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Research Article

An Artificial Neural Network Model to Predict the Thermal Properties of Concrete Using Different Neurons and Activation Functions

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Growing concerns on energy consumption of buildings by heating and cooling applications have led to a demand for improved insulating performances of building materials. The establishment of thermal property for a building structure is the key performance indicator for energy efficiency, whereas high accuracy and precision tests are required for its determination which increases time and experimental costs. The main scope of this study is to develop a model based on artificial neural network (ANN) in order to predict the thermal properties of concrete through its mechanical characteristics. Initially, different concrete samples were prepared, and their both mechanical and thermal properties were tested in accordance with ASTM and EN standards. Then, the Levenberg–Marquardt algorithm was used for training the neural network in the single hidden layer using 5, 10, 15, 20, and 25 neurons, respectively. For each thermal property, various activation functions such as tangent sigmoid functions and triangular basis functions were used to examine the best solution performance. Moreover, a cross-validation technique was used to ensure good generalization and to avoid overtraining. ANN results showed that the best overall R^2 performances for the prediction of thermal conductivity, specific heat, and thermal diffusivity were obtained as 0.996, 0.983, and 0.995 for tansig activation functions with 25, 25, and 20 neurons, respectively. The performance results showed that there was a great consistency between the predicted and tested results, demonstrating the feasibility and practicability of the proposed ANN models for predicting the thermal property of a concrete.

1. Introduction

Building and construction sector has an important role in global energy consumption in terms of heating and cooling applications. Especially in Turkey, this amount approximately corresponds to 37% of the total energy consumption [1]. The main purpose of a heating or cooling system is to maintain conditions that provide thermal comfort for the building occupants and conditions that are required by the products and processes within the space. The net rate at which heat must be removed from a space to maintain a constant space air temperature at comfort level is called the cooling load [2]. The heat gain through the building envelope at most buildings, which contains walls and roofs, constitutes a major portion of the total cooling load of a space due to their large surface area [3]. Concrete is the most economical building material used in a building construction sector twice as much as the total of all other building materials, including wood, steel, and plastic [4]. To minimize energy consumption of the buildings, it is very important to enhance the insulation characteristics of concrete which greatly depend on its thermal properties. The thermal property is defined as a property that measures the response of a material to the application of heat. The energy may be transported to cooler regions of the specimen if temperature gradients exist [5]. For building heat transfer, important thermal properties are thermal conductivity, specific heat, and thermal diffusivity. Especially, a low value of thermal conductivity is desirable because of the associated ability to provide thermal insulation. Moreover, a high value of specific heat is desirable due to the associated ability to retain heat [6]. Besides, thermal conductivity of a concrete is strongly affected by microstructure, mineralogical composition, proportion, supplementary materials, moisture content, and porosity [7]. Especially, aggregate materials, which generally constitute about 70–80% by volume of concrete, can be expected to have a more important impact on thermal properties of concrete structures [8]. On the contrary, the compressive strength is a significant mechanical property in the construction and design; hence, these structures also need to have suitable mechanical properties.

Since the heat transfer mechanism in a concrete is complicated due to the contribution of the each component (aggregate, composition, etc.) to the heat transfer, it is difficult to find the ideal thermal properties of concrete structures. High accuracy and precision tests are required for its determination which increases time and experimental costs. Hence, a lot of work has been carried out by many researchers to find thermal properties of concrete using definite simple models. The effect of thermal conductivity and the mixing ratio of the lightweight materials on the heat insulation properties were investigated by Wang et al. [9]. The results demonstrated that there was an inverse relationship between porosity and thermal conductivity with R^2 of 0.81. The comparison of the thermal conductivity and its trend with the 28-day compressive strength was depicted with R^2 of 0.96 in a study [10]. The compressive strength and the thermal conductivity were found to reduce with a decrease in the density of the concrete. Sengul et al. [11] investigated the effect of expanded perlite on the mechanical properties and thermal conductivity of lightweight concrete. The results showed that there was a linear relationship between density and thermal conductivity with R^2 of 0.98. In another study, Nandi et al. [12] studied various thermal properties of anisotropic shale from Tennessee, which is commonly used as building stones and bricks. The regression analyses were conducted between heat capacity and significant independent variables including porosity, density (unit weight), and compressive strength test values of shale samples.

