Application of Artificial Neural Networks in Polymer materials science.

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Abstract

Artificial Neural Networks is a robust and efficient mathematical tool inspired by the biological nervous system, and can be used to simulate a wide variety of complex scientific and engineering problems. A powerful ANN function is determined largely by the interconnections between artificial neurons, similar to those occurring in their natural counterparts of biological systems. In polymer composites a good number of experimental results are required to predict its properties hence after the network has learned solve the problems, further data can be predicted without performing the long and time consuming experiments. ANNs can also be used for systematic parameter studies in the optimum design of functionally specific composite materials. In the present paper, an artificial neural network (ANN) approach was applied to predict a few of the properties of polymer composites.

Introduction

The use of polymer composites is rapidly becoming the latest in Hi-Tech materials especially in the automobile industry. In order to meet the application specific criteria of these materials have to be designed by selecting the correct composition and choosing the appropriate manufacturing process. A polymer composite can be designed and manufactured differently for different applications. As an example Fig. 1 illustrates the general principles for the systematic design of wear resistant polymer composites.

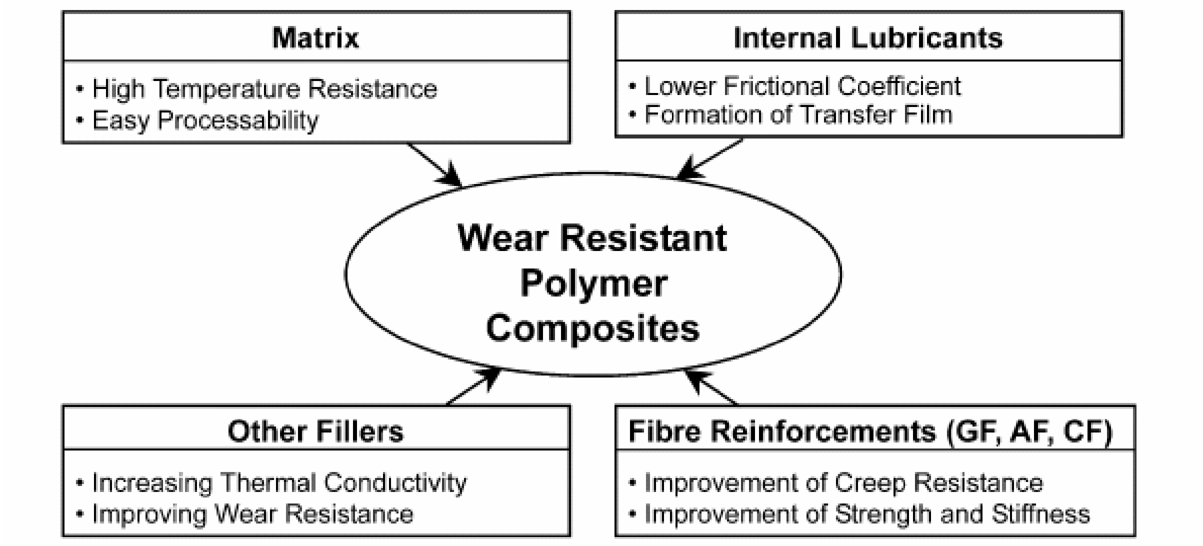

Fig. 1, Schematic presentation how to design the composition of wear resistant polymer composites

As shown in Fig. 1 each part of the polymer composite should have a specific property to form a good wear resistant polymer. Property investigation plays a key role in materials science to evaluate composites designed for special engineering applications. The understanding and evaluation of the effects of these factors is a crucial factor in these composites in order to meet the requirements of its applications.

Modeling of such relationships usually involves the formulation of a mathematical model derived from tedious experimental data. Pioneers have used semi-empirical relations but in most cases they are pretty complicated. To reduce further load of experimentation artificial neural networks (ANN) have been recently used in the field of polymer composites. Inspired by the biological nervous system ANNs can be used to solve a wide variety of scientific and engineering problems. Just like the biological system ANNs can learn from therefore can be trained to find solutions of the complex non-linear, multi-dimensional functional relationships without any prior assumptions about their nature; further, the network learns directly from experimental data by its self-organizing property and hence reduces experimental time.

Artificial neural networks

Working principle and background.

