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Journal of Macromolecular Science, Part A
Pure and Applied Chemistry

ISSN: 1060-1325 (Print) 1520-5738 (Online) Journal homepage: http://www.tandfonline.com/loi/lmsa20

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To cite this article: Ashkan Reisi-Dehkordi & Reza Eslami-Farsani (2015) Prediction of High Performance Fibers Strength Using Back Propagation Neural Network, Journal of Macromolecular Science, Part A, 52:8, 642-647, DOI: 10.1080/10601325.2015.1050636

To link to this article: http://dx.doi.org/10.1080/10601325.2015.1050636

Published online: 24 Jun 2015.

Journal of Macromolecular Science, Part A: Pure and Applied Chemistry (2015) **52**, 642–647

ISSN: 1060-1325 print / 1520-5738 online
DOI: 10.1080/10601325.2015.1050636

Prediction of High Performance Fibers Strength Using Back Propagation Neural Network

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Received December 2014, Accepted February 2015

Nowadays, quantification of the effects of basic parameters such as precursor, temperature oxidation, residence time, low temperature carbonization (LTC) and high temperature carbonization (HTC) on production process polyacrylonitrile based carbon fibers is not completely understood. In this way, there is not a completely theoretical model that accomplishes to quantitatively describe production process carbon fibers very accurately which needs to be used by engineers in design, simulation and operation of that process. This paper presents the development of a back propagation neural network model for the prediction of carbon fibers produced from PAN fibers. The model is based on experimental data. The precursors, temperature oxidation, residence time, LTC and HTC have been considered as the input parameters and the strength as output parameter to develop the model. The developed model is then compared with experimental results and it is found that the results obtained from the neural network model are accurate in predicting the strength of carbon fibers.

Keywords: High performance fibers, production process, back propagation neural networks, regression model

1 Introduction

At present, three precursors, including polyacrylonitrile (PAN)-based, rayon-based, and pitch-based fibers, are mainly used for the production of carbon fibers (1). Due to its high degree of molecular orientation, higher melting point, and greater yield of carbon fibers, PAN fiber has been found to be the most suitable precursor for making carbon fibers (1–4). PAN fiber is a form of acrylic fiber, composed of acrylonitrile units in at least 85% wt. The remaining 15% consists of neutral and/or ionic co-monomers, used to improve the properties of the fibers (3–6).

Developing carbon fiber from PAN fiber is generally subjected to three processes, namely stabilization, carbonization, and graphitization under controlled conditions (4). The PAN fiber is first stretched and simultaneously oxidized in a temperature range of 200–300°C (1, 4, 5). After oxidation, the fibers are carbonized at about 1000°C in inert atmosphere which is usually nitrogen (1, 4). Then, in order to improve the ordering and orientation of the crystallites in the direction of the fiber axis, the fiber must be heated at about 1500–3000°C (4). High temperature process generally leads to higher modulus fibers which expel impurities in the chain as volatile by-products (1, 3–7). During heating treatment, the fiber shrinks in diameter, builds the structure into a large structure and upgrades the strength by removing the initial nitrogen content of PAN precursor and the timing of nitrogen (1, 4, 5, 8).

As previously discussed, many parameters have effects on performance of production process carbon fibers. According to previous studies, five parameters were selected. It is believed that they have the greatest effects on production process including precursor, temperature oxidation, residence time, LTC and HTC (1, 4, 5, 9–12).

However, costly and time-consuming experiments are required in order to determine the optimum production process parameters due to the complex and nonlinear nature of the production process of carbon fiber. Therefore, a more efficient method is needed to determine the optimum production process parameters. Technique of neural networks offers potential as an alternative to standard computer techniques in control technology and has attracted a widening interest in their development and application (13–16). The advantages of the neural

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networks is that the network can be updated continuously with new data to optimize its performance at any instance, the networks ability to handle a large number of input variables rapidly, and the networks ability to filter noisy data and interpolate incomplete data (14, 16–18).

