



Thermal Properties of Multiwalled Carbon Nanotubes Toughened Quartz Nanocomposite Using Artificial Neural Network (ANN)

Yusuf Tijjani

Department of Mechanical Engineering,
Faculty of Engineering, Bayero University, Kano, Kano, Nigeria

ABSTRACT

Sequel to the experimental results acquisition using the established test procedures as outlined in the previous study on the mechanical and thermal properties of CNT-Reinforced quartzite Nanocomposite for Furnace Lining, the present research has been centered on the implementation and evaluation of an artificial intelligence model for the characterization of the multiwalled carbon nanotubes (MWNTs) reinforced quartz ceramic nanocomposite. A multi input and multi output Artificial Neural Network (ANN) model was developed using the Levenberg Marquardt Back Propagation (LMBP) algorithm to predict the thermal properties of the MWNTs/quartz nanocomposite bricks developed in the previous study. The predicted model was compared with the experimental test results in order to evaluate the power and the accuracy of the artificial intelligence model for the characterization of the entire series of the nanocomposite bricks developed. The developed model adequately predicts the thermal properties; specifically specific heat capacity and thermal conductivity of MWNTs/quartz nanocomposite with a coefficient of determination (R^2) of 1.00.

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INTRODUCTION

Artificial intelligence modeling

In recent times, artificial intelligence has been shown to be a dominant approach which has fascinated both the academic and industries in expanding the attainable study output through the enhancement of inputs from the experimental results (Duan *et al.*, 2017; Gokceoglu *et al.*, 2009). The needs for artificial intelligence have been rooted as mentioned in the previous study by Basheer and Hajmeer (2000) for its nonlinearity, noise-insensitivity, high parallelism, learning and flexibility, and generalization.

One of such artificial intelligence tool which has been employed extensively in addressing numerous scientific problems is the artificial neural network (ANN) (Gardner and Dorling, 1998). The artificial neural network is a computer-based programs inspired by the ability of the human brain in processing information. An outstanding attribute of the ANN is offering high

computational power to model sophisticated nonlinear processes by repeated training of a set of data until the output provides an agreeable value that correlates with the expected target rather than depending on mere computer programs (Jain *et al.*, 1996). Generally, the artificial neural network technique is highly powerful and provides satisfactory level of accuracy. Beside this, ANNs are very useful in preliminary prediction of characteristics of new materials prior to experimental study.

ANN model structure and training algorithm

As shown in Figure 1, is the flow chart depicting a sequence and procedural steps in the development of the ANN models for the characterization of CNTs-reinforced quartz refractory nanocomposites. As demonstrated in the figure, the predictive modeling in the present study can be categorized by three fundamental steps consisting of data acquisition, model training, and predictions.

