Artificial Neural Network Modelling of PP/PET Blends

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Abstract- In this study, comparison between the dynamic mechanical properties of polymer blends and the results of artificial neural networks (ANN) modeling has been conducted. The glass transition temperature and storage modulus values of PP(polypropylene)/PET(polypropylene terephthalate) polymer blends was used for ANN modelling. The observations on ANN results and the experimental results has shown sufficient accuracy mutually. At the same time, these results were supported by scanning analyzes. The artificial intelligence modeling studies for this article proves the applicability of dynamic mechanical properties of PP/PET blends. These results shows that artificial neural networks can be a helpful tool for experimental work of dynamic mechanical properties of polymer materials

Keywords- PP/PET blends, dynamical mechanical properties, artificial neural network

1. Introduction

Nowadays, natural material resources are decreasing daily. Therefore, polymer materials are used as an alternative to natural materials and the applications of polymer are increasing. Nonetheless, neither the theoretical calculations nor the modelling of chemical and physical properties of polymer materials are easy because they are highly non-linear systems. The structure has an important effect on material properties and and characterization process of polymer material is expensive and time consuming besides many difficulties.

Hence, in recent years many researchers have begun to apply artificial intelligence to determine the behaviour of these materials and the interest in ANN modelling has increased in material science [1,2]. ANN is a powerful tool especially for determining relationship conditions between parameters and the relevant parameters of the interaction, which is very complex in highly nonlinear systems. These applications are often used in situations where even large systems involving complex processes exist and where certain mathematical models are not available [3]. Most of the polymer materials that are being used in applications are homopolymers. However, more complex materials are required in complex applications. The process to develop new polymer systems and to create this suitable material is expensive and long.

In this paper PP/PET blends are used because polymer blending is an alternative method to develop new polymer systems, which obtains two or more physically mixed polymers [4]. Creating a polymer blend allows to combine unique properties of different polymers.The properties and concentration of materials involved and final physical structure of mixture determine performance of mixture.

Although PP and PET are widely used alone, there are very few studies in industry and literature regarding polyolefin / polyester blends Increasing interest in polyolefins and PET blends is due to improved mechanical properties due to poor partnership [5].

Tensile strength is the most important advantages of PP, which is widely used in textile and technical applications. However, disadvantages of PP's are low young modulus and recycling problems [6]. Whereas PET is not only abrasion resistant but also has high elastic modulus and conformational stability. PET is not affected by acids but is sensitive to alkaline [7,8].

The melting point and glass transition temperature (Tg) of PET and PP are very different. Therefore, at high temperature it is reinforced by increasing the tensile strength of PET and PP [9]. If the morphologies of the PP/PET blends are optimizable, these blends could potentially have an application as packaging material. In addition, this could contribute to the reduction of environmental pollution and conservation of resources by using thermoplastic recycling technology [10].

1.1. Artificial neural Networks

ANN structure and function are learning computer algorithms based on the structure and learning behavior of biological neural networks. ANN is based on the human brain, and YSA consists of artificial nerve cells called "perceptron"that are like brain nerve cells. These artificial cells are the component soft neural network connected with each other [11]. neural network structures have the ability to adapt to changing processes and environmental conditions [12.]

In neural cells, as shown in Figure 1, change in an input value, creates a particular change in the output and this change depends on the weight coefficient of the input value [13].

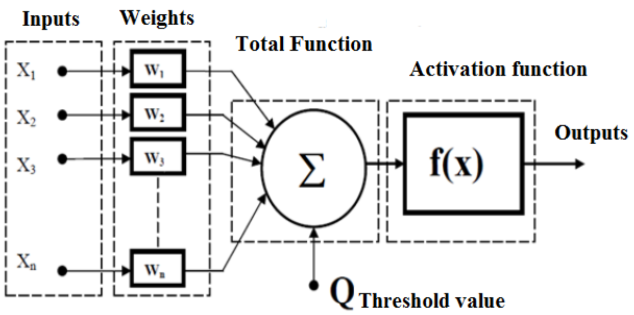

Fig. 1. Nervecell [14]

In Figure; x_i the input values, w_i is a weight factor which that is determined for each input value, Σ is the total function and Q is the threshold value. Each x_i input value is multiplied by the wi weight factor, then each product value is summed to form the threshold value. The threshold value is processed by the activation function denoted by f(x) to form the output value [15].

