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NEURAL NETWORK MODELING FOR PREDICTION SIZE OF SILVER NANOPARTICLES IN MONTMORILLONITE/STARCH SYNTHESIS BY CHEMICAL REDUCTION METHOD

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Silver nanoparticles (Ag-NPs) have attracted considerable attention for chemical, physical, and medical applications due to their exceptional properties. In this study, artificial neural network (ANN) was employed to develop an approach for the evaluation of size of silver nanoparticles (Ag-NPs) in montmorillonite/starch bionanocomposites (MMT/Stc BNCs) synthesized by chemical method. The suitable ANN model is found to be a network with two layers that first layer has 10 neurons. This model has four inputs include of $AgNO_3$ concentration, temperature of reaction, weight percentage of starch, and $NaBH_4$ concentration. It can capable for predicting the size of Ag-NPs synthesized by chemical reduction method for a wide range of conditions with a mean absolute error of less than 0.04 and a regression of about 0.99. Also linear and multiple linear regression models verified that $AgNO_3$ concentration content has significant effect on size of Ag-NPs. ANN generalization results denoted that the selected ANN successfully predicts the behavior of size of nanoparticles as functions of operating variables.

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Keywords: Artificial neural network, silver nanoparticles, montmorillonite, modelling, bionanocomposites.

1. Introduction

The synthesis of nanomaterials is one of current interest due to their wide variety of applications in fields such as electronics [1], photonics [2], catalysis [3], medicine [4], etc. Most of the applications are due to the fact that matter at the nanometer scale has different properties as compared with the bulk state. For this reason, many research groups around the world are trying new methods of synthesis of different materials at the nanoscale. One goal is to control the size and shape of atomic clusters or nanoparticles (NPs) and their ordering in one, two or three dimension arrays [5].

A variety of preparation routes have been reported for the preparation of metallic nanoparticles [6, 7], notable examples include, salt reduction [8], microwave dielectric heating reduction [9], ultrasonic irradiation [10], radiolysis [11], electrochemical synthesis [12, 13], etc. In recent years many metal nanoparticles have been found to exhibit interesting antibacterial activities [14].

Among of metals nanoparticles the silver nanoparticles (Ag-NPs) have been found to exhibit interesting antibacterial activities [15–17].This may perhaps have numerous applications in the fields of dentistry, clothing, catalysis, mirrors, optics, photography, electronics and food industries [18]. Because of such broad variety of applications, wide ranges of different preparation methods have been developed. However, the developing methods of Ag-NPs preparation, must give preference to control size of Ag-NPs. Therefore, nanosilver with small particle size and

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devoid of aggregation between particles is favorable in this purpose. There are several ways to reduce Ag^+ for instance, application of physical methods using of γ-rays, UV-irradiation, ultrasonic irradiation, microwave irradiation, heating and electrochemical reduction [19], application of reducing chemicals, such as hydrazine, sodium borohydride [20–24], polyethylene glycerol [25], N,N-dimethyl formamide [26], glucose [27], ethylene glycol [28], formaldehyde [29], sodium in liquid ammonia, etc [30].

Several studies on the synthesis of metal NPs by using natural polymers have been performed. The polyelectrolyte's, such as starch, are particularly interesting for metal NPs synthesis, due to their interactions with metal ions and metal NPs. Among natural polymers, starch is one of the most promising biocompatible and biodegradable materials because it is a renewable resource that is universally available and of low cost [31].

A novel invention of nanocomposites materials which indicate a promising field in the frontiers of nanotechnology materials and life sciences are bionanocomposites. Bionanocomposites are composed of a natural polymer matrix and organic/inorganic filler with at least one dimension on the nanometer scale [32]. A number of researchers have presented work in the field of starch-based bionanocomposites which can be obtained by filling a thermoplastic starch matrix with nanofillers such as layer silicates like montmorillonite and kaolinite are the usual layer silicates used in starch-based bionanocomposites [33].

In recent years artificial neural network (ANN) models have been applied for the modeling of chemical processes related to different area , for example the extraction of various compounds from different liquid and solid phases [34], also in nanocomposites [35], bio-sorption process [36], nanoparticles-activated carbon [37, 38] and nanofibers [39]. ANN is a modeling tool to solve linear and nonlinear multivariate regression problems [40]. ANNs may provide accurate results for very complex and non-linear problems that demand high computational costs [42–44]. One of the most employed learning algorithms is the back-propagation and its main advantage is the use of output information and expected pattern to error corrections [45]. The main advantages of ANN techniques include learning and generalization ability of data, fault tolerance and inherent contextual information processing in addition to fast computation capacity [46]. It is important to mention that since 90's many studies have related advantages of applying ANN techniques when compared to other statistical methods [47–49]. Employing neural network models would lead to saving time and cost by predicting the results of the reactions so that the most promising conditions can then be verified [50–53]. Therefore the objective of this paper is to develop an ANN model to predict the size of Ag-NPs, based experimental data; also investigating effect of important variables on size of nanoparticles.

In this article, we study that the artificial neural network algorithm is present for the prediction of size of Ag-NPs with the inputs of $AgNO_3$ concentration, temperature of reaction, weight percentage of starch, and $NaBH_4$ concentration.

2. Experimental Section

2.1 Materials

Silver nitrate ($AgNO_3$, 99.98%), used as the silver precursor, was obtained from Merck (Darmstadt, Germany). Montmorillonite powder (MMT), used as a solid support for the Ag-NPs, was purchased from Kunipia-F (Tokyo, Japan). Sodium borohydride ($NaBH_4$, 98.50%) and soluble starch (99.89%) used as a reduction agent, and stabilizer respectively, were obtained from Sigma-Aldrich (St Louis, MO). All the aqueous solutions were used with double-distilled water.