Artificial Neural Networks (ANNs) are model free formulators that have exceptional ability to perform complex multidimensional, nonlinear vector mappings and complex pattern recognition or classification. The artificial neural networks, inspired by the biological nervous system are the simple clustering of the primitive artificial neurons. These clusters are in turn connected to one another, the topology of which also varies. Basically there are three classes of neurons. One which takes input from the user second is the hidden neuron (which in turn forms the hidden layer) and the third one being the ones which give the output. Similar to nature the network function is determined mainly by the interconnections between the neurons and they need not be linear in nature. Each input to a neuron has attached to it a synaptic weight factor that determines the contribution of that connection to the overall result. In fact the training of these ANNs take place by the adjustment of these weights so as to get optimum result in the training set so that they perform well with the actual test data .This is the key behind ANN’s self learning and memory. For this reason, ANNs were defined by Aleksander and Morton as “A massively parallel-distributed processor made up of simple processing units, which has a natural propensity for storing experiential knowledge and making it available for use”.

Training Process.

In most cases a multi-layered neural network is preferred. A back propagation algorithm can be used to train these multilayer feed-forward networks with differentiable transfer functions to perform function approximation, pattern association, and pattern classification. The term backpropagation refers to the computation ad correction of network error with respect to weights and biases. The training of ANNs by backpropagation involves three stages (i) the feed forward of the input training pattern, (ii) the calculation and backpropagation of the associated error, and (iii) the adjustment of the weights.
The process has to be optimized for the application and this can be achieved using various optimization strategies.

Fig. 2shows the multi-layer feed-forward ANN configuration in the upper part. As explained earlier the neural network is made up of three basic layers, i.e., input, hidden and output layers. Each layer has different number of neurons and the behaviour of the network depends on the interconnection between the elements. The hidden layers consist of one or more number of hidden neurons depending on the application.

The lower part of Fig. 2shows a systematic representation of a single neuron. The relationship between the output vector $X_j^{(n)}$ and the input vector $X_j^{(n+1)}$ is given by the following equation (eq. 1)

$$X_j^{(n+1)} = F\left(\sum_i W_{ji}^{(n)} X_i^{(n)}\right) \qquad (1)$$

Where F(x) is the tan sigmoid function $F(x) = \dfrac{1}{1+e^{-x}}$ or other nonlinear transfer function, e.g. log-sigmoid function, and $X_j^{(n+1)}$ is output of unit j in the nth layer, $W_{ji}^{(n)}$ is a weight from unit i in nth layer to unit j in (n+1)th layer.

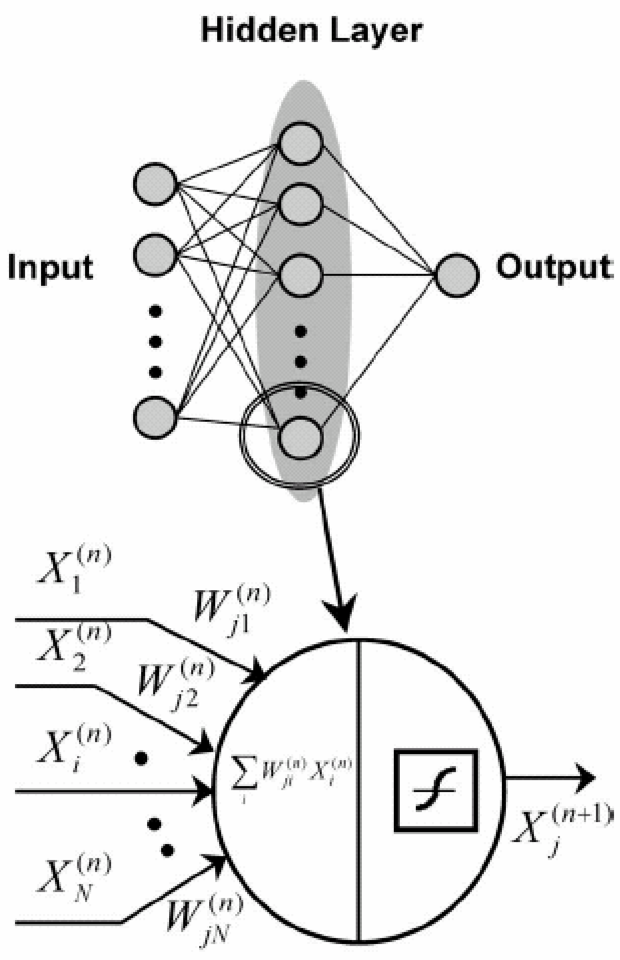

Fig.2, Artificial neural network configuration (upper part). The lower part gives a schematic description of the relationship between the input and output vectors of one neuron.