The back propagation network system is one of the families of artificial neural network techniques used to determine the production process of carbon fiber parameters for various production processes. The network is a multilayer network that contains at least one input layer in addition to input and output layers. Number of input layers and number of neurons in each hidden layer is to be fixed, based on the application, the complexity of the problem, and the number of inputs and outputs (17–20).

The objective of this research is to investigate the possibility of employing neural network models to accurately strength of carbon fibers produced from PAN Fibers. Network connection weights are also interpreted quantitatively to determine the relative importance of precursor (PAN Fibers), temperature oxidation, residence time, LTC and HTC on strength of carbon fibers.

2 Experimental

2.1 Materials

2.1.1 *Fibers precursor*

Polyacrylonitrile (PAN) is an important commercially useful polymer used in a wide range of industrial applications such as carbon fibers. Producing best quality carbon fibers from commercial PAN fibers through the common processing routines is not possible. But in recent years, there have been successful attempts in making carbon fibers from these fibers types through several chemical and mechanical treatments before and after stabilization (19, 20). Experiments were carried out using a commercial PAN fibers precursor from Polyacryl Iran Corporation (PIC). Specification and properties of commercial PAN fibers utilized in this paper are shown in Table 1.

2.2 Method and Procedure

The PAN fibers used were converted into carbon fibers at two stages as follows:

a) Stabilization in a batch furnace with air circulation system at temperatures ranging from 180–260°C.
b) Carbonization of the stabilized PAN fibers in a horizontal tubular furnace with a ceramic tube under high purity nitrogen atmosphere (99.999%) at a temperatures ranging from 1200–1450°C.

The schematics of stabilization and carbonization furnaces are shown in Figures 1a and 1b, respectively. During the experiments, supervision was carefully done to control stabilization temperature, stabilization duration time, carbonization temperature and carbonization duration time. All of the adjustments and measurements for the experiments were the same.

2.3 Artificial Neural Networks

A commercially available software program (Matlab neural network toolbox v. 6.1, 2006) was applied to implement supervised neural network on a personal computer. The network was trained in three stages: (1) feed forward of the input training pattern, (2) calculation and back propagation of the associated error, and (3) the adjustment of the weights. The neural network output corresponding to the input patterns were then compared with the target values and the weights were adjusted to reduce the sum of square of errors (16, 17, 19).

2.3.1 *Theory*

Back propagation learning is a supervised learning which needs to know the inputs and the desired outputs in advance. This network is well established as a method for data mapping. Data estimated from the experiments and regression models are provided to a network at the learning stage, e.g., production process parameters. During network learning, the network output is compared with the desired output and the connector weights inside the network adjust to minimize the difference. The error is then propagated backwards through the network and weights are changes based on the back propagation-learning algorithm. This learning process is an iterative process and learning will stop once an acceptable error is achieved. When the trained network is presented with new input

Table 1. Specification and properties of commercial PAN fibers used

Type	*Shape of cross section*	*Cross sectional area* (μm^2)	*Density* (g/cm^3)	*Linear density (tex)*	*Tensile strength (MPa)*	*Elongation (%)*	*Chemical analysis (%)*		
							AN	*MA*	*SMS*
Commercial PAN fibers fabricated by dry spinning	Dog-bone	423	1.18	0.5	244	41	93	6	1