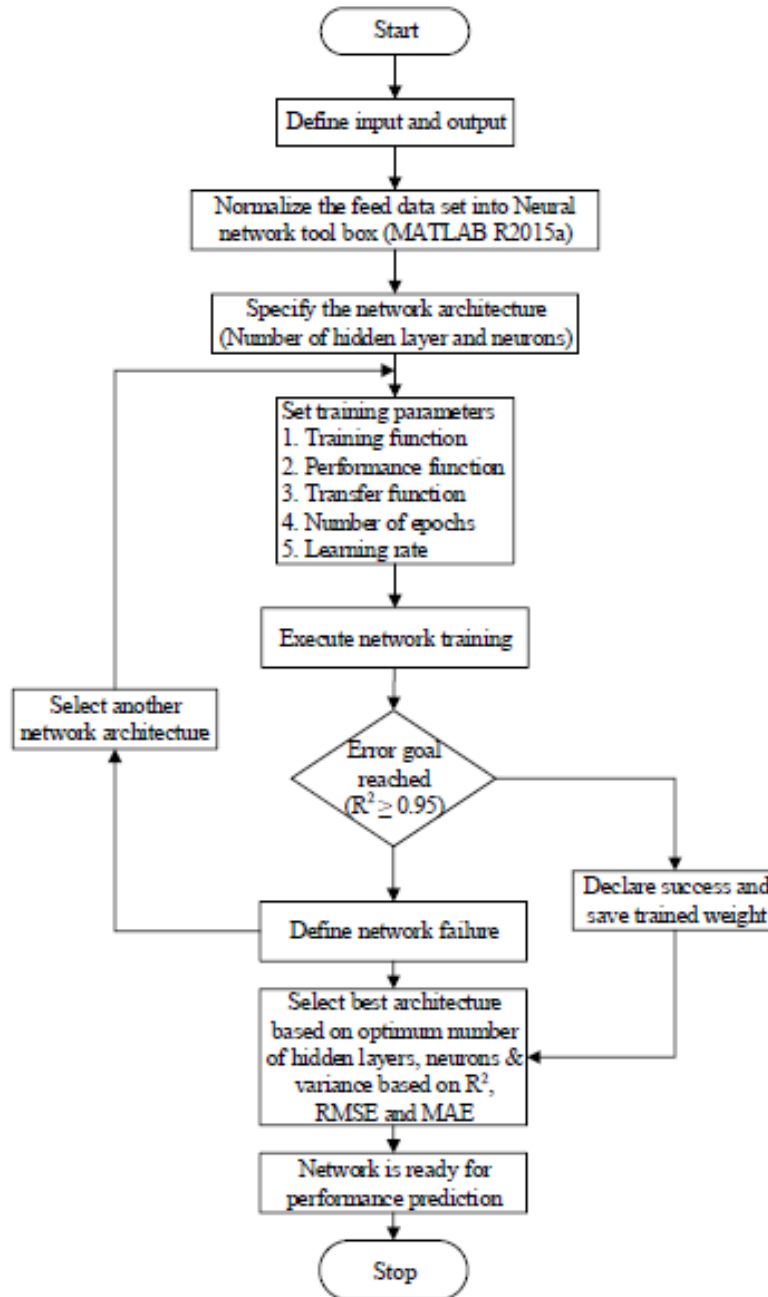


Figure 1: The flow chart for developing the neural network models

THE ANN MODELING

A total of 417 datasets; input and output, sourced from all sample formulations were employed in training the ANN. The overall data in the present model were divided into three classes, consisting of 80% training, 10% validation and 10% testing. Also, the input and output data have been normalized between 0 and 1 with the aids of the equation (1), to establish the proper implementation of the sigmoid transfer function.

$$X_{norm} = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (1)$$

Where X_{norm} is the normalized value, X is the true value of the variable, X_{min} & X_{max} are the minimum & maximum values of the dataset respectively.

The network model ANN, was programmed by a supervised multilayer perceptron (MLP) trained with the back propagation (BP) algorithm (Levenberg Marquardt (LM) algorithm) using the neural network toolbox of MATLAB R2015a. For the ANN; Figure 2, MLP ANN has three input parameters (Quartzite content, MWNTs content and Temperature) and two output parameters (specific heat capacity and thermal conductivity) was developed and evaluated.