The activation function is One of the most important factors in the success of modeling in the YSA method.This function collects data from the external environment, and then processes it and produces output corresponding to the input data.

There are different kinds of activation functions used in YSA models. It is decided which activation function should be used according to the structure of the problem. In YSA models, logarithmic sigmoid function is generally used to estimate a value, while tangent sigmoid function is used when data is selected [16,17].

In this paper for ANN modeling back propagation network is used and back propagation network minimizes a predetermined error function to find the right weights that would create an output vector $Y = (y_1, y_2, . . . y_p)$ as close as possible tothe target values of output vector $d = (d_1, d_2, d_3 . . . d_p)$ with a selected accuracy. A predetermined error function has the following equation [18]

$$E = \sum_p \sum_P (y_i - d_i)^2 \qquad (1)$$

Where y_i is the constituent of an output vector, di, is the constituent of a target output vector and pis the number of output neurons and P is the number of training patterns [13]. The least square error technique, along with a generalized delta rule, is used to optimize the network weights. The gradient descent method with momentum term, along with the chain rule of derivatives, is employed to modify network weights as

$$V_{ij}(n) = -\delta \frac{\partial E}{V_{ij}} + \alpha V_{ij}(n-1) \qquad (2)$$

where the learning degree that is used to increase the chance of avoiding the training procedure being trapped in a local minimum instead of a global minimum [19].

2. Experimental and Method

2.1 Materials and apparatus

PP and PET polymers were used in this study and %3 Maleic anhydride functionalized polypropylene (PP-MA) was used as a compatibilizer. Average thickness of 300-700 micron film samples is provided from Mir Research and Development Inc. Five different blends of PP/PET (wt%) are used to examine the morphology of the surface of PP/PET blends, SEM images have been magnified X3000 with Phenom Pro brand SEM device. The samples were broken in liquid nitrogen and then were coated with gold.

The samples are carried out in Q800 DMA device at 1 and 5 Hz, with a 2 ^{0}C/min temperature increase from 30 ^{0}C to 120 ^{0}C in film clamp apparatus with a constant voltage at 1 and 5 Hz frequency.

2.2 ANN Modelling

DMA experimental results are used for artificial neural network modelling and the temperature and PET additive ratio of the samples were determined as input parameters for artificial neural network modelling.

Output parameter in the DMA, E (storage modulus) and tan δ (Tan Delta) were subjected to training in different networks separating the results obtained in two different ways. In this experiment, 80% of the results of the Tan Delta and Storage Modulus results are used for training and 20% for testing.In order to improve the success of the training input data was normalized. ANN modelling was conducted in a Matlab software.

3. Ethical and Safety Oriented Remarkable Issues Caused By Artificial Intelligence

3.1 SEM Results

PET and PP are incompatible because of their differences in chemical structure and polarity. Incompatible blends are being observed as two distinct phases [3,20].SEM analysis of the images that are obtained from the main sign is PP. PET polymers that are formed by PET droplets are available in different diameters and, this heterogeneous structure shows that there is no significant adhesion. In Figure 2, PET particles appear as droplets in the structure of structures in PP+20% PET blend. It seems that the PP+30 % PET sample is the homogeneous structure. In this example, it can be assumed that the voids have decreased and the PET droplets have settled into the voids. Also it was observed that in this sample, the fibril structures begin to emerge gradually. The fibrillar appears to be more clearly enlarged in PP+40% PET blend.

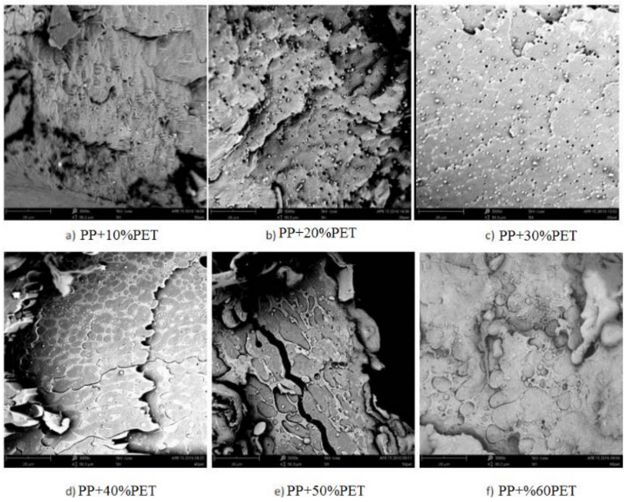

Fig. 2. Different magnification (X3000) SEM images

The homogeneity has begun to deteriorate again, and voids have begun to form again in the structure of PP+50% PET sample. It has been observed that PET particles have completely covered the main structure and transformed the droplet form to the fibril structure. This event shows a structural phase change.

