International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 10 (2018) pp. 7261-7266
© Research India Publications. http://www.ripublication.com

Modeling and Simulation of the Polymer Behavior Filed by Nano Particles Using Artificial Neural Network

A. A. Alshennawy [1,2*], Ageel F. Alogla[1], Ayman A. Aly [1,3]

[1] *Mechanical Engineering Department, College of Engineering, Taif University, Taif, Kingdom of Saudi Arabia.*

[2] *Production and Mechanical Design Department, Faculty of Engineering, Tanta University, Tanta, Egypt.*

[3] *Mechatronics Sec., Mechanical Engineering Department, Faculty of Engineering, Assiut University, Assiut, Egypt.*

Abstract

The polymeric compositions filled with Nano particles is the most important and faster research axes for development of engineering materials. The objective of having two or more constituents is to take advantage of the superior properties of both materials without compromising on the weakness of either. A soft plastic can become harder and stronger by the addition of a light weight high stiffness material. The mathematical model of such behavior is very difficult to be determined. An alternative solution to predict the polymer behavior filed by Nano particles is using soft computation technique such as Artificial neural networks (ANN), which is based on the information processing system of the human brain. In general, it is composed of three layers of neurons; (a) input layer neurons that may receive external data, (b) output layer neurons that send data out of the ANN, and (c) hidden layer neurons whose signals remain within the ANN and connect the input layer neurons to output layer neutrons. The hidden neurons may form one or more hidden layers.

In the present work, the main objective is to study the polymer behavior filed by nano particles using the ANN considering description of the different ANN structures, selection of the suitable ANN model based upon minimizing the least square error between the predicted and target outputs and finally validate of the proposed ANN model

Keywords: Polymer Composites, Artificial neural networks (ANN), Mechanical Properties, Modeling and simulation.

INTRODUCTION

With the booming of nano-phased materials in the re-cent years, attempts are being made to develop nano- particle filled-polymer composites with improved tribologi- cal performance of the materials. It is expected that good tribological properties can be obtained for the polymers filled with nano-scale fillers compared to those filled with micro-scale particles [20,21]. Due to their lower strength and stiffness compared with synthetic fibers, natural fibers use in polymer composites has been limited to non-tribological applications. Very little information concerning the tribological performance of natural fiber reinforced composite materials has been reported [22].

Polytetrafluoroethylene (PTFE) exhibits many desir- able tribological characteristics, including high melting temperature, low friction, and chemical inertness. PTFE is an excellent solid lubricant and used commonly in bearing and seals applications [23] Unfortunately, PTFE exhibits high wear rate under normal friction conditions, which limits its application fields. Therefore, many kinds of PTFE-based composites have been produced to improve the wear resistance of PTFE [24,25]. It was found that some micro-scale inorganic fillers showed distinct effect on the friction and wear behaviors of PTFE composites [26].

There are several different methods for dispersing carbon nano particles, and the determination of the ideal method proves challenging. These methods utilize polymers, surfactants, acids, or a combination of several different materials to disperse carbon nano-tubes [1-15]. Several of these methods tend to utilize hazardous materials and lengthy procedures to produce the desired result, while others require less dangerous materials with shorter durations to produce a similar result [5-6,13-25]. Therefore, these less dangerous methods used to disperse carbon nano-tube may not be thought of as “ideal methods.” Typically, all of the methods utilize some degree of sonification, from a few minutes to several hours, to initially mechanically disperse the carbon nano-tubes. This method of mechanical dispersion in conjunction with these surface-active agents reduces the van der Waals forces, provided that, the dispersing agent can separate the carbon nano-tubes to prevent re-aggregation [22- 23].

Due to the interactions of the polymer chains with the supporting surface and the air interface, the thinner films required for such applications have distinctly different properties than those of the well-defined bulk systems.