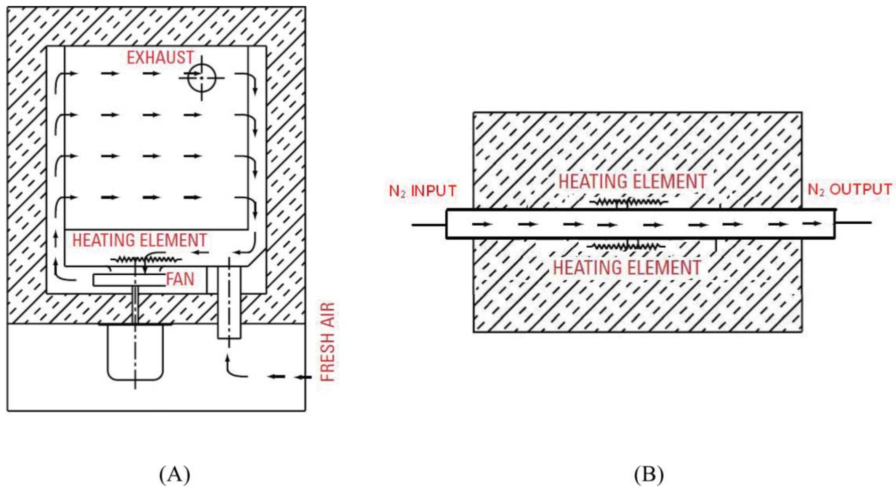

Fig. 1. The schematics of (a) stabilization furnace and (b) carbonization furnace.

(beyond training), the network responds according to the knowledge it has acquired (17–20).

The process operating parameters of the production process of carbon fiber are fed as input to the input layer of the network. Each of the inputs, Ii is multiplied by weights on inter-layer connections of a hidden layer neuron, Wij1 and added to bias, φ to produce activation. Also, α can be represented by the Equation 1.

$$\alpha_1 = W_{ij}{}^1 I^T + \varphi \tag{1}$$

where I_i is the output of the input layer, and $W_{ij}{}^1$ is the weight structure between input and hidden layers.

A log-sigmoid activation function that transforms activation of hidden layer neurons to a scaled output O_1 can be written as Equation 2.

$$O_1 = \frac{1}{e^{\alpha 1}} + 1 \tag{2}$$

Outputs from hidden layer neurons are treated as inputs to output layer neurons. Summation of product of all hidden layer outputs and weights between hidden and output layers added to bias constitutes activation a_2 of output layer neurons. Log-sigmoid transfer function is applied and output O_2 is computed. Error is estimated as difference between actual and computed outputs. This procedure constitutes forward flow of back propagation phase and error computed is back propagated through same network to update weights. Weights are updated using generalized delta rule as given in Equation 3:

$$W_{new} = W_{old} - \eta E_T I \tag{3}$$

where W_{new} is weight after modification, W_{old} is the weight structure before modification, η is the learning rate, usually taken between 0 and 1, and ET is the error calculated. ET is described using the following equation:

$$ET = X_{experimental(i)} - X_{calculated(i)} \tag{4}$$

where $X_{experimental(i)}$ and $X_{calculated(i)}$ are the ith experimental and ANN predicted data correspondingly.

Weight change is determined for all connections. Errors for all patterns are summed and the algorithm is run till error falls below a specified value. Back propagation algorithms attempts to minimize the error of mathematical system represented by neural network's weights and thus walk downhill to the optimum values for weights. Unfortunately due to the mathematical complexity of even simplest neural network, there are many minima, some deeper than others (16, 17, 19).

2.3.2 *Variable learning rate algorithm*

With standard steepest descent, the learning rate is held constant throughout training. The performance of the algorithm is very sensitive to the proper setting of the learning rate and can be improved if we allow the learning rate to change during the training process. An adaptive learning rate will attempt to keep the learning step size as large as possible while keeping learning stable. First, the initial network output and error are calculated. At each epoch new weights and biases are calculated using the current learning rate. New outputs and errors are then calculated. If the new error exceeds the old error by more than a predefined ratio max-perf-inc (typically 1.04), the new weights and biases are discarded. In addition, the learning rate is decreased (by multiplying by lr-dec). Otherwise, the new weights, etc., are kept. If the new error is less than the old error, the learning rate is increased (by multiplying by lr-inc). This procedure increases the learning rate, but only to the extent that the network can learn without large error increases. The gradient is computed by summing the gradients calculated at each training example, and the weights and biases are only updated after all training examples have been presented (MATLAB 6.1) (16, 18, 19).

2.4 Model Development

2.4.1 *Experimental data processing*

Five input process parameters, precursor, temperature oxidation, residence time, LTC and HTC are used in the present study to predict one output parameter, strength. Experiments have been carried out for different combinations of inputs.