The models indicated in the literature are generally in regression forms and obtained from physicomechanical properties such as porosity, bulk density, and compressive strength which have primary effect on thermal properties. However, thermal properties of building materials are affected by many independent mechanical properties; using a simple regression method to investigate the effect of each mechanical property on thermal property produces less accuracy results and requires more assumption. Artificial neural network (ANN) is considered to be an innovative solution to overcome this problem. In the literature, the principles of ANN have been briefly introduced and summarized in several studies. Nikoo et al. [13] and Chopra et al. [14] both conducted an experimental study about the prediction of concrete compressive strength by using evolutionary artificial neural networks as a combination of ANN and genetic algorithms. The results of simulation verify that the recommended ANN model enjoys more flexibility, capability, and accuracy in predicting the compressive strength of concrete. Liang et al. [15] employed a neural network for the prediction of compressive strength of concrete in the wet-dry environment. The performance results show that the model is practical to predict the concrete mechanical performance. Safiuddin et al. [16] studied the modeling of compressive strength for self-consolidating high-strength concrete incorporating palm oil fuel ash. The predicted compressive strength values obtained from the trained ANN model were much closer to the experimental values of compressive strength, which was R^2 of 0.9486. Alshihri et al. [17] used the ANNs to predict the compressive strength of lightweight concrete mixtures after 3, 7, 14, and 28 days of curing. It is concluded that the cascade correlation neural network model predicated slightly accurate results and learned very quickly as compared to the back-propagation procedure. So far, many studies have been conducted to predict 28-day compressive or tensile strength of concrete using ANNs [18–22]. However, there have been only a few studies conducted to investigate the thermal property of concrete materials. Gencel et al. [23] predicted the thermal conductivity of concrete with vermiculite by using ANN with 20 data set. Experimental results were compared with those of the ANN model. It was found that the radial basis neural network model is superior to the other models. The thermal conductivity of rock was predicted through physicomechanical properties in a study conducted by Singh et al. [24]. It was evident from the study that ANN modeling had good prediction capability to determine the very complex rock parameter like thermal conductivity. Lee et al. [25] presented a study about an effective prediction of thermal conductivity of concrete using ANN. The model was trained by 124 data sets with eleven parameters: 9 concrete composition parameters and 2 concrete state parameters. The result indicated that the proposed method was effective at predicting the thermal conductivity of concrete.

Although many researches have attempted to use the ANN method to predict the mechanical behavior of concretes, there has not been much research about investigating the thermal properties. Besides, there is no study in the literature to predict the thermal properties using mechanical properties of concretes. Both accurate and simple methods are required to describe the ideal thermal insulation properties of those structures. Therefore, an ANN model has been used to predict the thermal properties of concrete utilizing its mechanical properties so as to reduce time and experimental costs. The concrete samples were prepared by changing the volume fraction of normal and lightweight aggregate materials in the cementitious matrix, which were exposed to the same conditions. The findings and results are presented in detail in the following sections.

2. Materials and Methods

2.1. Concrete Mixtures, Materials, and Test Methods. Concrete is a composite material composed of aggregate material embedded in a hard matrix of material that fills the space between the particles and glues them together [26]. Several materials were used to produce concrete materials which were locally available ordinary Portland cement (CEM I 42.5R), silica fume, superplasticizer, air-entrained mixture, and fine and coarse aggregates such as gravel, sand, rubber, perlite, and pumice aggregates. In the experimental setup, concrete samples were designed with a constant water-cementitious material ratio of 0.48 and total cement content of 350 kg/m^3. Normal aggregates (sand and gravel) were replaced by lightweight aggregates (rubber, perlite, and pumice) at different volume fractions varying between 10% and 100%. In total, 264 concrete samples were produced, and their mechanical tests, which are the compressive strength (ASTM C39), split-tensile strength (as shown in Figure 1, ASTM C 496), ultrasonic pulse velocity (as shown in Figure 2(b), ASTM C597), bulk density (ASTM C138), and porosity (ASTM C1202-12) tests, were performed in accordance with ASTM standards on air-dried samples aged 28 days (ASTM C330-99). The minimum strength requirements for building blocks are most commonly set at 2.5 MPa (BS 6073: Part 1); therefore; the produced samples whose compressive strengths are under the limit are not included in the study.