The learning procedure is based on a least sum squares optimality criterion of the errors between the predicted and actual values.

$$E = \sum_{p=1}^{P} (d_p - o_p)^2 \tag{2}$$

In Eq. 2, E is the total sum squared error averaged over the whole of the training set. Here d_p is the ANN predicted output and o_p is the actual output as per experiments for the p^{th} pattern in the training data set. In order to minimize this error the weights of all connecting nodes are adjusted until the desired error level is reached or the maximum number of allowable cycles is reached. Equations 3 shows the learning algorithm used for the weights,

$$W_{ji}^{n}(t+1) = W_{ji}^{n}(t) + \Delta W_{ji}^{n}(t) \tag{3}$$

The correction for the above error used is shown in equation 4.

$$\Delta W_{ji}^{n}(t+1) = -\eta \frac{\partial E}{\partial W_{ji}^{n}} + \mu \Delta W_{ji}^{n}(t) \tag{4}$$

where $W_{ji}^{n}(t)$ is the training signal of the correct answer at the tth learning step, $\Delta W_{ji}^{n}(t)$ is the correction of the weight at the tth learning step, η is the learning rate, and μ is the momentum factor. η is a small parameter to adjust the correction each time, and μ reduces an oscillation and aids rapid convergence. Appropriate values of these parameters aid network learning. An example of a feed forward neural network trained by BP algorithm is shown in fig. 3.

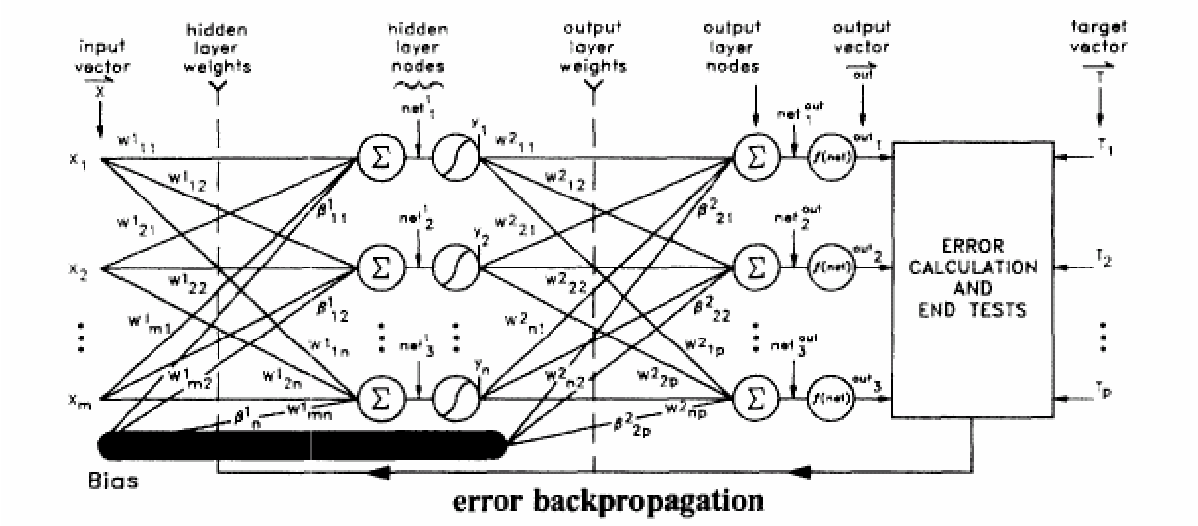

Fig. 3 Example of the topology of a feed-forward neural network trained with the backpropagation algorithm.

The successful areas of applications of ANNs have the following characteristics,

1. A large training database is available
2. Mathematical modeling of the problem involves complex and time consuming calculations.
3. Experimentation time is large.
4. The data set involves lot of noise and complexity.

Some properties of polymer composites such as wear, creep, fatigue etc have the above characteristics which is why they can be easily modeled using ANNs. The approach to solve such problems through ANN's has been elucidated in this paper.

Application of ANNs to Polymer Composites.

Fatigue life.

Fatigue presents one of the most complex problems in polymer composites. The failure mechanisms of these composites are still not well understood. This presents an ideal case for prediction using ANNs as there is no mathematical model to foreknow its behaviour and also there is extensive data available. ANN predicts the fatigue behaviour without being linked to mechanistic arguments. Hence ANNs are gaining greater importance in predicting the fatigue life.