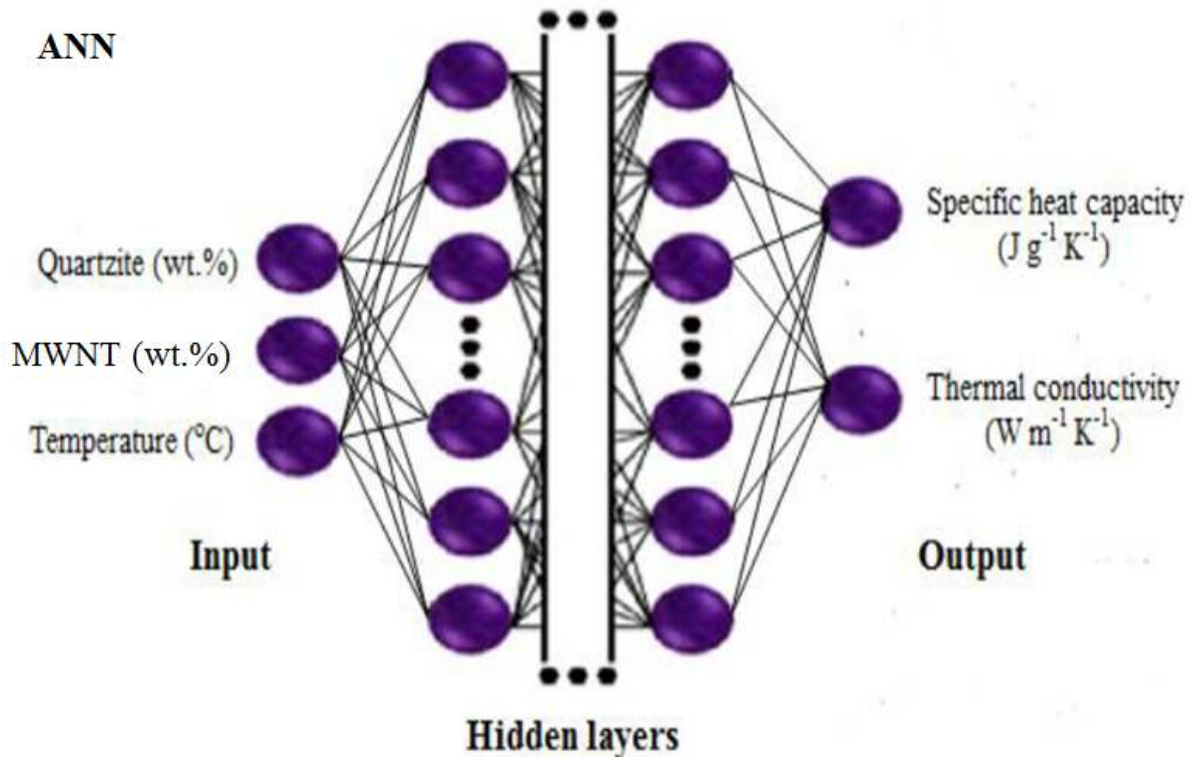


Figure 2: The ANN model for characterizing the MWNTs/quartz refractory nanocomposite

Due to the lack of standards for obtaining the required hidden layers and neurons, preliminary study revealed that two hidden layers provided the optimum performance value; minimum absolute error values for the training and testing datasets compared to one hidden layer. Hence, while evaluating the best

number of neurons needed for building the neural network models, the number of hidden layers was set at two for the ANN model. Furthermore, after many iterations the optimum ANN topologies were chosen based on: (i) The hyperbolic tan-sigmoid transfer function; equation (2) in both hidden layers. (ii) A linear transfer

function; equation (3) in the output layer. (iii) And best performance criteria: which is the function of goodness of fit of the different ANN topologies tested and based on the three statistical parameters; coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE), equations 4, 5 and 6 respectively.

$$Tansig(n) = \frac{2}{(1 + \exp(-2n)) - 1} \quad (2)$$

$$Purelin(n) = n \quad (3)$$

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_{Pred}^i - y_{targ}^i)^2}{\sum_{i=1}^N (y_{Pred}^i - \bar{y})^2} \quad (4)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_{pred}^i - y_{targ}^i)^2}{N}} \quad (5)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_{pred}^i - y_{targ}^i| \quad (6)$$

Where y_{pred}^i is the predicted value, y_{targ}^i is the real value retrieved from the experimental data, \bar{y} is the average of the actual observation and N is the number of observations.

Levenberg-Marquardt back propagation (LMBP) algorithm

Levenberg Marquardt (LM) algorithm; a trust region, type of Gauss-Newton method is a second order back propagation algorithm which has been recommended as the preferred supervised training algorithm (Mukherjee and Routroy, 2012). With a view to minimizing the error function until a specified minimum or stopping gradient is reached, the algorithm trains a neural network through repeated modification and update of the weight and bias values (Wilamowski and Yu, 2010). Therefore, in spite of consuming a relatively higher memory and processing resources than other algorithms, the LMBP has been adopted in the current study as the training algorithm due to its high efficiency and accuracy. Figure 3 outlines the standard LMBP algorithm.

