Artificial neural networks in prediction of mechanical behavior of high performance plastic composites

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Abstract. Using a feed-forward artificial neural network (ANN), the tensile strength of a series of poly(phthalazinone ether sulfone ketone)(PPESK) blended with different contents of polyetheretherketone(PEEK), polysulfone(PSF), polyphenylene sulide (PPS) and reinforced with various amounts of whisker(TK) composites has been predicted based on a measured database. Compared with the experimental results, the maximum error obtained is not more than 0.8%. It is concluded that the predicted data are well acceptable. A well-trained ANN is expected to be very helpful mathematical tool in the structure-property analysis of polymer composites. Finally, using ANN modeling data and experimental data, the tensile strength properties related to whisker weight percent were established.

1. Introduction

Recently, a new programming paradigm, artificial neural networks (ANN) has been proposed to model complicated multi-parameter material behavior. The basic advantage of artificial neural network lies in the fact that it is able to automatically map a relationship from the supplied input and output parameters. Artificial neural networks learn through examples. The examples are presented in the form of input and corresponding output parameters. The network then attempts to learn, or in other words map the relationship between the input and output from the examples presented to it. The input-output parameter can be generated from experimental results. As a result, the material behavior is captured directly from the experiments without describing the exact relationship between the parameters. The ‘trained’ network would contain adequate information about the material behavior to qualify as a material model. Therefore, complicated relationships between various parameters can be found out by the network. Moreover, ANN is a model free estimator. Therefore, the parameters that are difficult to measure experimentally can be avoided.

In the present paper we show the tensile strength of artificial neural networks in capturing the behavior of high performance poly(phthalazinone ether sulfone ketone) composites. The result from experimentation has been used directly to train the network. Therefore, all the complicating effects have been included directly in the model. The results have been very encouraging.

2. Collecting the experimental data

A series of poly(phthalazinone ether sulfone ketone)(PPESK) based composites blended with different contents of polyetheretherketone(PEEK), polysulfone(PSF), polyphenylene sulide(PPS) and reinforced with various amounts of whisker(TK) was prepared using a model TSSJ-25/33 twin screw extruder. The moulding pellets of PPESK, PEEK, PPS, PSF and TK were dried in a vacuum oven at 150°C for 3h before extrusion. The moulding pellets produced from the extruder were subsequently dried prior to injection moulding( model JM128MK3-C). According to ASTM D638, the examples were tested.
The technological parameters such as PPESK weight percent, PEEK weight percent, PSF weight percent, PPS weight percent, and TK weight percent are input variables and measured tensile strength of composites is the output parameter. In this section 24 pairs of experimental data points under process condition were collected out of which 20 data points were used to train the neural network and the remaining 4 data points were used for testing the neural network, the partial sample data was not shown.

3. Results and discussion

The final architecture of the networks used, the optimum set of network parameters and learning parameters adopted in this study are discussed in detail below.

3.1 Network performance with different network parameters

In order to study the effect of network parameters, the number of neurons was varied from 4 to 30 neurons in the hidden layer at interval of one neuron, the effect of the number of neurons in the hidden layer on the network performance being shown in Fig. 1. From Fig. 1 it is evident that as the number of neurons is increased, the RMS error is decreasing, which shows the predicted values are close to the experimental values. It can be also observed that after reaching some optimum number of neurons, the RMS error is not decreased further. It has been observed that the RMS error is minimum with 18 neurons in the hidden layer.

![Fig. 1 The influence of hidden neurons on the RMS error (\(\eta=0.01, \alpha=0.9\), iteration limit =30,000).](image)

3.2 Network performance with different learning parameters

![Fig. 2 The influence of iteration limit on the RMS error. (\(\eta=0.01, \alpha=0.9\))](image)
In addition to the number of neurons in the hidden layer, the network performance depends also on other parameters such as the number of training iterations (note that the number of training iterations is different from the number of training set), the learning coefficient (η), the momentum factor (α), etc. In order to study the effect of these parameters, the number of training iterations has been varied from 1000 to 30,000, the learning coefficient varying from 0.01 to 0.9 with a step of 0.1 and the momentum factor, from 0.2 to 0.9 with a step of 0.1. The RMS error of the network with different learning parameters has been shown in Figs. 2-4.