From experimental point of view and due to some inconsisteny on this subject in the literature, the objective of this study is to develop an Artificial Neural Network (ANN) model to predict the behaviour filed by nano based on experimentally measured values gathered from different published articles. The advantages of ANN compared to classical methods are its high speed, simplicity, and large capacity which reduce engineering efforts. The ANN has been applied successfully in various fields of modeling and prediction in many thermal engineering applications [27-29]. In the present study, the performance of the proposed ANN model is assessed by comparing the predicted results with the experimental data.

The present paper aims to model the effect of adding different percentages of carbon nano-particulates (CNP_S) to polystyrene

International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 10 (2018) pp. 7261-
© Research India Publications. http://www.ripublication.com

(PS) on the mechanical properties of nano-composites produced using ANN technique.

EXPERIMENTAL PROCEDURES

Coating into the four stages of deposition, spin-up, spin-off, and evaporation (Fig.1). By taking both the force of spinning and the concentration-controlled evaporation into account, these researchers were able to predict film thickness. This model was extremely useful because it included the surface chemistry and the type of polymer used. Solutions in toluene were prepared at 0.2%, 0.5%, 0.7%, and 1.0% by weight of CNP_S.

The silicon wafers were positioned on the spin coater and several drops of solution were placed on the wafer. Immediately, each sample began rotating at a constant speed to acquire the desired film thickness (2500 rpm). The samples were spun for one minute.

Figure 1: Spin coating.

Test rig

For measuring the friction and wear resistance a test rig was built. The test specimen assembly was carried on the compound cross slide of the lathe, which automatically operated for positioning purposes in the direction of adhesion, driven by controlled speeds. The test specimen was mounted on a platen supported on the tool post and restrained by a load cell, which senses tangential force on the test surface in the direction of sliding. The details of the test rig are shown in Fig. 2. The indenter, used in experiments, was a spherical and hardened steel ball having diameter of 1.588 mm, (see Fig.2). The friction force was measured by the deflection of the load cell. The ratio of the friction force to the normal load was considered as friction coefficient. The load was applied by weights. The test speed was nearly controlled by automatically turning the power screw feeding the indenter in the adhesion direction. The adhesion velocity was 0.05 mm/s. All measurements were performed at 28 ± 2 ° C and 50 ± 10 % humidity.

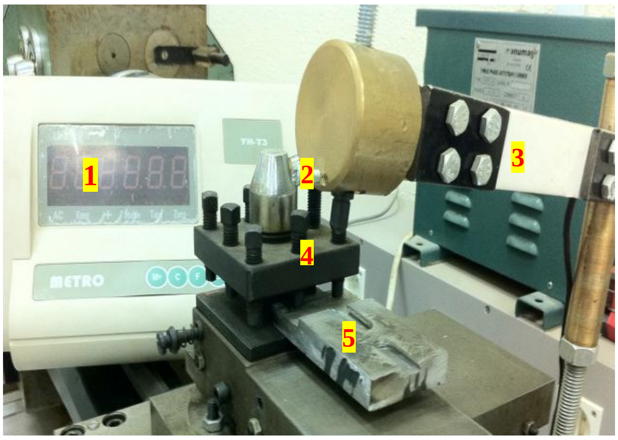

Figure 2. Measurements test rig

(1: screen, 2: indenter holder, 3: load cell, 4: ball indenter, 5: specimen holder).

The effect of the CNP_S content on the friction coefficient of composites is shown in Fig. 3 at different applied loads (4, 5 and 6 N). Generally, the figure shows scattering values for the frictional behavior of PS nano-composites containing different CNP_S contents.