The thermal properties tests, which are thermal conductivity, specific heat, and thermal diffusivity, were performed on the same state with the age of 35 days according to EN 12667 [27]. In this study, ISOMET 2104 device (Figure 2(a)) was used to measure the thermal conductivity of concrete samples on the basis of the transient plane source (TPS) method. In comparison with stationary or steady-state methods, the advantage of transient methods is to give a full set of thermal properties within a single rapid measurement. Moreover, the Matest 24048 test device is used for the determination of ultrasonic pulse velocity. The technical specifications of the used devices are given in Table 1.

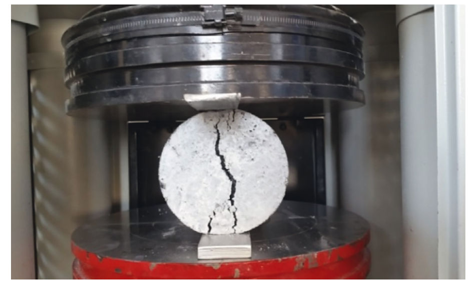


Figure 1: Split-tensile strength test.

2.2. Construction of Artificial Neural Network Model. ANNs are one of the most important methods used in machine learning. The neural networks algorithm is generally a useful tool for recognizing patterns, fitting a function, and clustering of data. The concept of neuron within the abbreviation of ANN is the brain-inspired systems based on the way people learn. It is very useful tool for the solution of problems caused by the inability of manual solution when the data are too much. The general neural network system consists of units such as input/output, weights, activation function, and hidden layer. The collected test data from experiments are multiplied by weights and transferred to the activation function. There are various activation functions, which are tangent sigmoid (tansig), linear (purelin), triangular basis (tribas), radial basis (radbas), and logarithmic sigmoid (logbas) transfer functions used in the networks [28, 29]. The indicated activation functions are shown in Table 2.

The mathematical expression of the basic neural network is presented as

$$o = f(wx + \text{bias}), \tag{1}$$

$$w = w_1, w_2, \ldots, w_n, \tag{2}$$

$$x = x_1, x_2, \ldots, x_n. \tag{3}$$

Weights and inputs are defined by equations (2) and (3). The transfer function of the neural network is defined in the following equation:

$$\text{net} = \sum_{i=1}^{n} w_i x_i + b, \tag{4}$$

where the index b is expressed as the bias value. If the sigmoid function is used as an activation function, the output of the network is expressed as

$$C_j = f\left(\text{net}_j\right) = \frac{1}{1 + e^{-(\text{net})}}. \tag{5}$$

The function shown in equation (5) represents that the functions can be derived from derivatives such as hyperbolic, sigmoid, and inverse hyperbolic. The error value in equation (6) is calculated by determining the difference between the expected output (B_k) and the calculated output (C_k) of the network. To reduce the error value, weights of the neurons in the network are changed until the error falls below a certain value:

$$E_m = B_k - C_k. \tag{6}$$

The total error is expressed as in the following equation:

$$TH = \frac{1}{2} \sum_m E_m^2. \tag{7}$$

The performance of the networks can be examined by using different training functions such as gradient descent, BFGS quasi-Newton, resilient back propagation, and scaled conjugate gradient; however, the Levenberg–Marquardt training function is generally preferred, which was also used in this study, due to its high accuracy and usability. By the way, using different neuron numbers on hidden layers will

(a) (b)

Figure 2: The measurement devices of ultrasonic pulse velocity and the thermal property.

Table 1: Technical specifications of devices for measuring parameters.