2.2 Synthesis of Ag-NPs in MMT/Stc BNCs

Schematic illustration of the synthesis of the Ag-NPs on MMT/Stc is shown in Figure 1. Starch solutions were prepared by soluble starch in the different temperature under constant stirring time. Then, different molar of $AgNO_3$ were added to the starch solutions under constant stirring for preparation of $AgNO_3$/Stc colloids. The $AgNO_3$/Stc colloids were added into the MMT

suspension and the mixture was further vigorously stirred for more than 3 h at certain temperature to obtain $[Ag(MMT/Stc)]^+$ composites that mention in Equations 1. Freshly prepared of $NaBH_4$ solutions with different molar were added to the $[Ag(MMT/Stc)]^+$ composites. The mixtures were heated to certain temperature and were maintained at each temperature for 24 hours. The suspension rapidly changed to light brown and dark brown that indicating the initial formation of Ag-NPs. Then, obtained suspensions of Ag/MMT/Stc BNCs were separated by centrifugation, washed with double distilled water twice and dried under vacuum overnight. Unless stated otherwise, all experiments were conducted at certain temperatures [27, 54]. The possible reaction between $NaBH_4$, silver ions and starch in the MMT suspensions can be written as follows Equations 2.

$$Ag+ + Stc + MMT \rightarrow [Ag\ (MMT/Stc)]^+ \quad (1)$$

$$2[Ag\ (MMT/Stc)]^+ + 4BH_4^- + 6H_2O \rightarrow 2[Ag\ (MMT/Stc)] + 4H_2BO_3^- + 2H^+ + 9H_2\uparrow \quad (2)$$

Stc= Starch

Therefore, according to these reactions mechanism the interactions between Ag-NPs in the interlayer space of MMT/Stc BNCs can be van der Waals interactions. The physical bonding appears between the oxygen groups of oxygen group of starch with positive charge of Ag NPs surface.

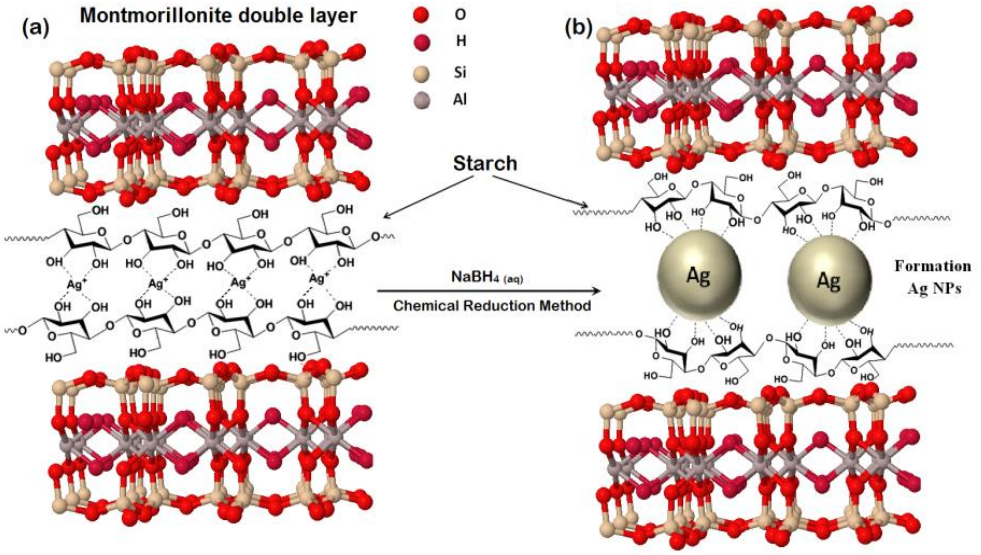

Fig.1: Schematic illustration of the synthesis of the Ag-NPs in MMT/Stc layers as bionanocomposites by chemical reduction method.

2.3 Characterization Method and Instrument

The Ag/MMT/Stc BNCs were characterized using transmission electron microscopy. Transmission electron microscopy observations were carried out on A Hitachi H-7100 electron microscope and the mean particle size distributions were determined using the UTHSCSA Image Tool version 3.00 program.

3. Modeling

Artificial neural networks (ANNs) are non-linear computational tools suitable to a great host of practical application due to their flexibility and adaptability [55, 56]. The massive interconnected structure make ANN an exceptional tool which learns through input data, while it

has the ability to model incomplete data without being affected by data noise. Such techniques have proved more efficient than standard modeling techniques such as the response surface methodology (RSM) [57, 58]. From a computational point of view, the simplest representation of an artificial neural network is that of a black-box which receives multiple inputs and produces multiple outputs (Figure2), this means that ANNs are just one of the possible ways to operate a non-linear mapping between an input and a target space [59].

Three subsets of data are used to build the network model: a training set and a testing set and validation set. The training phase needs to produce a neural network that is both stable and convergent. The training phase is carried out by adjusting the strength of connections between neurons with the aim to adapt the outputs of the entire network to be closer to the desired outputs or to minimize the sum of the training data.

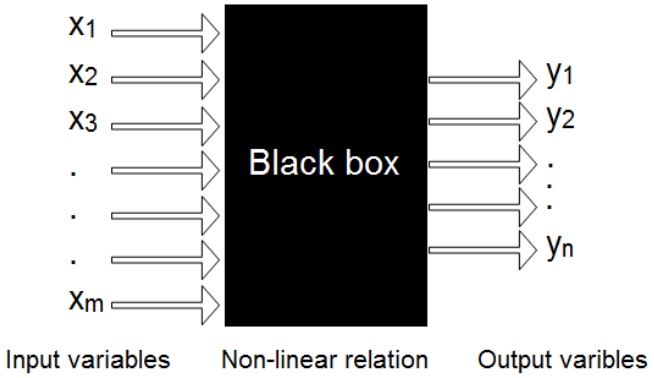

Fig. 2: Artificial neural network as a black-box

The training is carried out by adjusting the strength of connections between neurons with the aim to adapt the outputs of the entire network to be closer to the desired outputs or to minimize the sum of the training data [60]. Validation phase is required to modify and optimize the ANN architecture (activation function, training function and number of hidden layers), and adjust the number of neurons for hidden layer.