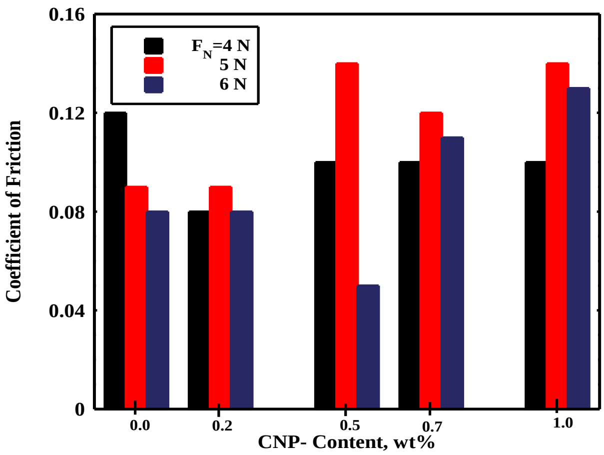

Figure 3: Friction coefficient of the carbon nano-particulates-PS composites.

It is clear that there are two different behaviors in the figure; one of them belongs to the unfilled specimens and the other concerning with filled specimens. The unfilled specimen exhibits a continuous decrease in the coefficient of friction with increasing normal load as a result of the frictional heating that reduced the shear strength of the PE specimens. Moreover, the topography of the surface becomes smoother with increasing the load causing a decrease in the values of friction. Whereas the second trend which concerning with the carbon nano-particulates filled PS based composites shows a variation of friction coefficient with increasing normal load. Friction coefficient of PS samples filled by carbon nano-particulates with different weight contents is shown in the previous Figure too. PS composites containing carbon nano-particulates of 0.5 wt. % showed the smallest coefficient of friction at applied load of 6 N while the maximum values always displayed at applied load of 5 N. The increase in the coefficient of friction during adhesion is attributed to increasing plowing of the coating by the indenter with increasing normal load but the abrupt decrease of friction at applied load of 6 N may be attributed to the direct contact with the carbon nano-particulates which its nature as a solid lubricant.

THE ARTIFICIAL NEURAL NETWORK MODEL

A computing system, made up of a number of simple, highly interconnected processing elements, which processes information by its dynamic state response to external inputs. The ANN is supposed to consist of artificial neurons or processing elements [13, 14].

If we denote the i^{th} input as x_i and the output as y, then it can write the mapping from the inputs to the output performed by the processing elements in this case as:

$$y = f\left(\sum x_i w_{ij} + b \right) \tag{1}$$

Layers are connected together composing an ANN. Inputs could be connected to many nodes with various weights, resulting in a series of outputs, one per node (Fig. 4). The connections are multiplied by the weights associated with that particular node with which they interconnect. They convey analog values. Note that there are many more connections than nodes. The network is said to be fully connected if every output from one layer is passed along to every node in the next layer.

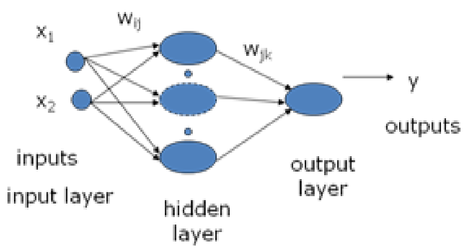

Figure 4. A schematic of multilayer neural network

Several studies have found that a three-layered neural network with one hidden layer can approximate any nonlinear function to any desired accuracy [15]. The network consists of input layer, hidden layer and output layer.

The method is based on an analysis of how a change in any particular weight influences the output of the network. After such analysis is done, the designer understands how to change the weights to achieve the specified values for the outputs.

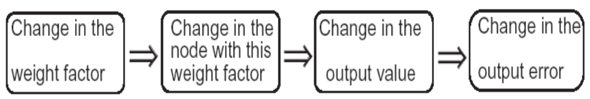

Figure 5. ANN analysis algorithm

First of all, one must construct a chain similar to Fig. 5. This chain examines the influence of any weight factor on the output value and, hence, on the error value. Where, the error is the difference between the actual output and the desired one.

The performance function is the sum square error (SSE) which is defined as the sum of square of the difference between target output (expected) and the actual output from the NN.

$$SSE = \sum_{k=1}^{m} (t_k - y_k)^2 \tag{2}$$

Learning rule gradually adjusts the weights until the performance function (SSE) falls below a certain threshold or minimised.