The fatigue life prediction approach using ANNs is different for unidirectional composites and laminate composites. In the former case ANN the maximum stress and the fiber orientation angle were used as the input, and the output is the number of cycles to fatigue failure. From literature it has been found that a 3-$[12]_1$-1 architecture was used with around 100 measured results. The prediction showed highly satisfactory results with root mean square error (RMSE) less than 20%. In the case of laminate composites. Three fatigue parameters, peak stress, minimum stress and probability of failure, and four monotonic mechanical properties, tensile strength, compression strength, tensile failure strain and tensile modulus, were selected as the ANN inputs, which were applied to predict the fatigue life of the composites as the output. A 7-$[21]_1$-1 architecture was finally optimized to model this property by changes in the RMS error of the output and corresponding changes in the number of neurons in the hidden layer. All the above data have been found form literature and in almost all the cases good predictions were observed.

Wear of composites

The earliest use of ANNs for wear of composites was made to predict the wear volume of short-fiber/particle reinforced thermoplastics. Here they used a 10-[25]1-1 network to calculate the wear volume of with a dataset of 72 independent wear volume measurements from experiments. The inputs were mechanical properties and test conditions, i.e. compressive strength, compression modulus, compressive strain to failure, tensile strength, tensile strain to failure, impact strength, environmental testing temperature, initial load, average load and average velocity. The optimization method used here was an automated version of the backpropagation algorithm called the "Bayesian regularization (BR)". This algorithm has the capability to automatically identify the optimum size of the network in its hidden layers. A fair amount of success was achieved in this first attempt although predictive quality needed to be improved.

Further studied were made with larger datasets and better input variables and modified output variables such as specific wear rate was measure instead of wear volume thus making it dimensionally independent. Also better optimization and training algorithms were used like the CGB algorithm Powell–Beale conjugate gradient algorithm (CGB), BFGS quasi-Newton method (BFG), Adaptive learning rate (GDX), and Levenberg-Marquardt algorithm (LM). BR is a better algorithm for the automated parameter regularization but it has its cons such as it is very time consuming. CGB however is better in this case as it is fast and high training quality is obtained. By the use of these algorithms the predictive quality clearly improved in almost all of the cases. Although it was found that better results could be obtained by increasing the training dataset.

Further studies have been done in prediction of erosive wear data of certain polymers. I was found out those studies done on erosive wear of polymers such as polyethylene (PE), polyurethane (PUR), and an epoxy modified by hygrothermally decomposed polyurethane (EP-PUR). Three different datasets were used to train the ANNs. For the first two polymers, the impact angle of solid particle erosion and some characteristic properties were selected as the input variables, whereas the third one, material compositions, i.e. epoxy and HD-PUR weight contents, were also taken as additional ANN input variables. In all these cases, the output parameter was the erosive wear rate. Satisfactory results have been achieved and with better training and optimization algorithms.

Summary and conclusions.

Conventional methods to model the properties of composites involve a step by step procedures based on a complex mathematical model with large time and memory complexity. Hence the application of ANNs offers a simple yet effective route to model complex systems with out much of mathematical complexities and hence large error. Further advantage with ANNs is that is has an automated learning process by the adjustment of the synaptic weights. Hence like the human brain it can learn seeing the trends in the data and hence can find solutions. Hence complex properties like creep, fatigue and wear where there is no rigid mathematical model, can be easily modeled without much complications. A further advantage being the saving of valuable experimentation time. It has hence been found out that very good results have been obtained using the ANN approach.

The ideal conditions concluded for the use of ANNs in polymer composite property prediction are:

1. A large training dataset is always useful for good predictions
2. A fast training algorithm is more suited for industrial applications
3. The more complex the non-linear relation between the input and output, the larger is the training dataset required.
4. The analysis of relationships between simple and complex properties provide additional help in prediction of data

The modeling of composites using ANNs is still in the basic stages and further research has to be done to ensure better prediction of data. Future work can include a fuzzy selection model incorporated with the ANN model in designing applications and also in the manufacture of these composites. The fuzzy model can select the appropriate process and the ANN can predict the property outcome thus the whole of the manufacturing and design property can be simulated before the actual process. Also genetic and evolutionary algorithms can be used to optimize the solutions obtained.

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