Modelling of effective thermal conductivity: A comparison of artificial neural networks and theoretical models

R. S. Bhoopal¹*, Manoj Tripathi², P. K. Sharma³, Ramvir Singh³

¹Department of Physics, JSS Academy of Technical Education, Noida 201301, India.
²Department of Mechanical Engineering, University of Malaya, Kuala Lumpur 50603, Malaysia.
³Thermal Physics Laboratory, Department of Physics, University of Rajasthan, Jaipur 302055, India.

Email – singhrajpal7@gmail.com

Abstract

Artificial neural networks (ANNs) are flexible computing networks and universal optimizers that can be applied to modelling of different material properties. Modelling of the effective thermal conductivity (ETC) of silicon (Si) powder filled high-density polyethylene (HDPE) composites by using ANNs algorithm. The ANN is trained using different training feed-forward backpropagation (FFBP) algorithms, hidden layers, and neuron numbers in hidden layers in order to check the system accuracy of each training algorithm at the end of learning. ANNs algorithm are based on FFBP network with training functions: Levenberg-Marquardt (LM), conjugate gradient with Powell-Beale restarts (CGB), Conjugate gradient backpropagation with Polak-Ribiere updates (CGP), Conjugate gradient backpropagation with Fletcher-Reeves updates (CGF) and one-step secant (OSS). Training algorithm for neurons and hidden layers for different FFBP networks runs at the uniform threshold function TANSIG-PURELIN for 1000 epochs. Our modelling confirms that the ETC of Si powder filled HDPE composites is predicted better agreement with experimental results and theoretical models proposed by Lewis-Nielson and Agari and Uno model. A comparison with other models is also made and found that the values of ETC predicted by using present model are in good correlation with the reported experimental values.

Key words: Effective thermal conductivity, Artificial neural networks, Modeling, Polymer-based composites.

1. Introduction

The addition of conductive filler in a polymer composites have been widely used in many fields of engineering applications and important in the technological developments because of their outstanding multifunctional properties compared to conventional conductive polymer composites. The different physical properties and the volume fraction of the filler materials must be known in order to determine the importance of the materials. It is therefore important, from a scientific and practical point of view, to understand the effects of metallic filler on the different properties of polymer composites. They have a lighter weight than metals and are less costly. The composites made by incorporation of powdery metal fillers into thermoplastic polymers combine the advantageous properties of metals and plastics, offering cost effectiveness and rapid fabrication rate with a wide range of design flexibility, lightweight, non-corrosiveness etc [1]. Commonly used plastics are electrical insulators with a low thermal conductivity. New discovered applications such as, like heat sinks, in radio frequency interference shielding or in electronic packaging [2-4] require new composites with higher thermal and electrical conductivity. Conductive filler/ polymer composites are massive used for electromagnetic interference shielding. The applications include encapsulations, die (chip) attach, thermal grease, thermal interface materials and electric cable insulation [5-6].

A number of experimental studies have been carried out, and various numerical and analytical models have been developed to predict the effective thermal conductivity of particle filled polymers [7-28]. An artificial neural network (ANN) approach is a powerful mathematical tool in recognizing and modelling of different material properties. ANNs have been used in diverse applications in control, robotics, pattern recognition, forecasting, power systems, manufacturing, optimization, signal processing, etc. The idea to solve engineering problems using neural networks was developed in the 1940s in the United States. It has been introduced into the fields of materials recently [29-31]. Gotlib et al. [32] investigated the problem of effective properties such as thermal conductivity, electrical conductivity and dielectric constant in the realm of disordered composites with the help of neural network.
Zhang and Friedrich [33] applied the ANN to predict certain properties of polymer composites. Turias et al. [34] estimated the effective thermal conductivity of a unidirectional composite by using ANNs. Kadi [35] studied the mechanical behavior of fiber-reinforced polymeric composite by using ANNs. Al-Haik et al. [36] predicted the non-linear viscoelastic behavior of polymer composites using ANN. Turan et al. [37] investigated heavy metal removal during landfilling of industrial waste and the effects of various liner materials, such as bentonite, natural zeolite, expanded vermiculite, and pumice on the removal of Cu (II) and Zn(II) are examined. Fuchs et al. [38] have examined the relationships between thermal conductivity and standard well-log data by a theoretical analysis and by using real subsurface data from four boreholes of the North German Basin. The theoretical approach comprised the calculation of thermal conductivity from well-log response values for artificial sets of mineral assemblages consisting of variable contents of 15 rock-forming minerals typical for sedimentary rocks. Tian et al. [39] obtained main factors and historical data of end life vehicles in China, its prediction models are established by multiple linear regressions (MLR), neural networks (NN) and optimized NN based on genetic algorithm (GA-NN) methods.