Amongst network functions, the popular feed-forward with back-propagation algorithm is assessed. A feed-forward network with I inputs, H hidden neurons and O outputs computes O nonlinear functions of its I input variables as compositions of the H functions computed by the hidden neurons (Equations 3):

$$y_j = g\left(\sum_{i=1}^{H} w_{ji} HN_i + w_{j0}\right) = g\{\sum_{i=1}^{H} w_{ji} f\left(\sum_{r=1}^{I} w_{ir} a_r + w_{i0}\right) + w_{j0}\} \quad (3)$$

Where g and f are the activation functions of the output and hidden layers, respectively, HN_i is the value of the ith hidden neuron, w_{ji} is the weight connecting the ith hidden and the jth output units, while w_{ir} is the weight associated to the connection of the ith input to the rth hidden neuron. Activation functions used for multilayer feed-forward networks are usually s-shaped functions like sigmoid or hyperbolic tangent, which satisfy the requisites of being non-linear and bounded [55, 59].

Before practical implementation, the network has to be trained so that the free parameters or connection weights are determined and the mapping between inputs and outputs is accomplished. The training method is called back-propagation, a supervised learning technique, which generally involves two phases through different layers of the network: a forward phase and a backward phase. In the forward phase, input vectors are presented and propagated forward to compute the output for each neuron. During this phase, synaptic weights are calculated and the mean square errors (MSE) and the coefficient of determination (R^2) of all the patterns of the training set are calculated by Equation (4, 5):

$$MSE = 1/n \sum_{i=1}^{n} (a_i - b_i)^2 \quad (4)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (a_i - b_i)^2}{\sum_{i=1}^{n} (a_i - a_m)^2} \quad (5)$$

Where "n" is the total number of training patterns a_i is the target value, b_i is the network output value and a_m is the average of the target values.

The backward phase is an iterative which is error reduction performed in a backward direction from the output layer to the input layer. The gradient descent method, adding a momentum term, is usually used to minimize the MSE as fast as possible [61–63].

4. Results and Discussion

The proposed method is implemented using Matlab 7.6 on a T6400, 2 GHz, 2 GB RAM computer. The data were randomly divided into three groups (70% for training, 15% for the testing and 15% for the validation set). The optimum ANN model with four neurons ($AgNO_3$ concentration, temperature of reaction, weight percentage of starch, and $NaBH_4$ concentration), one neuron (size of nanoparticles) and 10 neurons in the hidden layer was found as fitness function, while the weight and bias values of each layer were determined. Then, optimal ANN architecture was determined as 4:10:1 with log-sigmoid transfer function for hidden and linear transfer function for output layers (Figure 3):

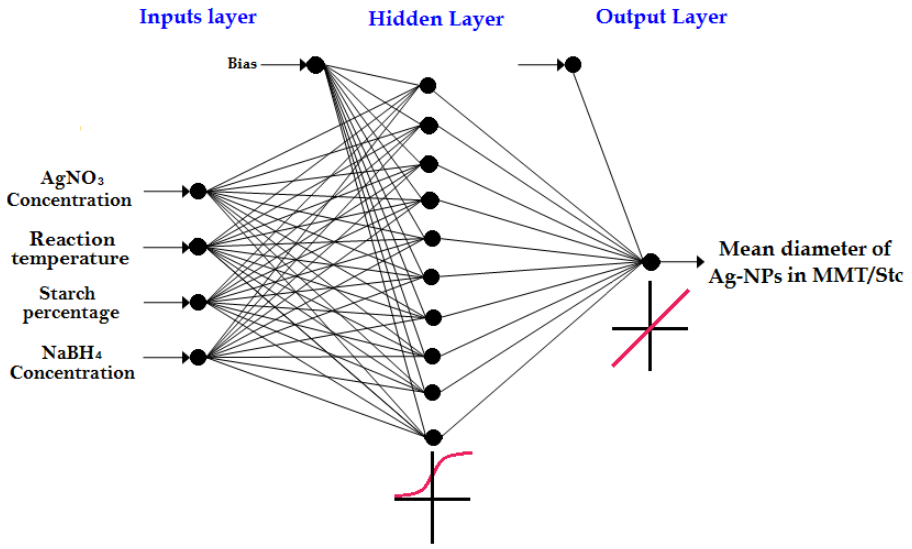

Fig. 3: The optimums ANN model for prediction the size of Ag-NPs in MMT/Stc BNCs

In Table 1 is presented the experimental data used for the training of the ANN model. The predicted particle size is compared to the observed particle size and the difference between the predicted and observed size is stated as particle size error based on the difference between these two values.

Table 2 shows the values of connection weights (parameters of the model) for the complete ANN model trained on the whole datasets. This information allows other researchers to compare present ANN models with their own experimental data.

The performances of ANN model on training, validation and testing data sets are evaluated by MSE and R^2. These resulting values are reported in Table 3 and this results show that the predictive accuracy of the model is high.

Table 1: Experimental values (training, validation, and testing data set),actual and model predicated of size of Ag-NPs.