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Step 1: The weights and parameter are initialize  $\mu$  ( $\mu = 0.01$  is suitable).
Step 2: The sum of the squared errors over all inputs  $F(w)$  applying equation (7) is compute:
 $F(w) = e^T e \quad (7)$ 
Where  $w = [w_1, w_2 \dots w_n]$  includes all weights of the network,  $e$  is the error vector containing the error for all the training examples.
Step 3: The weight increment  $\Delta w$  is computed via equation (8):
 $\Delta w = [J^T J + \mu I]^{-1} J^T e \quad (8)$ 
Where  $J$  is the Jacobian matrix,  $\mu$  is the learning rate that is to be updated employing the  $\beta$  based on the outcome. Specifically,  $\mu$  is multiplied by decay rate, where  $\beta$  ( $0 < \beta < 1$ ).
Step 4: Applying  $w + \Delta w$  as the trial  $w$ , and judge:
IF performance index  $F(w) < F(w)$  in step 2 THEN
 $W = w + \Delta w$ 
 $\mu = \mu \cdot \beta$ 
go back to step 2
ELSE
 $\mu = \mu / \beta$ 
go back to step 4
END IF

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Figure 3: Pseudocode for LMBP Algorithm (Nazari and Riahi, 2013; Tijjani *et al.*, 2019)

Performance of the LMBP-ANN models

In order to validate the performance of the LMBP ANN in characterizing the different

grades of MWNTs reinforced quartz ceramic nanocomposites developed in the previous study (Tijjani, 2018), various ANN topologies were

deployed in training the network by adjusting the number of hidden neurons. Table 1, highlight the network performance for each of the ANN topology; hidden neuron configuration employed in developing the ANN model. 15 different ANN

topologies were tested by systematically varying the number of neurons in the hidden layers between 4 and 20 (Dele-Afolabi *et al.*, 2018, Tijani *et al.*, 2019).

Table 1: Variation of hidden neurons utilized in developing the ANN model

Hidden neurons	Train			Validation			Test		
	R ²	RMSE	MAE	R ²	RMSE	MAE	R ²	RMSE	MAE
4-6	1.0000	0.0035	0.0025	1.0000	0.0030	0.0021	1.0000	0.0029	0.0019
4-16	1.0000	0.0033	0.0029	1.0000	0.0030	0.0025	1.0000	0.0031	0.0027
4-20	1.0000	0.0012	0.0010	1.0000	0.0011	0.0009	1.0000	0.0009	0.0007
6-15	1.0000	0.0013	0.0011	1.0000	0.0014	0.0011	1.0000	0.0013	0.0010
8-17	1.0000	0.0009	0.0007	1.0000	0.0008	0.0006	1.0000	0.0007	0.0006
9-12	1.0000	0.0026	0.0022	1.0000	0.0028	0.0025	1.0000	0.0028	0.0023
9-17	1.0000	0.0007	0.0006	1.0000	0.0008	0.0007	1.0000	0.0009	0.0007
10-14*	1.0000	0.0009	0.0007	1.0000	0.0010	0.0008	1.0000	0.0010	0.0008
10-18	1.0000	0.0007	0.0006	1.0000	0.0007	0.0006	1.0000	0.0010	0.0007
10-20	1.0000	0.0020	0.0016	1.0000	0.0020	0.0016	1.0000	0.0019	0.0015
11-7	1.0000	0.0011	0.0008	1.0000	0.0013	0.0009	1.0000	0.0015	0.0009
12-12	1.0000	0.0032	0.0023	1.0000	0.0031	0.0024	1.0000	0.0037	0.0028
18-12	1.0000	0.0014	0.0012	1.0000	0.0012	0.0010	1.0000	0.0013	0.0011
19-14	1.0000	0.0013	0.0010	1.0000	0.0013	0.0010	1.0000	0.0011	0.0009
19-18	1.0000	0.0011	0.0008	1.0000	0.0011	0.0009	1.0000	0.0010	0.0007

* Best model based on the training, validation and test data.