From Fig. 2 it is evident that, for a smaller number of training iterations the RMS error has been found to be quite high. Once the optimum number of training iterations is reached, the RMS error is found to be minimum. Even though the number of training iterations is increased beyond the optimum number of training iterations, there is no significant improvement in the prediction accuracy. So the optimum number of training iterations is 30,000.

From Fig. 3 it is clear that at higher learning coefficients the RMS error is somewhat higher, resulting the prediction values are away from the experimental results. Once there is no further improvement in the network performance after the optimum learning coefficient ($\eta=0.01$) is reached.

Fig. 3 The influence of $\eta$ (learning parameter) on the RMS error ($\alpha=0.9$, hidden=18, iteration limit =30,000).

Fig. 4 The influence of alpha (momentum factor) on RMS error ($\eta=0.01$, hidden neuron=18, iteration limit=30,000).
From Fig. 4 it appears that the momentum factor has a considerable effect on the network’s performance. The RMS error is found to be minimum for an optimum value of momentum factor. In general, with all other factors held constant, increasing either the momentum factor or the number of training iterations or decreasing the learning rate, resulted in a decrease in the RMS error up to a particular level, thereafter resulting in unstable behavior. The RMS error remains constant or increase after reaching certain values of learning parameters. Once the RMS error is found to be minimum, we should stop training and select the value of learning parameter of minimum error. In this study, it has been identified that the optimum number of training iterations is about 30,000, the number of neurons in the hidden layer is 18, learning coefficient is 0.01, and the momentum factor of 0.9.

With this optimum network parameters the developed back propagation ANN is trained with the training data set until the desired error limit is reached, once the training is over the connection weights of the network is saved on a text file, which is further used for predictions of the output parameters.

3.3 Comparison of predictions with experimental results
The final and most important step in this work of neural networks is to test the programs designed. The knowledge parameters, which have been saved after training the network, can be used for predictions of the tensile strength properties of composites. The programs were tested using different input and output values that were not given for training previously. The verified results reveal that the predicted values are coincide well with the experimental results as shown in Fig. 5. From such an analysis, it may be deduced that the predicted values can satisfy the demand in practice, and that performing experiments according to the predicted value can provide a satisfactory and promising effect.

![Fig. 5 Comparison between the experimental and predicted values.](image)

3.4 Prediction and analysis
The results of modeling revealed that the well-trained network can be used in prediction of new tensile strength of the composites with considerable cost and time saving. In this way amount of experimental work can be significantly reduced. This result was previously cited in literature, zang et al\cite{2,7} emphasized that well-trained network is expected to be very helpful and powerful for the composite design.
Fig. 6 demonstrates the prediction model for the tensile strength properties as a function of whisker content. It is evident that the tensile strength properties showed a general increasing trend with increase in whisker percent. Furthermore, tensile strength properties reached maximum for the composites at about 10% whisker and then decreasing with increase in whisker percent. From this prediction, it is clear that the optimization of tensile strength properties would occur for the composites containing 10% weight percent of whisker.

![Graph showing tensile strength properties as a function of whisker content.](attachment:image.png)

Fig.6 ANN prediction for tensile strength of composites as a function of weight content of TK.

4 Conclusions

In this paper, tensile strength of a series of whisker reinforced PPESK/PEEK/PSF/PPS composites has been developed by making use of ANN, by means of which the effect of the variation contents of high performance plastic composites on tensile strength can be predicted successfully. Compared with the experimental results, the maximum error obtained is not more than 0.42%. It is concluded that the proposed neural network model is capable of predicting the tensile strength of high performance plastic and satisfies the practical demand well.

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