Run No	$AgNO_3$ (M)	Temperature (°C)	Starch (%w/w)	$NaBH_4$ Con. (M)	Size of Silver (Actual) (nm)	Size of Silver (Predict) (nm)	Error= Actual-Predict (nm)
1	0.5	25	0.25	0.5	25.47	25.282	0.18788
2	0.5	25	0.25	1	23.42	23.842	-0.4221
3	0.5	25	0.25	1.5	22.87	22.624	0.24597
4	0.5	25	0.25	2	21.59	21.598	-0.00802
5	0.5	25	0.25	2.5	20.81	20.736	0.07408
6	0.5	25	0.25	3	20.03	20.012	0.01794
7	1.0	30	0.5	1	19.25	19.608	-0.35812
8	1.0	30	0.5	2	18.47	18.458	0.01200
9	1.0	30	0.5	3	17.72	17.6	0.12015
10	1.0	30	0.5	4	17.07	16.928	0.14188
11	1.0	30	0.5	5	16.36	16.369	-0.00881
12	1.0	30	0.5	6	15.61	15.871	-0.26089
13	1.5	35	1	1.5	14.85	14.893	-0.04287
14	1.5	35	1	3	14.14	14.203	-0.06283
15	1.5	35	1	4.5	13.75	13.506	0.24425
16	1.5	35	1	6	12.69	12.768	-0.07787
17	1.5	35	1	7.5	11.84	11.978	-0.13778
18	1.5	35	1	9	11.22	11.141	0.07937
19	2.0	40	1	2	10.25	10.25	0.0000
20	2.0	40	1.5	4	9.49	9.4871	0.00293
21	2.0	40	1.5	6	8.23	8.6317	-0.40165
22	2.0	40	1.5	8	7.51	7.7574	-0.24743
23	2.0	40	1.5	10	6.72	6.7223	-0.00232
24	2.0	40	1.5	12	5.38	5.3772	0.00280
25	5.0	50	2	5	4.76	4.7617	-0.00173
26	5.0	50	2	10	4.53	4.7206	-0.19055
27	5.0	50	2	15	4.24	4.2419	-0.00192
28	5.0	50	2	20	4.01	4.0101	-0.00013
29	5.0	50	2	25	3.87	3.9347	-0.06468
30	5.0	50	2	30	3.86	3.8608	-0.00078

Table 2: Values of connection weights for the complete ANN model (parameters of the model)

	Node1	Node2	Node3	Node4	Node5	Node6	Node7	Node8	Node9	Node10	Bias 2
Input 1	0.78695	1.0277	0.61168	0.35598	-0.22961	2.0693	2.0109	-1.8701	0.30248	0.50168	
Input 2	-0.78233	-0.4063	1.37	-0.23377	-2.0116	0.97917	0.40739	-2.8302	-1.5875	-0.051288	
Input 3	1.7222	-2.2102	-0.05875	-2.2749	0.97927	-1.5422	1.2763	0.3165	1.7796	-1.8787	
Input 4	0.20915	-1.2791	1.0375	-2.2808	-0.90458	0.30561	2.8448	-0.91541	-0.5772	-3.1984	
Output	-0.67863	-3.589	-1.767	0.10127	-0.069593	0.20272	-1.2494	0.64627	2.3205	-5.693	
Bias 1	-0.46376	0.23879	0.25792	-0.33878	1.9209	1.3256	0.17776	0.29823	1.3054	3.3051	1.8277

Table 3: The performances of ANN model on training, validation and testing data sets

Data	RMSE	R^2
Train	0.0185	0.9979
Validation	0.0441	0.9952
Test	0.0557	0.9984

In Figure 4 is also shown the scatter diagram of predicted values in comparison with actual values. It shows that the model prediction fits well with the experimental observations.

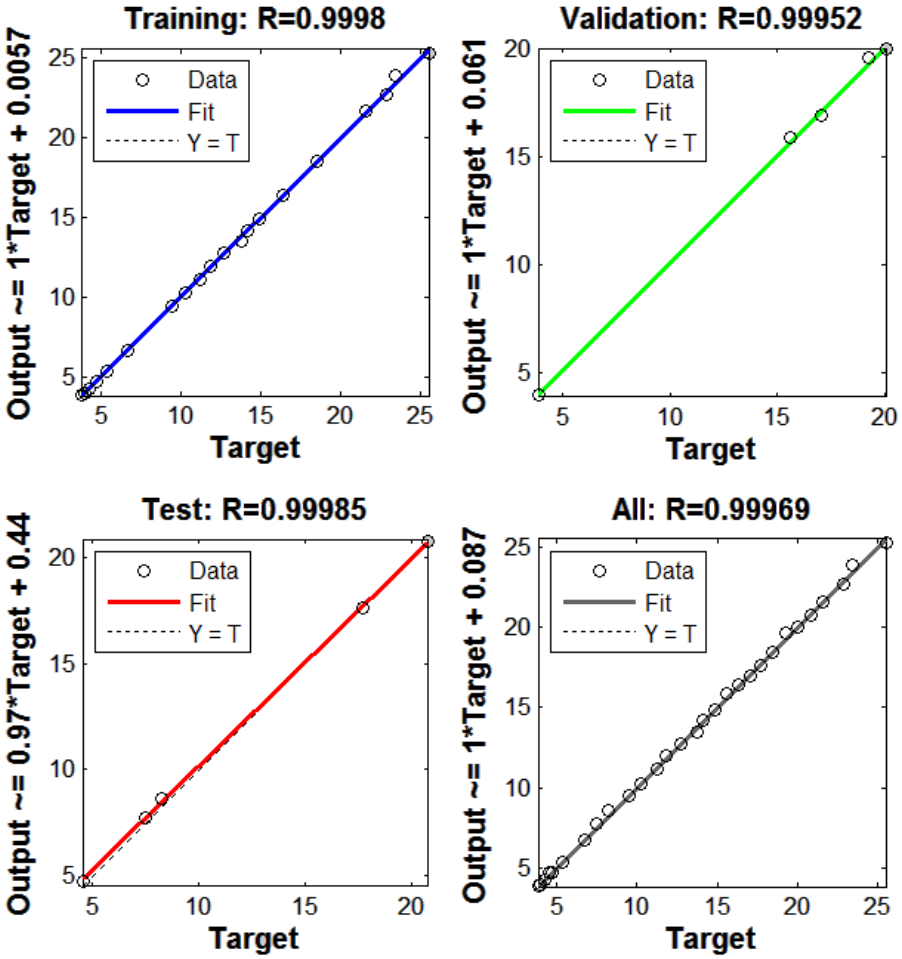

Fig. 4: The scatter plots of ANN model predicted versus actual values for training, validation, testing and all data sets.