However, the application of ANN to model the non-linear thermal behavior of engineering materials is limited in the literature. No research has been carried out to utilize the input–output data mapping capability of ANN computing technique in modeling of ETC of Si powder filled in HDPE. Since ANN approach seems to have good effort to save time and cut expenses in solving various scientific, engineering and industrial problems. In the present communication is to optimize the ETC of Si powder filled in HDPE. In general, the different training feed-forward backpropagation algorithms are used in the training of ANN approach.

2. Theoretical models for ETC
Over the past years, numerous theoretical models have been reported to predict the precise value of the thermal conductivity of two phase and multiphase composites. By solving Laplace’s equation and assuming absence of any interactions between the filler particles, Maxwell [7] calculated the effective thermal conductivity of a random distribution of spheres in a continuous medium which worked well for low filler concentrations. The Maxwell’s Eq. (1) is given below:

\[ K_e = K_m + \frac{2K_m + 2\phi(K_f - K_m)}{K_f + 2K_m - \phi(K_f - K_m)} \]  

(1)

Bruggeman [8] derived another exact model for the effective thermal conductivity, under different assumptions for permeability and field strength. The Bruggeman’s Eq. (2) is given below:

\[ (1-\phi)\frac{(K_f - K_m)(K_f/K_m)^{1/3}}{(K_f - K_m)} \]  

(2)

Hamilton and Crosser [9] extended Maxwell’s model to include an empirical factor ‘n’ to account for the shape of the particles (\( n = 3 \) for spheres and \( n = 6 \) for cylinders). It may be noted that both Maxwell, nor, the Hamilton and Crosser model contains any dependence on particle size, and they also imply that the temperature dependence of the thermal conductivity is approximately the same as that of the base fluid. The modified Eq. (3) is given below:

\[ K_e = \frac{K_f + (n-1)K_m - (n-1)(K_f - K_m)\phi}{K_f + (n-1)K_m} \]  

(3)

Meredith and Tobias suggested a useful theoretical model for high filler-loaded composites [10]. Meredith and Tobias’s Eq. (4) is given by:

\[ K_e - K_m = \left\{ \left[ \frac{2K_f + 2\phi}{K_f + 2K_m - \phi} \right]^{1/3} - 1 \right\} \left[ \frac{K_f}{K_m} \right]^{1/3} \]  

(4)

A semi-empirical model was reported by Lewis and Neilson [12], which was based on modification of the Halpin–Tsiok equation [13-14]. Their proposition takes into account the effect of the shape and the orientation of the particle or, the type of packing for a two-phase system. The constant \( \alpha \), in their equation, takes care of the particle shape and how they are oriented with respect to the direction of the heat flow, while the type of packing is accounted by the term \( \theta_m \). This model has been reported to be more successful for low and medium filler-loaded composites (<20%). The Lewis and Neilson’s Eq. (5) is given below:

\[ K_e = \frac{K_f + \alpha \phi \theta_m}{1 + \beta \phi \theta_m} \beta = \frac{K_f}{K_m} - 1 \text{ and } \alpha = \frac{1}{1 + \phi \theta_m} \]  