It was seen that when the additive ratio exceeds 40% PET, the homogeneity is again lowered. The homogeneous structure again begins to decompose in PP+50% PET and PP+60 % PET samples

3.2 Dynamic Mechanical Analysis (DMA) Results:

In Figure 3, tan δ results showed that Tg increased with increasing amount of PET and increased peak width and severity.

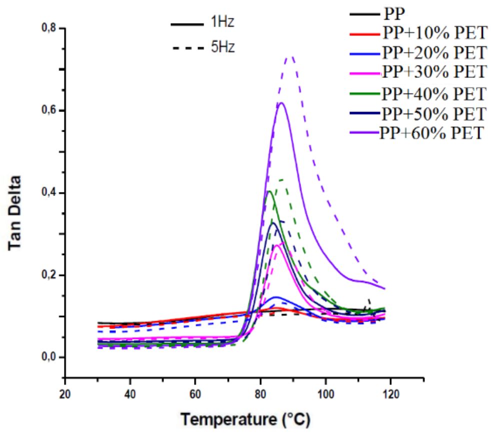

Fig. 3. Dependence of Tan Delta on temperature

In addition, the frequency increases with the increasing Tg as shown figure 4 and this still seems to be the peak of the increased intensity. Storage module which is an indicator of hardness did not show a significant change in the ratio 0-20% PET, and exhibit higher growth rates of 20-40% PET. PET ratio of 50% shows this value shows a significant declined. This decrease in storage modulus are due to the absence of a structural phase transition at this rate.SEM images also support this.

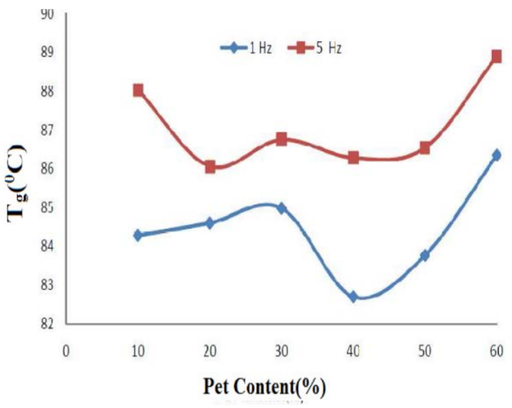

Fig. 4. Dependence of Tg on PET ratio (frequency of 1 Hz and 5 Hz)

The storage modulus is increasing again in PP+60% PET sample.There was no significant change in the storage module after PP+60% PET sample. Storage modules for all samples increases with the increasing frequency as presented in Figure 5.

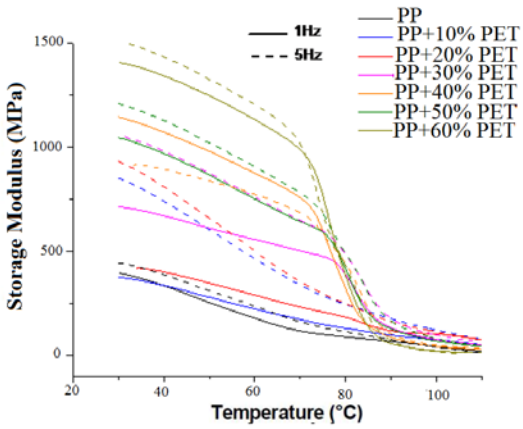

Fig. 5. Dependence of storage modulus on temperature

3.3 ANN Modeling of DMA

Storage Modulus ANN Modeling tests performed with different number of intermediate layer neuron number, activation function and number of iterations training results with one hidden layer, 8 intermediate neurons and log-sigmoid activation function. Furthermore, training made using 1000 iterations were found to be the most successful, in which the R training value reached 0.9967and the test results reached a value of 0.985

The ANN test results and the experimental results of the storage module are shown in Figure 6 to illustrate the compatibility between them.