In Figure 5 is shown the errors histogram of train, validation and test sets. These results show errors three data sets is less than 0.86. These results indicate that the experimental data has been fitted with good accuracy using the obtained ANN model.

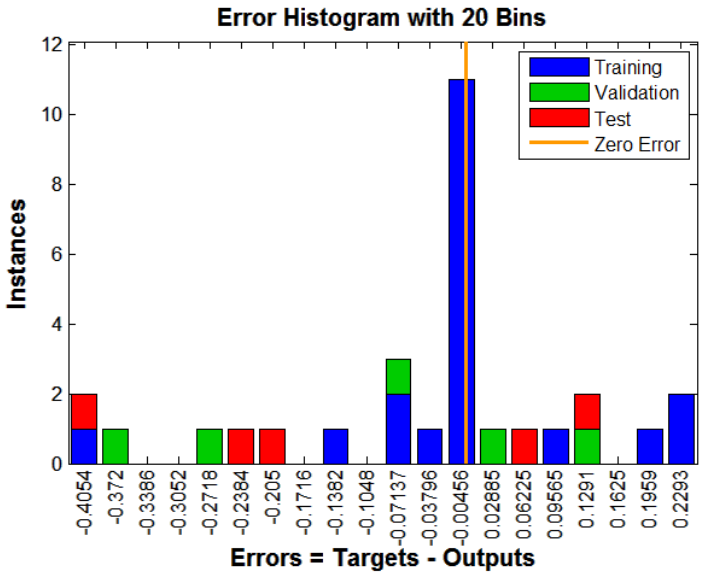

Fig. 5:Error histogram of training, validation, and test datasets

Figure 6 presents the MSE of training, test, and validation datasets for 20 iterations, and the best validation performance is found to in 0.004 in the 20th epoch (iteration). The results presented in Figure 6 show other reasons for validating the final obtained ANN model.

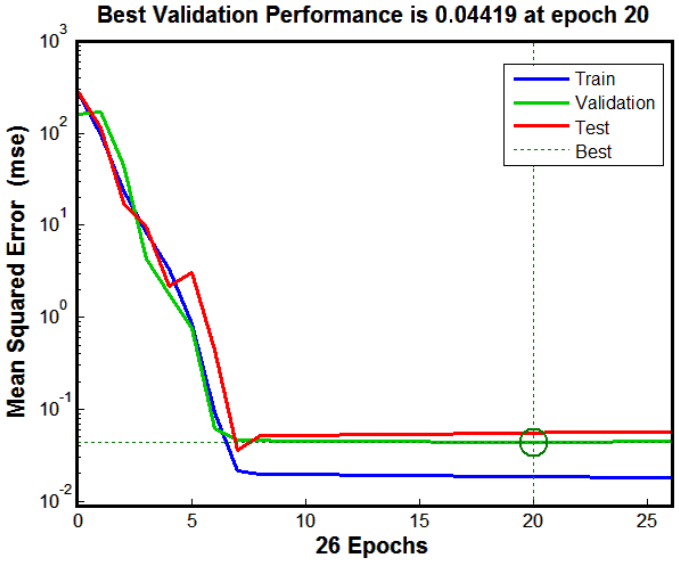

Fig. 6. Mean squared error of training, validation, and test datasets

4.1 Model Fitting and Statistical Analysis

Data fitting is the process of fitting models to data and analyzing the accuracy of the fit. Engineers and scientists apply data fitting techniques, including nonparametric methods, mathematical equations and, to model acquired data. Two-dimensional plots for presenting the effects of each input variable on output (size of Ag-NPs) based on regression models have been exhibited in Figure 7(a-d).