(5)

Agari and Uno [15] also proposed another semi-empirical model, which is based on the argument that the enhanced thermal conductivity of high filler-loaded composites originates from forming conductive channels or, chains of fillers. Their expression contains two parameters \( C_1 \) and \( C_2 \), which respectively accounts for the effect of the crystallinity of the polymer and the ease in formation of conductive chains of fillers. Agari and Uno’s model Eq. (6) is:

\[ \log K_e = \phi C_1 \log K_f + (1 - \phi) \log C_1 K_m \]  

(6)

In Eqs. (1-6), ETC of composite is \( K_e \), \( K_m \) and \( K_f \) are the thermal conductivity of matrix and filler, respectively and \( \phi \) is the volume fraction of filler. \( \phi_m \) is the maximum packing fraction of dispersed particles. \( \alpha \) is constant depends on the shape and oriented of the dispersed particles. \( C_1 \) is a factor influencing the effect of crystallinity of the polymer. \( C_2 \) represents ease in formation the conductive chains of the filler particles.

Singh and Kasana [16] have considered a two-phase medium made up of solid material and a fluid phase filling the pore space. The matrix was supposed to be made up of layers oriented parallel and perpendicular to the direction of heat flow. The corresponding expressions for parallel and perpendicular layers were given as:

\[ \lambda_{II} = \phi \lambda_f + (1 - \phi) \lambda_m \]  

(7)
\[
\lambda_\perp = \frac{\lambda_s \lambda_f}{(1 - \phi)\lambda_f + \phi\lambda_s} \tag{8}
\]

where thermal conductivity of solid phase is \(\lambda_s\), \(\lambda_f\) is thermal conductivity of fluid phase and \(\phi\) is the volume fraction of fluid phase. The \(\lambda_{eff}\) and \(\lambda_\perp\) are the upper and lower bounds on the ETC of a two-phase system. As these relations do not predict the ETC of a real two-phase system correctly, a different kind of weighted geometric mean was proposed by them as

\[
\lambda_e = \lambda_{eff}^F \lambda_\perp^{(1-F)}; F \geq 0, 0 \leq F \leq 1 \tag{9}
\]

Where \(F^th\) fraction of the material is oriented in the direction of heat flow and remaining \((1 - F^th)\) fraction is oriented in the perpendicular direction. Eq. (9) was solved for \(F\) in terms of \(\lambda_e, \lambda_{eff}\) and \(\lambda_\perp\) as

\[
F = \frac{\ln\left(\frac{\phi \lambda_e^{\perp} + (1-\phi) \lambda_e^{\perp}}{\lambda_f^{\perp} + \frac{\lambda_f^{\perp} - 2}{1 + \phi(1-\phi) \lambda_e^{\perp} + \lambda_f^{\perp}}}ight)}{\ln\left(1 + \phi(1-\phi) \lambda_e^{\perp} + \lambda_f^{\perp} - 2\right)} \tag{10}
\]

The correction term \(F\) may be a function of ratio of thermal conductivity of the constituent phases and porosity of the system. Using curve fitting technique, they developed the expression for \(F\) as

\[
F = C \left(0.3031 + 0.0623 \ln \left(\frac{\lambda_e^{\perp}}{\lambda_f^{\perp}}\right)\right) \tag{11}
\]

Here, the average value of \(C\) is constant. We have calculated constant value of \(C\) is 0.1293 for HDPE/Si system.

3. Artificial neural network (ANN)

Artificial Neural Networks are powerful nonlinear mapping structures and are especially useful for modelling relationships which are unknown. ANNs function similar to the human brain and can solve problems involving data that is complex, nonlinear etc. ANNs were developed as generalized mathematical models to represent the biological nervous system. A model of “computing elements” called Mc-Culloch-Pitts neurons, which performs weighted sum of the inputs to these elements followed by a threshold logic operation. Combinations of these computing elements were used to realize several logical computations [40]. A learning scheme for adjusting a connection weight based on pre and post synaptic values of the variables which became a fundamental learning rule in neural network literature [41]. The perceptron model has weight adjustable by the perceptron learning law [42]. It is possible to adjust the weight of a multilayer feed forward neural network in a systematic way to learn the implicit mapping in a set of input and output patterns pairs. The learning law is called generalized delta rule or error back propagation [43].