The process parameters included in performing the experiment are three levels of precursor (A, B and C), four levels of temperature oxidation (200, 210, 220 and 230°C), three levels of residence time (30, 60 and 90 min), four levels of LTC (450, 500, 550 and 600°C) and HTC at 1000, 1100, 1200, 1300 and 1400°C. All other parameters except these under consideration are fixed. During the experiments, temperature oxidation, residence time, LTC and HTC were carefully controlled.

Various experiments have been carried out for different combinations of inputs and the production process parameters have been found. Seventy-five tests are taken to develop the back propagation neural network model, of which, sixty-four tests are used for training the back propagation neural network model and eleven tests are used for testing.

2.4.2 *Network experimentation*

A schematic representation of the back propagation neural network model is shown in Figure 2. The hidden network structure contains two layers and a bias node. The neural network employed in this case is a feed forward back propagation rule with 'Traingda' as it is a Matlab command for a particular type of gradient descent algorithm (with adaptive capacity).

The input layer has five neurons (since five input parameters) and the output layer has one neuron (17–21).

The inputs and the outputs are normalized in the range [0,1]. A log-sigmoid transfer function is used for both the layers as the outputs are ranging between zero and one. The network was created in MATLAB 6.1 using the function net1=newff (minmax (p), (5, 4, 2), {'logsig','logsig','logsig'}, 'traingda'). Then it was imported to GUI network/data manager for training and testing the results (15–17, 20, 21).

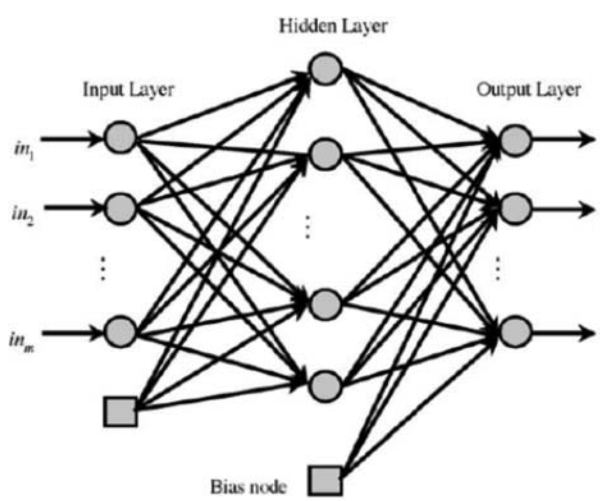

Fig. 2. The topological structure of a typical back-propagation neural network (17).

3 Results and Discussion

In this section, the production process of carbon fiber is modeled by a back-propagation artificial neural network with five inputs (precursors, temperature oxidation, residence time, LTC and HTC) and one output (strength). A trial-and-error method is used in the optimization of neural network production process. A back propagation neural network model to predict production process is developed in this work. To ensure the accuracy of the back propagation neural network model developed to predict strength, density and linear density, the experimental results and the predicted results using the developed back propagation neural network model are compared. A correlation value is calculated to measure the relationship between experimentally measured output and the output predicted by the back propagation neural network model. However, a high correlation value is not necessarily equivalent to accurate predictions since the slope of the measured vs. predicted plot is not reflected. Consequently, percentage difference is also included to measure the spread of prediction error. The following sections show the results obtained by the back propagation neural

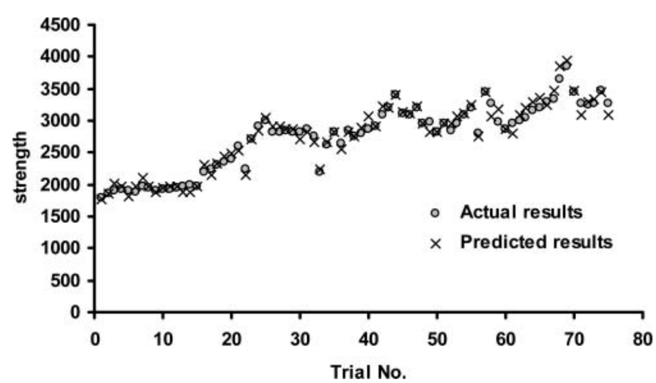

Fig. 3. Comparison of predicted and actual results in predicting strength of carbon fibers while training using back propagation neural network model.