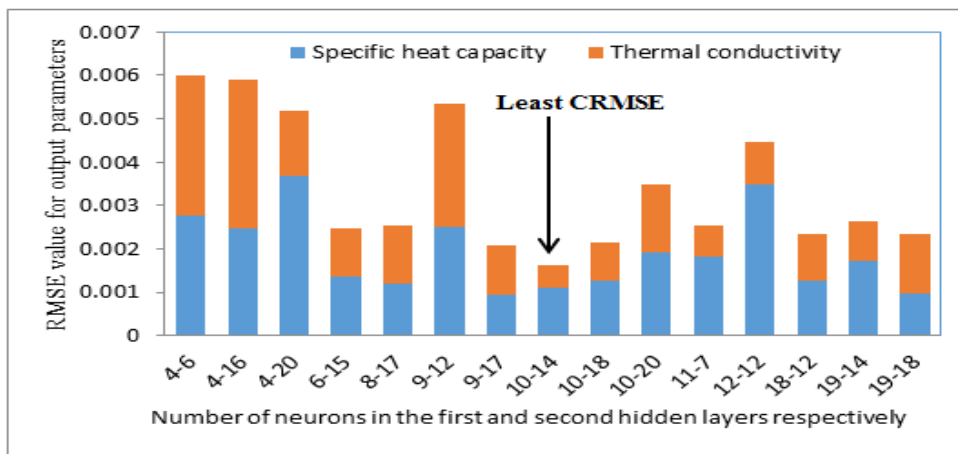


Figure 4: The performance of the ANN in characterizing MWNT/quartz nanocomposites in terms of RMSE value (where CRMSE; cumulative root mean square error)

Based on the cumulative RMSE values of the ANN topologies tested, the performances of the ANN model in predicting the output parameters are graphed in Figures 4. From both the Table 1 and Figure 4, it is evident that the best hidden neuron configurations based on the highest coefficient of determination (R^2), lowest cumulative training, validation and testing error (RMSE and MAE), and least cumulative RMSE of the predicted output parameters is 10-14 for the dataset trained in the ANN model. Hence, 3-10-14-2 was selected as the preferred and the most

accurate ANN architecture deployed in training and predicting the output parameters of the ANN.

As can be observed from Figure 5, the predicted values determined by using the optimum ANN topology in the model conform to the experimental results. The conformity could be attributed to ample experimental dataset (417) employed for training the ANN model. R^2 value of approximately 1 was obtained for the output parameters; specific heat capacity and thermal conductivity.

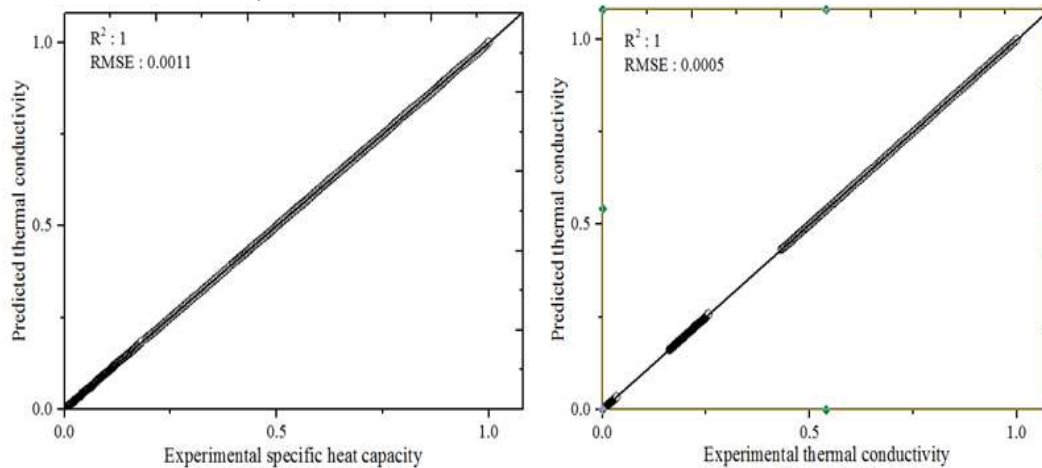


Figure 5: Comparison between predicted and experimental results for the MWNT/quartz nanocomposites

CONCLUSION

As shown in Figure 5, the excellent fit between the experimental values (the straight line) and the predicted values (the bolted data points) signifies that the proposed ANN model has the ability to adequately predict with a minimal/no error, the thermal properties; specifically, specific heat capacity and thermal conductivity of MWNT/quartz nanocomposites having formulations within the range of those values employed in the experimental process as mentioned in the study by Tijjani (2018).

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