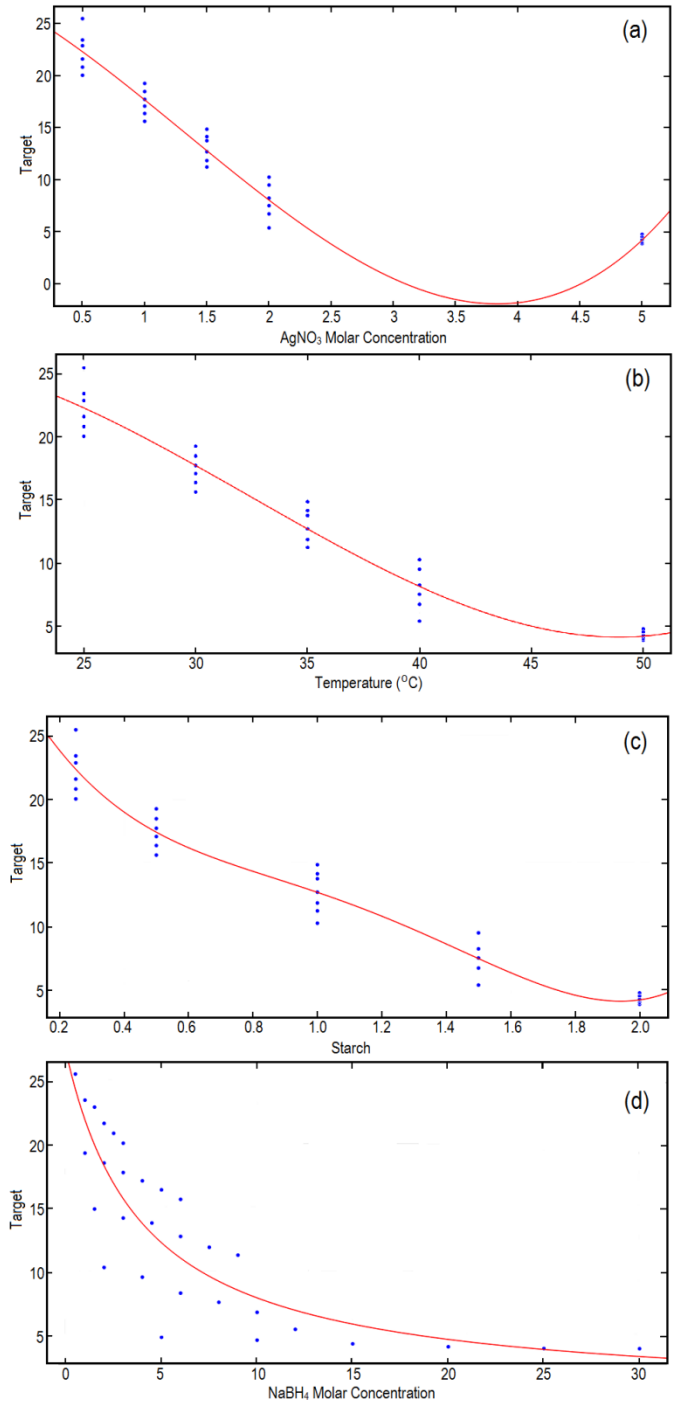

Fig. 7: Two-dimensional plots effects of $AgNO_3$ concentration (a), temperature of reaction (b), starch percentage (c), and $NABH_4$(d) on size of Ag-NPs

It was observed that measurement of size of Ag-NPs increased rapidly with the increase in the amount of $AgNO_3$ concentration, starch percentage, and amount of $NaBH_4$ concentration [35].

The Figure 8 (a–f) shows the combined effects of the four input variables, on the size of nanoparticles. The size of nanoparticles on based the amount of starch and $AgNO_3$ concentration is presented in Figure 8 (a), and shows both factor are important.

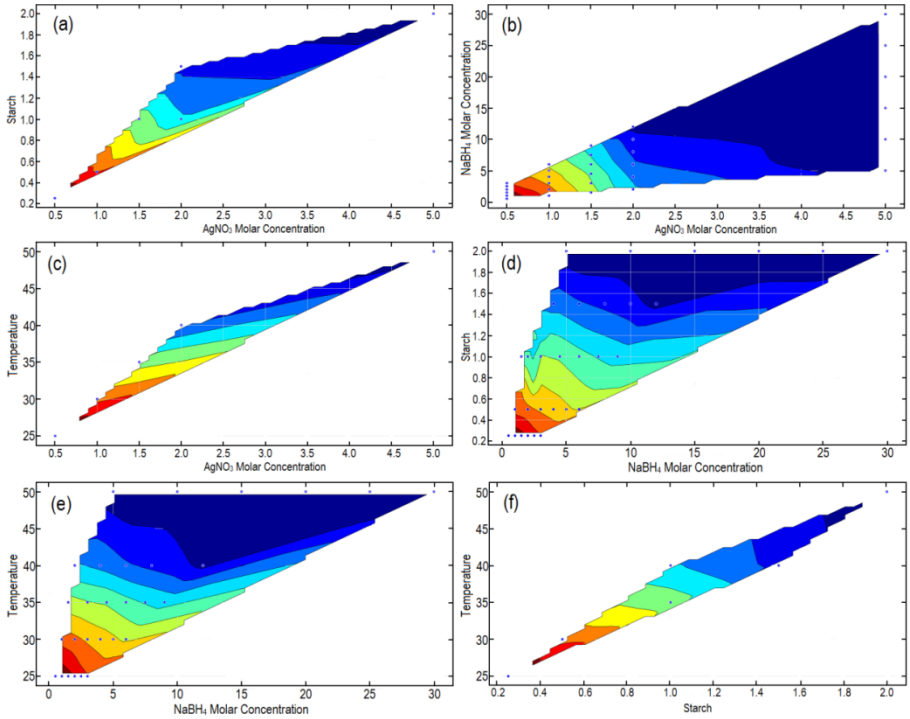

Fig. 8:Two-dimensional surfaces plots: effects of $AgNO_3$ concentration and starch percentage (a), effects of amount of $AgNO_3$ and $NaBH_4$concentrationsand (b), effects of temperature of reaction and $AgNO_3$ concentration (c), effects of starch percentage and amount of $NaBH_4$ concentration (d), effects temperature of reaction and amount of $NaBH_4$ concentration (e), and effects of starch percentage and temperature of reaction (f) on size of Ag-NPs.

In Figure 8 (b) the points are inside the light green, yellow, red and dark blue areas present for low amount of $AgNO_3$ concentration (<2), the factor of $NaBH_4$ concentration is more important than $AgNO_3$ concentration; and for (2–5) factor of $AgNO_3$ concentration is more important than $NaBH_4$ concentration. The effects of concentration$AgNO_3$ and temperature of reaction on the size of nanoparticles is shown in Figure 8 (c). It shows both factors are important in determining nanoparticle size.