Measurement property	Measurement range	Accuracy
Thermal conductivity, λ	0.015–6 W/m·K	5% of reading + 0.001 W/m·K
Specific heat capacity, ρc_p	4×10^4–4×10^6 J/m^3·K	15% of reading + 1.103 J/m^3·K
Ultrasonic pulse velocity, UPV	0–3000 μs	±0.1 μs

Table 2: Equation of different types of activation functions.

Name of activation function	Function equation
Sigmoid (logsig) function	$y = 1/1 + e^{-x}$
Linear function (purelin)	$y = x$
Triangular basis (tribas) function	$y = \begin{cases} 1-\lvert x\rvert & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$
Radial basis (radbas) function	$y = e^{-x^2}$
Tangent sigmoid (tansig) function	$y = \tanh(x)$

also have an impact on the results. For this purpose, 5, 10, 15, 20, and 25 neurons were tested in the single hidden layer, respectively.

Figure 3 shows the proposed ANN model for 5 inputs and 1 output with a single hidden layer. The mechanical properties of the concrete obtained from the experimental study are used as an ANN input, and three different neural network structures with a single hidden layer are designed to predict the thermal properties and are used as an output. Consequently, in order to determine best performance values, a single hidden layer ANN model with five activation functions and five different neuron numbers was designed to perform the prediction of the thermal properties of concretes.

Cross validation is a method to assess the prediction performance and to investigate how they perform outside the sample to a new data set also known as testing data. The technique is used to ensure good generalization and to avoid overtraining [30, 31]. In this paper, the fold number k is set to 10 considering the computational time and the recommendations in the literature. Therefore, the training data were divided into 10 subsets, of which 8 were used for training, while the remaining one was used for cross validation. In the training phase, experimental data are shown to the network by shifting 10 times. Then R^2 values are calculated by taking the average of R^2 values obtained from each shift.

2.2.1. Normalization Process. Some activation function values vary from 0 to 1. For this reason, it is required to use some data in this range for training. To achieve this, a process called normalization should be applied. The equation shown below is used to perform the normalization process [32]:

$$X_i^{\text{norm}} = \frac{X_i - X_i^{\min}}{X_i^{\max} - X_i^{\min}}, \tag{8}$$

where X_i^{norm} is the normalized value, $X_i^{\max}$ is the maximum value, $X_i^{\min}$ is the minimum value, and X_i is the actual value.

2.2.2. Performance Evaluation of the ANN. In order to evaluate the performance of developed models, the coefficient of determination (R^2) is used as a common criterion to judge about the "accuracy" of a specific model based on its prediction, while the root-mean-square error (RMSE) and mean absolute percentage error (MAPE) are commonly used to show the "precision" of a model based on residual analysis. Therefore, it is preferred to use a combination of criteria to conclude and/or compare overall performance of models. In this study, the stated metrics are used to evaluate the prediction performance of an ANN. The first performance indicator is the mean absolute error (MAE) which measures the average magnitude of the errors without considering their directions [33]. The MAE performance function is expressed as

$$\text{MAE} = \frac{1}{n}\sum_{k=1}^{n} \lvert y(k) - t(k)\rvert. \tag{9}$$

The root-mean-squared error performance function is computed as follows:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{k=1}^{n} [y(k) - t(k)]^2}. \tag{10}$$