The ANN is trained to detect a pattern between the input data and the related output data. After training the set, the ANN can be used to predict the result of a newly input data. There is various types of ANNs including feed forward, recurrent neural network and probabilistic network. The ANN structure used in this thesis is referred to as feedback oriented propagation multilayer perception. The ANNs can be categorized on the basis of two major criteria: (i) the learning rule based and (ii) the connections between processing elements. Based on learning rules, ANNs can be divided into supervised and unsupervised networks. In supervised learning, the network is presented by a historical set of inputs and desired outputs. The actual output of the network is compared with the desired output and an error is calculated. This error is used to adjust the connection weights between the inputs and outputs to reduce the error between the historical outputs and those predicted by the ANN. In unsupervised learning, the network is only presented with the input stimuli and there are no desired outputs. The network itself adjusts the connection weights according to the input values. Based on connections between processing elements, ANNs can be divided into feedforward and feedback networks. In feedforward networks, the connections between the processing elements are in the forward direction only, whereas, in feedback networks, connections between processing elements are in both the forward and backward directions. Sometimes, feedforward network called multilayer perceptron (MLP), which is generally trained with the backpropagation or error algorithm, learning vector quantization, radial basis function, etc. A multilayer feedforward network learns by backpropagation, in which error propagates back is called feedforward backpropagation (FFBP).

In this paper, the FFBP network has been used with training functions: Levenberg-Marquardt (LM), conjugate gradient with Powell-Beale restarts (CGB), Conjugate gradient backpropagation with Polak-Ribiere updates (CGP), Conjugate gradient backpropagation with Fletcher-Reeves updates (CGF) and one-step secant (OSS).

3.1. Training process of FFBP

The neural network model is a three-layer feedforward neural network, which is the most widely applied neural network. Each layer has different numbers of neural elements, which is fully connected to the succeeding layer through the connection weights as shown in Figure 1.

The training rule of ANNs by FFBP involves three stages: (i) the feedforward of the input training pattern, (ii) the calculation and back propagation of the associated error and (iii) the adjustments of the weights.

First of all, assumed the activation function used for units in the hidden and output layers is a Tangent sigmoid function (TANSIG), which is non-linear function given by

\[
y_j = \frac{2}{(1 + \exp(-2X_j))} - 1 \tag{12}
\]

and pure linear function (PURELIN), where linear function is
Algorithm is summarized in terms of the following stages:

(i) Set all weights and thresholds to small random values

(ii) Present input and desired output, and target output

(iii) Calculate actual output and passes that as input to the next layer.

(iv) Adapt weights, start from the output layer

\[
Y_{jk} = f \left( \sum_{i=0}^{n-1} W_{ij} x_i \right)
\]

\[
W_{ij}(p+1) = W_{ij}(p) + \eta \delta_{jk} o_{jk}
\]

where \(W_{ij}(p)\) represents the weights from \(i\) to \(j\), \(\eta\) is a gain term, and \(\delta_{jk}\) is an error term.

(a) For output unit

\[
\delta_{jk} = k o_{jk} (1-o_{jk}) (y_{jk} - o_{jk})
\]

(b) For hidden units

\[
\delta_{jk} = k o_{jk} (1-o_{jk}) \sum_p \delta_{kp} W_{kp}
\]

where the sum is over the \(p\) nodes in the layer above node \(k\). The details about the theory are available in the literature [44].