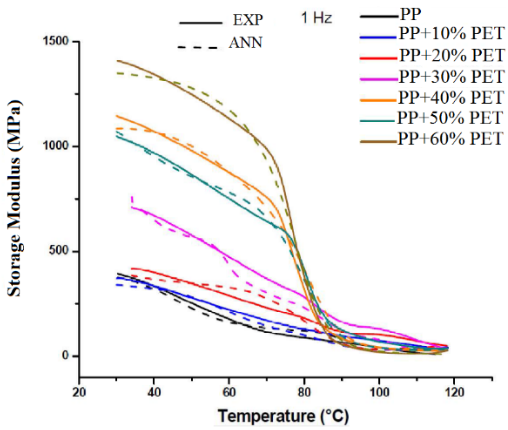

Fig. 6. Comparing test results of ANN and storage modulus

As presented in figure 6, Tan Delta ANN Modeling tests performed with various numbers of intermediate layer neuron, activation function and number of iterations for training results in with one hidden layer, 8 intermediate neurons and log-sigmoid activation function. The training was performed by using 1000 iterations which is found to be the most successful number of iterations, and the correlation coefficients (R^2) for training value reached 0.955with test results of 0.856 for correlation coefficients (R^2).

PP/PET blend and Tan Delta results in comparison to the ANN modeling test results are presented in Figure 7, Tg values obtained from the DMA analysis with temperature increase for the different samples were used in the artificial neural network model

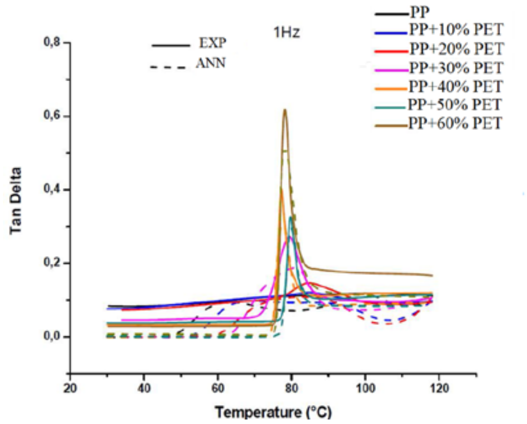

Fig. 7. Comparison of experimental results and Tan Delta

In the ANN model, the frequency values and the PET contribution rate of the samples were used as input parameters, whereas the Tg value was the output parameter.When number of hidden layers is 1, number of intermediate neurons is 12, and the activation function is the log-sigmoid function, which is selected during training stage, it is seen that the education success of the network is sufficient. The value of the correlation coefficients (R^2)is 0,99 for training and 0,977 for test.

Experimental Tg results and comparison of ANN modeling results for different frequency and PET additive ratios of PP/PET blends are presented in Figure 8.

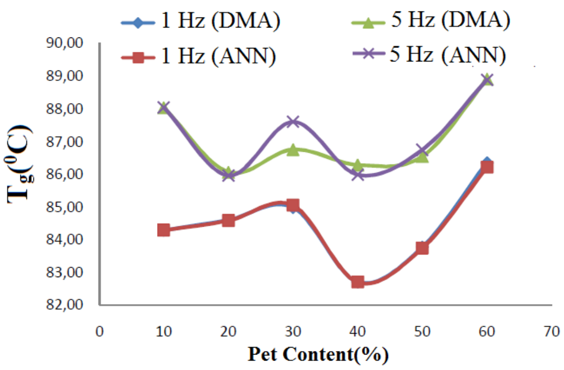

Fig. 8. Comparison of Tg ANN and Experimental Results

It is also another ethical issue if it should be allowed one intelligent machine to create – develop other ones autonomously. That's a rising issue because it is still unclear how after-learned, intelligently done behaviors can result to differences in new type of machines developed as benefiting from experiences – after-learned data of previous, ancestor machines.

4. Conclusion

This article proves the applicability of The artificial intelligence modeling studies into dynamic mechanical properties of PP/PET blends. These results shows that artificial neural networks can be a helpful tool for experimental work on dynamicmechanical properties of polymer materials

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