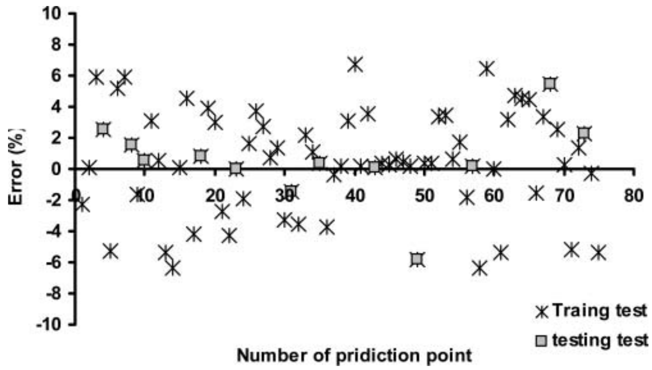

Fig. 4. Comparison of % error of predicted results using back propagation neural network model for strength of carbon fibers.

network model and their comparison with the experimental results.

A comparison plot of the analysis data and verification data of the strength in the multiple regression analysis is provided in Figure 3. It can be found from Figure 3 that the results obtained by back propagation neural network model are in close agreement with the experimental results for training tests. The percentage difference to measure the spread of prediction error obtained by the back propagation neural network model for all the testes in predicting the strength is calculated.

According to results of presented in Figure 4, it can be observed that the ability of the back propagation neural network model to predict production process is well within the allowable error. The regression analysis is performed to find out the correlation value. The coefficient value (R^2) is used to measure the relationship between the measured and predicted values. It is found out that a regression value of 0.9722 is obtained while predicting the strength by back propagation neural network model, for training testes proving that accurate prediction is possible through the input parameters using this model. The line of best fit using the plotted points is estimated using the regression and is depicted in Figure 5.

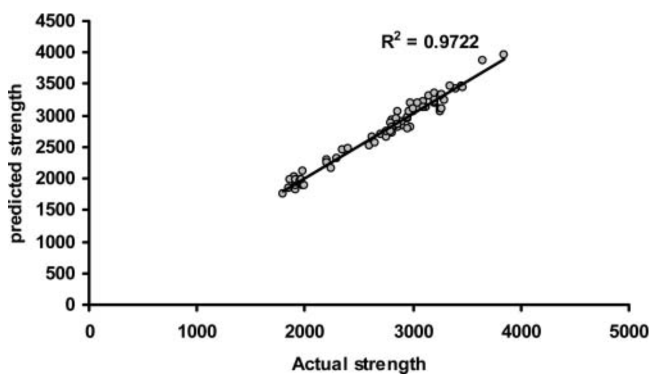

Fig. 5. Line of best fit for predicted strength and the actual strength of carbon fibers by back propagation neural network model for training testes.

To determine the accuracy of the back propagation neural network model for predicting the outputs when an unknown input is given, a regression analysis is performed on the network and line of the best fit is obtained for testing testes of the back propagation neural network model (Fig. 5). A correlation value of 0.9722 is determined for the training testes while predicting the strength.

4 Conclusions

The present study focused on the modeling and comparison of strength of PAN-based carbon fibers by artificial neural networks during production process. Neural network approaches seem to have an important role in the prediction of strength of carbon fibers. The results obtained from each modeling approach showed that the excellent agreement between experimental data and predicted values of strength could be achieved at any conditions of precursors, temperature oxidation, residence time, LTC and HTC. Although Back Propagation neural network results fitted better to observed strength in terms of correlation values. By using elaborated back propagation neural network modeling, it is able to predict the production process of carbon fiber at a high accuracy from process variables such as temperature oxidation, residence time, LTC, HTC and precursor type. Back propagation back propagation neural network as a modeling tool could be used in production process system performance and evaluation of experimental conditions. In addition, this modeling technique could be applied as a simulation tool to improve the operating conditions of production process by predicting the system performance.

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