.20	94.20	100
11	0.050	0.570	0.01	60	59.50	59.50	100
12	0.075	0.687	0.01	90	97.50	97.50	100
13	0.025	0.570	0.02	90	77.60	77.60	100
14	0.050	0.687	0.02	30	82.50	82.50	100
15	0.075	0.500	0.02	60	89.20	90.27	101
16	0.025	0.687	0.03	60	80.10	80.10	100
17	0.050	0.500	0.03	90	91.90	91.33	99.38
18	0.075	0.570	0.03	30	98.10	98.10	100
19	0.025	0.500	0.01	30	94.20	94.20	100
20	0.050	0.570	0.01	60	59.50	59.50	100
21	0.075	0.687	0.01	90	97.50	97.50	100
22	0.025	0.570	0.02	90	77.60	77.60	100
23	0.050	0.687	0.02	30	82.50	82.50	100
24	0.075	0.500	0.02	60	89.20	90.27	101
25	0.025	0.687	0.03	60	80.10	80.10	100
26	0.050	0.500	0.03	90	91.90	91.33	99.38
27	0.075	0.570	0.03	30	98.10	98.10	100

Table 10. Compare MLR and ANN models by the statistical analysis for prediction of coating yield%

Source		DF	SS	MS	F-value	P- value
MLR model	X1	4	796.8	199.2	1.55	0.223
	Error	22	2831.8	128.7	-	-
ANN model	X1	1	1210	1210	5874.1	1.6939e-11
	Error	7	1.442	0.206	-	-

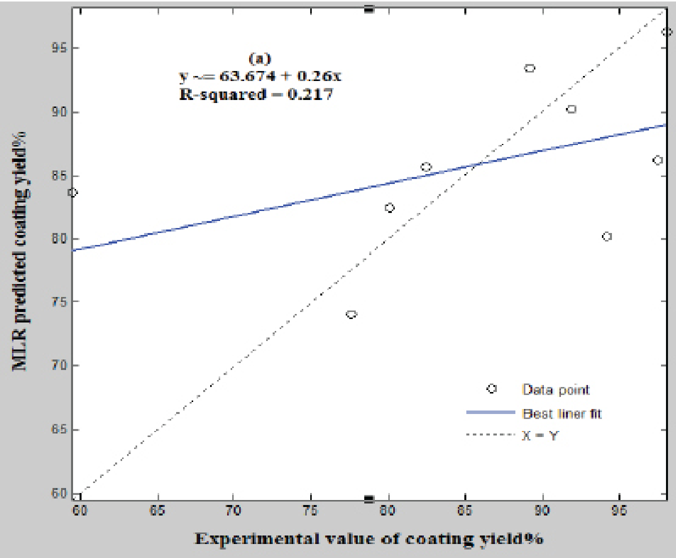

Figure 3. Predicted values against experimental values for coating yield MLR model.

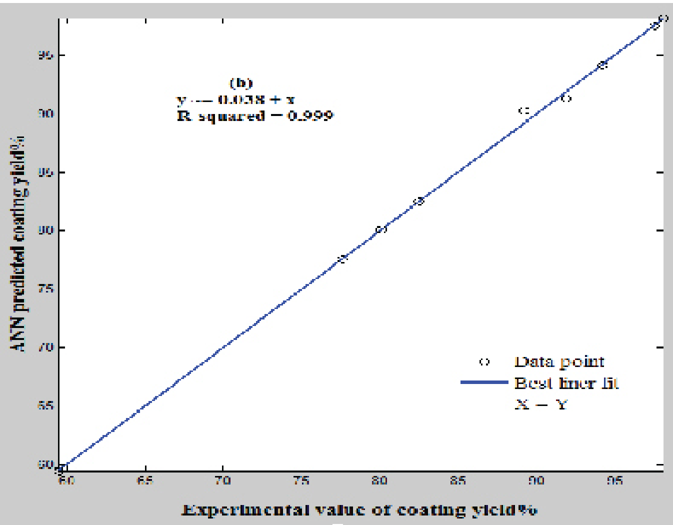

Figure 4. Predicted values against experimental values for coating yield ANN model.

Conclusion

In the present study, the predictive capability of MLR and ANN were aimed for graphene coating rate. The experimental design Taguchi results doing as input for these models, experimental design Taguchi results had been used. The Taguchi results were check by the choice of the best run by examining the S/N and ANOVA. The results show GO concentration and contact time are highly effective in coating rate. For MLR and ANN models, we chose the best parameters in the software and so optimized it. Results exposed the attitude of the inputs and output wasn't linear. Therefore, the ANN model is an excellent predicted performance compare to the MLR model for coating rate graphene on cotton.

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