Back-propagation learning updates the network weights and biases in the direction in which the performance function decreases most rapidly, i.e., the negative of the gradient.

$$\overline{w}_{k+1} = \overline{w}_k - \alpha_k \overline{g}_k \tag{3}$$

where w_{k+1} are updated weights, w_k are current weights, g_k is current gradient of performance function, and α_k is the learning rate. In this paper the network has two input elements and one outputs. Ten element hidden layers are assigned. For more details, Appendix –A illustrates the Back-Propagation Algorithm which was used for design the ANN model.

RESULTS AND DISCUSSION.

To validate the ANN model in predictive mode a set of experimental data (15 values) was used to test the model. Figure 4 shows the predicted results from the ANN model versus experimental measurements for friction coefficients with different CNPs. The figure show excellent agreement between the predicted values and the experimental data. The accuracy of the predicted results is the same as that of the trained data.

The error analysis of the data is presented in Fig. 5 with different CNPs and different applied forces. With applied force of 4N, it is found that the maximum error is around $2\text{x}10^{-8}$ as illustrated in Fig.5-a. The error friction coefficients with 5N force is about $12\text{x}10^{-4}$ as shown in Fig.5-b while less than $2.5\text{x}10^{-4}$ as shown in Fig5.-c. The most important value of applying the ANN model is that it makes it possible to evaluate the friction coefficients in terms of the other two properties (applied force and CNPs) at any value within the treated range of data. In Fig.6-a, with applied force of 4N and CNPs values more than 1% is predicted via ANN model and less than 1% is the reference values which the ANN was built by them. The values of the applied force was changed to be 5N in Fig.6-b and 6N in Fig.6-c. It very useful to find extension of the results using the ANN Model.

International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 10 (2018) pp. 7261-
© Research India Publications. http://www.ripublication.com

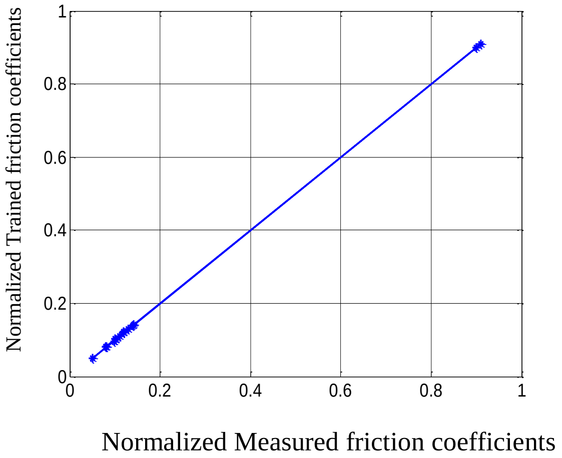

Figure 5: Comparison of experimentally measured and ANN-trained values of friction coefficients

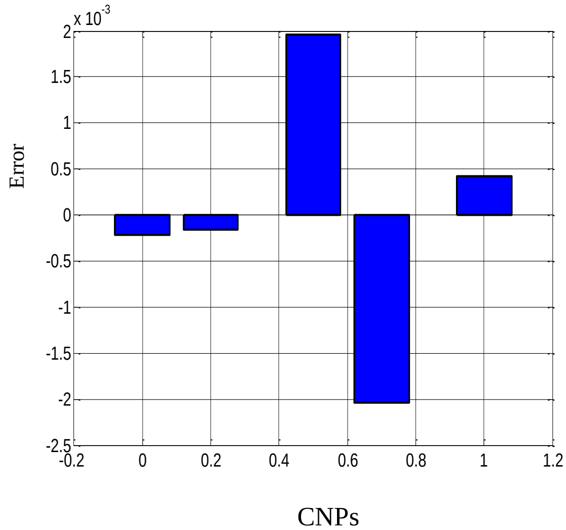

Figure.5-a Error between trained and measured friction coefficients with applied force of 4N.