4. Results and discussion

In the present study, five training functions (Levenberg-Marquardt (LM), Conjugate gradient with Powell-Beale restarts (CGB), Conjugate gradient backpropagation with Polak-Ribiere updates (CGP), Conjugate gradient backpropagation with Fletcher-Reeves updates (CGF) and one-step secant (OSS) of FFBP network are used for prediction of nonlinear behavior of ETC of Si powder filled in HDPE. The network's input range from one to three \([1, 3]\). The first layer has two TANSIG (tangent sigmoid function) neurons, and the second layer has one PURELIN (pure linear function) neuron at the uniform threshold function TANSIG-PURELIN run for 1000 epochs and third layer is output layer for five training functions of feedforward backpropagation network.

The experimental effective thermal conductivity of HDPE/Si composites [45] and those predicted by the different training functions of ANN and various theoretical models over a wide range of volume fraction of dispersed phase (filler) between 0 to 20% are plotted in Figures 2–6. The ETC of composites increases considerably with the increase of volume fractions of inclusions. This enhancement in the ETC of HDPE/Si composites is mainly because the thermal conductivity of the filler (Si) is significantly higher \(\lambda_{Si} = 140\text{ W/m K}\) than that of HDPE \(\lambda_{HDPE} = 0.362\text{ W/m K}\). The maximum value of ETC 0.833 \(\text{W/m K}\) (TRAINLM, TRAINCGB, TRAINCGF, TRAINCGP, TRAINOSS) is achieved for HDPE containing 20% volume fraction of Si, which is more than double of pure HDPE.

Fig. 1. A three-layered FFBP artificial neural network

\[ Y_j = A X_j \]

Fig. 2. Variation of ETC with volume fraction in HDPE/Si for training function TRAINLM and various theoretical models

Fig. 3. Variation of ETC with volume fraction in HDPE/Si for training function TRAINCGB and various theoretical models

Fig. 4. Variation of ETC with volume fraction in HDPE/Si for training function TRAINCGP and various theoretical models
Fig. 5. Variation of ETC with volume fraction in HDPE/Si for training function TRAINCGF and various theoretical models

Fig. 6. Variation of ETC with volume fraction in HDPE/Si for training function TRAINOSS and various theoretical models

Fig. 7. Deviation between the modelled data of ETC in the different training functions

concentration except Agari et al. [15]. According to Agari and Uno model best suited to predicted data better than 2% for both the concentration values. The constants $C_1$ and $C_2$ found from best fit of the Eq. 6 are 0.98092 and 0.66116, respectively. The parameters $C_1$ and $C_2$ should be in between 0 and 1 as per Agari and uno model [15]. After fitting the parameter $C_1$ found close to 1, which gives the evidence that the introduction of Si into HDPE does not have any influence on the crystallinity of the polymer. Further, the closure $C_2$ values are to 1; more easily the conductive chains/channels are formed in composites. It may be noted that, depending on the dispersion state of the particulates, the thermal conductivity of the composites may be different, even if the composition of the composites is same [45].

Figure 7 show that the percentage deviation in ETC using different training functions (TRAINLM, TRAINCGB, TRAINCGF, TRAINCGP, TRAINOSS) for the HDPE/Si composites over a wide range of volume fraction of dispersed phase (filler) between 0 to 20%. The
TRAINCGP is the most deviation amongst in all the used training functions. The Percentage deviations obtained are within acceptable limits. The developed ANN model can be used to estimate the ETC of different three-phase systems for a wide range of physical conditions.

Conclusions

ANN approach is very powerful in finding solutions of various engineering problems and will be useful for solving many physical problems, both numerically and analytically equations. We have used different five training functions TRAINLM, TRAINCGB, TRAINCGP, TRAINCGF, and TRAIINOSS of feedforward backpropagation network which have been used for prediction of ETC of HDPE/Si composites. The ANN approach predicted results are obtained here; conform to its good agreement with the experimental results and Agari and Uno model. The used different models of ANN show the capability to use the ANNs for future predictions of ETC of various complex structures.

References

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