5. Conclusion

In this research, a suitable method was presented for simulating the structural features on size of Ag-NPs in MMT/Stc BNCs by the optimized artificial neural network. The Ag-NPs were synthesized from $NaBH_4$ as a strong reducing agent between silicates layer structures of MMT/Stc. With input vectors molar concentration of $AgNO_3$, temperature of reaction, percentage of starch, and amount of molar concentration of $NaBH_4$, consisting of one hidden layers (4:10:1) was adopted to predict the size of Ag-NPs. ANN generalization results denoted that the selected ANN successfully predicts the behavior of size of nanoparticles as functions of operating variables. Also, it was found out that the technique of ANN modeling has many satisfactory features like high accuracy, generalization and simplicity; consequently it is an excellent way for modeling such complex systems. Furthermore in this paper, fitting models was employed to model the impacts of numerous independent variables on the dependent variable. As shown in experimental results, the importance factors in identify of size of NPs respectively are the $AgNO_3$ concentration, temperature of reaction and $NaBH_4$. The modeling results revealed that the size of nanoparticles decreases with increasing the $AgNO_3$ concentration as well as the percentage of starch and amount of $NaBH_4$concentration. Therefore, employing neural network and fitting models would lead to

saving time and cost by predicting and evaluation the results of the reactions. The final models are presented as being useful for other researchers by preventing unnecessary experiments.

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References

[1] T.C. Karni, R. Langer, D.S. Kohane. ACS Nano. **6** (2012) 6541–6545.
[2] Z. Zalevsky, V. Mico, J. Garcia. J. Nanophotonics. **3** (2009) 1–18.
[3] S.B. Kalidindi, B.R. Jagirdar. Chem. Sus. Chem. **5** (2012) 65–75.
[4] M.L. Etheridge, S.A. Campbell, A.G. Erdman, C.L. Haynes, S.M. Wolf, J. McCullough. Nanomed: Nanotech. Biol. Med. **9** (2013) 1–14.
[5] E. Rodríguez-León, R. Iñiguez-Palomares, R. Elena Navarro, R. Herrera-Urbina, J. Tánori, C. Iñiguez-Palomares, A. Maldonado. Nanoscale Res. Lett. **8** (318) (2013) 1–9.
[6] A. Pal, S. Shah, S. Devi. Colloids Surf. A. **302** (2007) 483–487.
[7] M.J. Rosemary, T. Pradeep. Colloids Surf. A. **268** (2003) 81–84.
[8] Z.S. Pillai, P.V. Kamat. J. Phys. Chem. B. **108** (2004) 945–951.
[9]K. Patel, S. Kapoor, D.P. Dave, T. Murherjee. J. Chem. Sci. **117** (1) (2005) 53–60.
[10] B. Soroushian, I. Lampre, J. Belloni, M. Mostafavi. Radiat. Phys. Chem. **72** (2005) 111–118.
[11] M. Starowicz, B. Stypula, Banaœ. J. Electrochem. Commun. **8** (2006) 227–230.
[12] J.J. Zhu, X.H. Liao, X.N. Zhao, H.Y. Hen. Mater. Lett. **49** (2001) 91–95.
[13] S. Liu, S. Chen, S. Avivi, A. Gendanken. J. Non-Cryst. Solids. **283** (2001) 231–236.
[14] A.R. Shahverdi, A. Fakhimi, H.R. Shahverdi, M.S. Minaian. Nonomedicine. **3** (2007) 68–171.
[15] M.B. Ahmad, K. Shameli, W.M.Z. Wan Yunus, N.A. Ibrahim, A.A. Hamid, M. Zargar. Res. J. Biol. Sci. **4** (9) (2009) 1032–1036.
[16] K. Shameli, M.B. Ahmad, E.A.J. Al-Mulla, P. Shabanzadeh, S. Bagheri. Res. Chem. Intermediat. (2013) 1–13.DOI: 10.1007/s11164-013-1188-y
[17] K. Shameli, M.B. Ahmad, W.M.Z. Wan Yunus, N.A. Ibrahim, M. Jokar. Proc. World. Acad. Sci. Eng. Technol. **64** (2010) 28–32.
[18] M.E. Sigman, S.S. Rives. J. Chem. Inf. Comput. Sci. **34** (1994) 617–620.
[19] Y. Zhang, F. Chen, J. Zhuang, Y. Tang, D. Wang, Y. Wang, A. Dong, N. Ren. Chem. Commun. **49** (2002) 2814–2815.
[20] K. Shameli, M.B. Ahmad, M. Zargar, W.M.Z. Wan Yunus, N.A. Ibrahim, P. Shabanzadeh. Int. J. Nanomed. **6** (2011) 271–284.
[21] K. Shameli, M.B. Ahmad, M. Zargar, W.M.Z. Wan Yunus, A. Rustaiyan, N.A. Ibrahim. Int. J. Nanomed. **6** (2011) 581–590.
[22] M.B. Ahmad, J.J. Lim, K. Shameli, N.A. Ibrahim, M.Y. Tay. Molecules. **16** (2011) 7237–7248.
[23] K, Shameli, M.B. Ahmad, W.M.Z. Wan Yunus, N.A. Ibrahim. Int. J. Nanomed.**5** (2010) 743–751.