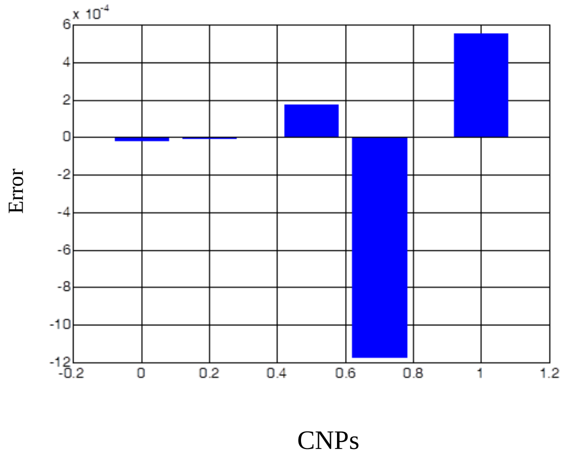

Figure 5-b Error between trained and measured friction coefficients with applied force of 5N.

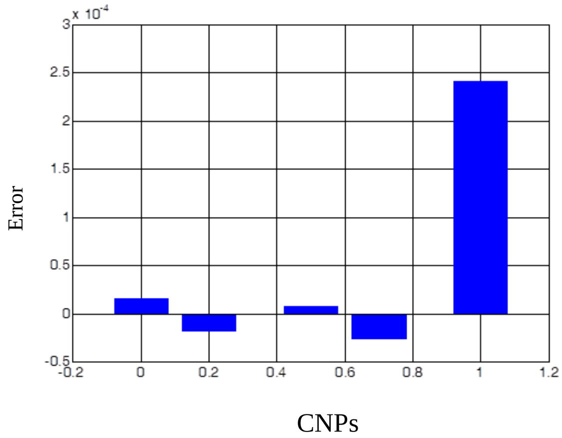

Figure.5-c Error between trained and measured friction coefficients with applied force of 6N.

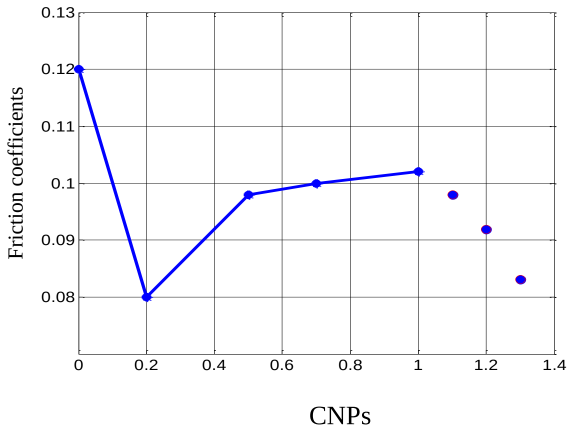

Figure 6-a Friction coefficients with applied force of 4N.

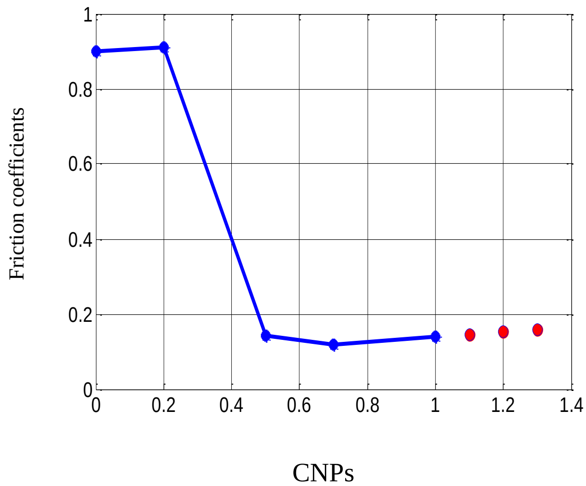

Figure 6-b Friction coefficients with applied force of 5N.

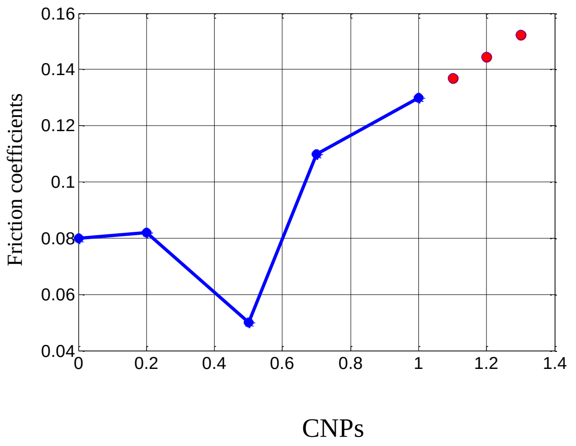

Figure.6-c Friction coefficients with applied force of 6N.

CONCLUSION

The problem associated with the application of a neural network (ANN) model to evaluate the instantaneous values of the friction coefficients is treated. The neural network model is implemented, and its feasibility is established. Good agreement between the outputs from the ANN model and the corresponding data is found. It is seen that the use of the proposed methodology results in some desirable characteristics. More accurate values of the friction coefficients can be obtained over a wide range of the CNPs and the applied force values without any need to empirical correlations.

ACKNOWLEDGEMENT

The authors would like to express their sincere gratitude to Taif University for its fully funding this research project (project number 5888/1438)**.**

APPENDIX A: Back-Propagation Algorithm

Back-propagation learning is one of the most popular types NN learning methods. It has two operational phases. In first phase, forwarding phase, we send input data from input layer to the output layer. In the second phase, back-propagation phase, we calculate the error (between target and output) and propagate the error backwardly to the input layer in order to change the weights of hidden layers by using the gradient descent method.

Several studies have found that a three-layered neural network with one hidden layer can approximate any nonlinear function to any desired accuracy [14]. The network consists of input layer, hidden layer and output layer. To explain the Back-propagation rule in detail a 3 layer network shown in Fig.6 will be used. The training phase is divided as follows:

1. forward-propagation phase: X=[Qp; PP] is propagating from the input layer to the output layer Y=[θp].

$$Z_q = f\left(\sum_{j=1}^{m} v_{qi} X_j\right) \tag{12}$$

$$Y_i = f\left(\sum_{q=1}^{l} w_{iq} Z_q\right) \tag{13}$$

2. back-propagation phase: (14) shows the error between the output, y, and the target, d.

$$E = \frac{1}{2}\sum_{i=1}^{n}\left(d_i - y_i\right)^2 \tag{14}$$

By using the gradient-descent method, the weights in hidden-to-output connections are updated as follows:

$$\begin{aligned}\Delta w_{iq} &= -\eta\frac{\partial E}{\partial W_{iq}} = -\eta\left[\frac{\partial E}{\partial Y_i}\right]\left[\frac{\partial Y_i}{\partial net_i}\right]\left[\frac{\partial net_i}{\partial W_{iq}}\right] \\ &= -\eta\left[d_i - y_i\right]\left[f'(net_i)\right]\left[Z_q\right] = \eta\delta_{oi}Z_q\end{aligned} \tag{15}$$

Following equations are the weight update on the input-to-hidden correction. Also chain rule and gradient-descent method are employed.

$$\begin{aligned}\Delta v_{qi} &= -\eta\frac{\partial E}{\partial V_{qi}} = -\eta\left[\frac{\partial E}{\partial net_q}\right]\left[\frac{\partial net_q}{\partial V_q j}\right] \\ &= \eta\delta_{hq}x_i\end{aligned} \tag{16}$$

$$\delta_{oi} = -\left[d_i - y_i\right]\left[f'(net_i)\right] \tag{17}$$

$$\delta_{hq} = \left[\frac{\partial E}{\partial Z_q}\right]\left[\frac{\partial Z_q}{\partial net_q}\right] \tag{18}$$

In Back-propagation learning rule, the two phases are iterated until the performance error decreased to certain small range.