[24] K. Shameli, M.B. Ahmad, M. Zargar, W.M.Z. Wan Yunus, N.A. Ibrahim. Int. J. Nanomed.**6** (2011) 331–341.
[25] K. Shameli, M.B. Ahmad, S.D. Jazayeri, P. Shabanzadeh, H. Jahangirian, M. Mahdavi, Y. Abdullahi. Int. J. Mol. Sci.**13** (2012) 6639–6650.
[26] I. Pastoriza-Santos, L. M. Liz-Marzán. Langmuir**15** (1999) 948–951.
[27] M. B. Ahmad, K. Shameli, W. M. Z. Wan Yunus, N. A. Ibrahim. Aust. J. Basic Appl. Sci.**4**(2010) 2158–2165.
[28] P. Setua, R. Pramanik, S. Sarkar. J. Phys. Chem. B.**114** (2010) 7557–7564.
[29] P. Praus, M. Turicová, M. Klementová. J. Braz. Chem. Soc.**20** (2009) 1351–1357.
[30] L. Sun, Z. Zhang, H. Dang. Mater. Lett.**57** (2003) 3874–3879.
[31]M. H. El-Rafie, M. E. El-Naggar, M. A. Ramadan, M. M.G. Fouda, S. S. Alyab, A. Hebeish. Carbohydr. Polym.**86**(2) (2011) 630–635.
[32] N.L. Zhou , Y. Liu, L. Li, N. Meng, Y.X. Huang, J. Zhang, S.H. Wei, J. Shen. Curr. Appl. Phys.**7**(1001) (2007) 58–62.
[33] M.B. Ahmad, K. Shameli, W.M.Z. Wan Yunus, N.A. Ibrahim, A.A. Hamid, M. Zargar. Res. J. Biol. Sci.**4**(9), (2009) 1032–1036.
[34] F. S. Mjalli. Chem. Eng. Sci.**60**(1) (2005) 239–253.
[35] P. Shabanzadeh, R. Yusof, K. Shameli. J. Ind. Eng. Chem.(2014) 1–9.http://dx.doi.org/10.1016/j.jiec.2014.09.007.
[36] A.W. Krowiak, K. Chojnacka, D. Podstawczyk, A. Dawiec, K. Pokomeda. Bioresource Technol.**160** (2014) 150–160.
[37] R.H. Nia, M. Ghaedi, A.M. Ghaedi. J. Mol. Liq.**195** (2014) 219–229.
[38] M. Ghaedi, A.M. Ghaedi, F. Abdi, M. Roosta, R. Sahraei, A. Daneshfar. J. Ind. Eng. Chem.**20** (2014) 787–795.
[39]A. Rabbi, K. Nasouri, H. Bahrambeygi, A.M. Shoushtari, M. R. Babaei.Fiber. Polym. **13**(8) (2013) 1007–1014.
[40] M. Khayet, C. Cojocaru, M. Essalhi. J. Membrane Sci.**368** (2011) 202–14.
[41] V.G. Maltarollo, K.M. Honorio, A.B. Ferreira da Silva, INTECH (2013) 203–224. http://dx.doi.org/10.5772/51275.
[42] E.O. Cerqueira, J.C. Andrade, R.J. Poppi. Quím. Nova,**24** (2001) 864–873.
[43] M.E. Sigman, S.S. Rives. J. Chem. Inf. Comput. Sci.**34** (1994) 617–620.
[44] T. Hsiao, C. Lin, M. Zeng, H.K. Chiang. Proceedings of the 20th Annual International Conference of the IEEE Engineering in Medicine and Biology Society **20** (1998) 1341–1343.
[45] A. K. Jain, J. Mao, K.M. Mohiuddin. IEEE Computer **29** (1996) 31–44.
[46] C. Borggaard, H.H. Thodberg. Anal. Chem. **64** (1992) 545–551.
[47] F. Zheng, G. Zheng, A.G. Deaciuc, C.G. Zhan, L.P. Dwoskin, P.A. Crooks. Med. Chem. **15** (2007) 2975–2992.
[48] B, Louis, V.K, Agrawal, P.V. Khadikar. Eur. J. Med. Chem.**45** (2010) 4018–4025.
[49] M. H. Fatemi, A. Heidari, M. Ghorbanzade. Bull. Chem. Soc. Jpn. **83** (2010) 1338–1345.
[50] K.M. Honório, E.F. de Lima, M.G. Quiles, R.A.F. Romero, F.A. Molfetta, A.B.F. Da-silva. Chem. Biol. Drug. Des. **75** (2010) 632–640.
[51] Y. Qin, H. Deng, H. Yan, R. Zhong. J. Mol. Graph. Model. **29** (2011) 826–833.
[52] A. Rahman, M. Basyaruddin, N. Chaibakhsh, B. Mahiran, A. Bakar, S. A. A. Rahman, R. N.Z. Raja. Appl. Biochem. Biotechnol. **158 (**3), (2009) 722–735.
[53]. X. Song, A. Mitnitski, C. Macknight, K. Rockwood. J. Am. Geriatr. Soc.**52**(2004)1180–1184.
[54] P. Shabanzadeh, N. Senu, K. Shameli, M. Mohagheghtabar. E-J. Chem**.305713**, (2013)1–8. http://dx.doi.org/10.1155/2013/305713

[55] F. Marini, R. Bucci, A.L. Magrì, A.D. Magrì. Microchem. J.**88** (2008) 178–185.
[56] P. Shabanzadeh, N. Senu, K. Shameli, F. Ismail. Dig. J. Nanomater. Bios. **8**(3) (2013)1133–1144.
[57] E. Vatankhah, D. Semnani, M.P. Prabhakaran, M. Tadayon, S. Razavi, S. Ramakrishna. Acta Biomaterialia.**10** (2014) 709–721.
[58] P. Shabanzadeh, N. Senu, K. Shameli, F. Ismail, M. Mohagheghtabar. Dig. J. Nanomater. Bios. **8**(2), (2013) 541–549.
[59] J. Zupan, J. Gasteiger. Neural Networks in Chemistry and Drug Design, 2nd ed. Wiley VCH Ed., Weinheim ISBN: 978-3527297795, 1999.
[60] M.A. Bezerra, R.E. Santelli, E.P. Oliveira, L.S. Villar, L.A. Escaleira. Talanta **76** (2008) 965–977.
[61] H. Baseri, S.M. Rabiee, F. Moztarzadeh, M. Solati-Hashjin. Mater. Design.**31** (2010) 2585–2591.
[62] H. Demuth, M. Beale, Neural Network Toolbox for Use with MATLAB, TheMathWorks, Inc., Massachusetts, 1998.
[63] P. Shabanzadeh, N. Senu, K. Shameli, F. Ismail, A. Zamanian, M. Mohagheghtabar. Res. Chem. Intermed. (2014)1–8. DOI: 10.1007/s11164-013-1431-6