REFERENCES

[1] L. E. Nielsen, R. F. Landel, “Mechanical Properties of Polymers and Composites,” 2nd ed., Marcel Deckker, New York, 1994.

[2] S. Nikkeshi, M. Kudo, T. Masuko, “Dynamic Viscoelastic Properties and Thermal Properties of Powder-Epoxy Resin Composites,” J Appl Poly Sci., Vol. 69, 1998), pp. 2593-2598.

[3] K. Zhu, S. Schmauder, “Prediction of the Failure Properties of Short Fiber Reinforced Composites with Metal and Polymer Matrix,” Comput Mater Sci., Vol. 28, 2003, pp. 743–748.

[4] I. H. Tavman, “Thermal and Mechanical Properties of Copper Powder Filled Polyethylene Composites,” Powder Technol., Vol. 91, 1997, pp. 63–67.

[5] T. Ahmad and O. Mamat, “The Development and Characterization of Zirconia-Silica Sand Nanoparticles

Composites," World Journal of Nano Science and Engineering, Vol. 1, No. 1, 2011, pp. 7-14..

[6] S. T. Peters, "Handbook of Composites," 2nd ed., Chapman and Hall, London, 1998.

[7] R. N. Rothon, "Mineral Fillers in Thermoplastics I Raw Materials and Processing," Adv. Polymer Sci., Vol. 139, pp. 67, J.Jancar, Ed., Springer, Berlin 1999.

[8] M. Sumita, T. Shizuma, K. Miyasaka, K. Ishikawa, "Effect of Reducible Properties of Temperature, Rate of Strain, and Filler Content on the Tensile Yield Stress of nylon 6 Composites Filled with Ultrafine Particles," Journal of Macromolecular Science, Physics Vol. B22 (1983), pp. 601-618.

[9] P. Ayak, S. K. Sahoo, A. Behera, P. K. Nanda, P. L. Nayak and B. C. Guru, "Synthesis and Characterization of Soy Protin Isolate/MMT Nanocomposite Film for the Control Release of the Drug Ofloxacin," World Journal of Nano Science and Engineering, Vol. 1, No. 2, 2011, pp. 27-36.

[10] Ayman A. Aly, El-Shafei B. Zeidan, AbdAllah A. Alshennawy, Aly A. El-Masry, Wahid A. Wasel, "Friction and Wear of Polymer Composites Filled by Nano-Particles: A Review," World Journal of Nano Science and Engineering, 2012, 2.

[11] M.S. Senthil Kumar, N. Mohana Sundara Raju, P.S. Sampath and L.S. Jayakumari, " Effects Of Nanomaterials On Polymer Composites - An Expatiate View", Rev.Adv.Mater. Sci. 38 (2014) 40-54

[12] M. C. Kuo, C. M. Tsai, J. C Huang, M. Chen, "PEEK Composites Reinforced by Nano-Sized SiO_2 and Al_2O_3 Particulates Materials," Chemistry and Physics, Vol. 90, 2005, pp. 185-195.

[13] T. E. Attwood, P. C. Dawson, J. L. Freeman, L. R. J. Hoy, J. B. Rose, P. A. Staniland, "Synthesis & Properties of Polyaryletherketones," Polymer, Vol. 22, 1981, pp. 1096-1103.

[14] P. K. Goyal, Y. S. Negi, A. N. Tiwari, "Preparation of High Performance Composites Based on Aluminum nitride/Poly(ether-ether-ketone) and Their Properties," European Polymer Journal, Vol. 41, 2005, pp. 2034-2044.

[15] P. Cassagnau, Payne, "Effect and Shear Elasticity of Silica-Filled Polymers in Concentrated Solutions and in Molten State," Polymer, Vol. 44, 2003, pp. 2455-2462.

[16] Y.H. Lai, M.C. Kuo, J.C. Huang, M. Chen, "Thermomechanical Properties of Nanosilica Reinforced PEEK Composites," Key Engineering Materials ,Vol. 351, 2007, pp. 15-20.

[17] Q. H. Wang, Q. J. Xue, W. M. Liu, J. M. Chen, "The Friction and Wear Characteristics of Nanometer SiC and Polytetrafluoroethylene Filled Polyetheretherketone," Wear, Vol 243, 2000, pp. 140-146.

[18] C. J. Schwartz, S. Bahdur, "Studies on the Tribological Behavior and Transfer Film–Counterface Bond Strength for Polyphenylene Sulfide Filled with Nanoscale Alumina Particles," Wear, Vol. 237, 2000, pp. 261-273.

[19] E. Reynaud, C. Gauthier, J. Perez, "Nanophases in Polymers," Rev. Metall., Vol. 98, 1999, pp. 169-176.

[20] Q. H.Wang, Q. J. Xue,W. C. Shen, "The Friction and Wear Properties of Nanometre SiO2 Filled Polyetheretherketone," Tribol. Int., Vol. 30, 1997, pp.193-197.

[21] M. Q. Zhang, M. Z. Rong, S. L. Yu, B.Wetzel, K. Friedrich, "Improvement of Tribological Performance of Epoxy by the Addition of Irradiation Crafted Nano-Inorganic Particles," Macromol. Mater. Eng, Vol. 287, 2002, pp.111-115.

[22] F. Li, K. Hu, J. Li, "The Friction and Wear Characteristics of Nanometer ZnO Filled Polytetrafluoroethylene," Wear, Vol. 249, 2002, pp. 877-882.

[23] W. G. Sawyer, K. D. Freudenberg, P. Bhimaraj, L. S. Schadler, "A Study on the Friction and Wear Behavior of PTFE Filled with Alumina Nanoparticles," Wear, Vol. 254, 2003, Vol. 573-580.

[24] Ayman A. Aly, Zeidan E. B., Hamed A. M., Ali W. Y., "Effect of Heat Treatment on the Abrasion Resistance of Thermoplastic Polymers," EGTRIB Journal of The Egyptian Society of Tribology Vol. 7, No. 4, 2010, pp.52 -64, .

[25] A. Hoshino, K. Fujioka, T. Oku, S. Nakamura, M. Suga, Y. Yamaguchi, K. Suzuki, M. Yasuhara, "Quantum Dots Targeted to the Assigned Organelle in Living Cells," Microbiology and immunology, Vol. 48, No. 12, 2004, pp. 985–994.

[26] Zhou Y. X., Pervin F., Jeelani S., Mallik P.K., "Experimental Improvement in Mechanical Properties of Carbon Nanofibers," Journal of Materials Processing Technology, 2008, 198, pp 445-453.

[27] YadollahAbdollahi, AzmiZakaria, NorAsrinaSairi, KhamirulAminMatori, HamidRezaFardMasoumi, AmirRezaSadrolhosseini, andHosseinJahangirian, "Artificial Neural Network Modelling of Photodegradation in Suspension of Manganese Doped Zinc Oxide Nanoparticles under Visible-Light Irradiation", Hindawi Publishing Corporation • e Scientific World Journal Volume 2014, Article ID 726101, 10 pages, http://dx.doi.org/10.1155/2014/726101 modeling

[28] Heydartaemeh, Panjipour and Karamoozian, "Artificial Neural Network (ANN) Approach for Modeling Co2+ Ion Adsorption from Aqueous Solutions by Loess Soil Nanoparticles", Heydartaemeh et al., Adv Recycling Waste Manag, 2017, 2:3, DOI: 10.4172/2475-7675.1000134 modeling

[29] Rasheed Atif, Fawad Inam, "Modeling and Simulation of Graphene Based Polymer Nanocomposites: Advances in the Last Decade", Graphene, 2016, 5, 96-142 Published Online April 2016 in SciRes.