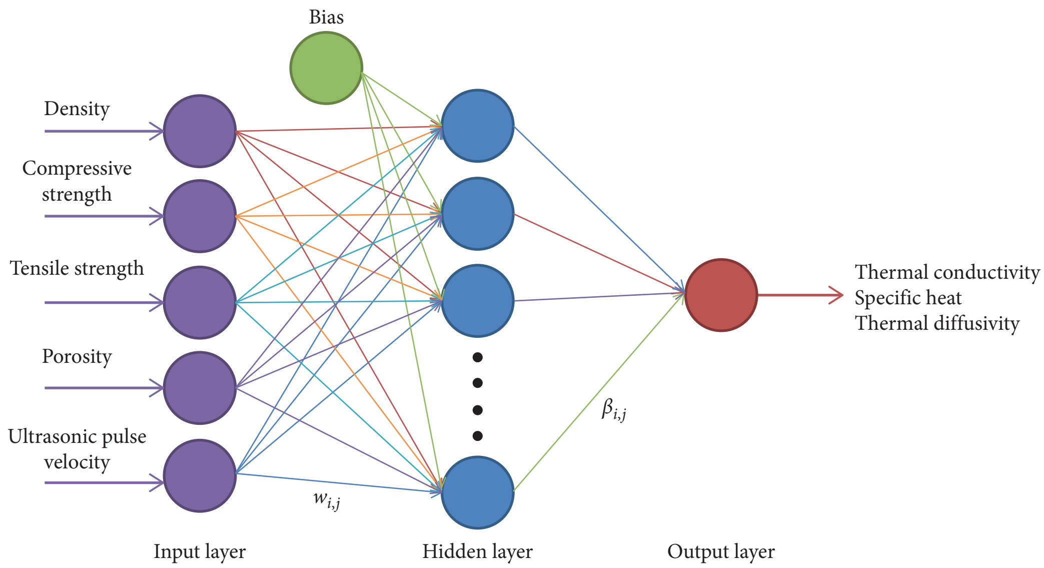


Figure 3: Construction of the ANN model.

The mean absolute percentage error is computed as follows:

$$\text{MAPE} = \frac{\sum_{k=1}^{n} \left| y(k) - t(k)/y(k) \right|}{n} \times 100. \quad (11)$$

The coefficient of determination criterion is computed as follows:

$$R^2 = \frac{\sum_{k=1}^{n} \left(y(k) - t(k)\right)^2}{\sum_{k=1}^{n} \left(y(k) - y_m(k)\right)^2}, \quad (12)$$

where n is the number of observations, $y(k)$ is the experimental data $t(k)$ is the predicted data, and $y_m(k)$ is the mean experimental data.

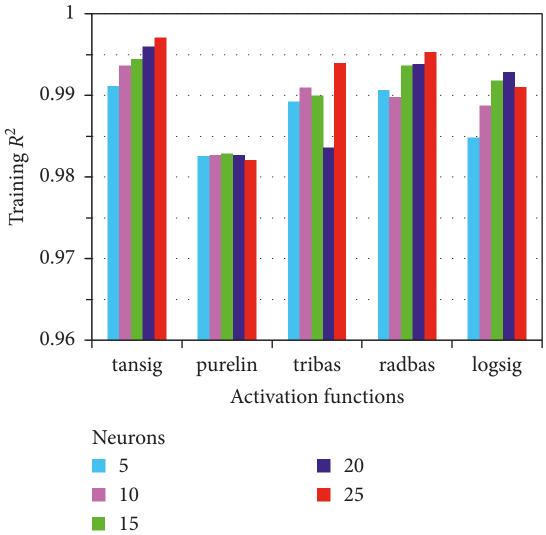
3. Results and Discussion

In this study, the ANN model has been used to predict the thermal properties of concrete by utilizing its mechanical properties. The mechanical properties of the concrete obtained from the experimental test data were used as inputs, and the thermal properties were used as outputs. In this regard, a single hidden layer neural network model with five different activation functions and different neuron numbers was designed, and their performances are examined. Due to the fact that the best performance results were obtained in the ANNs with single hidden layer, in this study, it was not required to design a multilayered ANN. The data were divided into two categories, training and testing subsets including 110 and 22 data (total of 132 data), respectively. In Figure 4, the coefficient of determination (R^2) values for prediction of thermal conductivity are indicated in training, validation, testing, and overall phases, respectively. As mentioned before, R^2 can take values between 0 and 1 where values closer to 0 represent a poor fit, while values closer to 1 represent a perfect fit. When overall R^2 values are examined, the tansig-based neural network with 25 neurons has the best R^2 performance with the value of 0.996. Although the best R^2 performance results are obtained in that network, other network results are also successful to predict the thermal conductivity values.

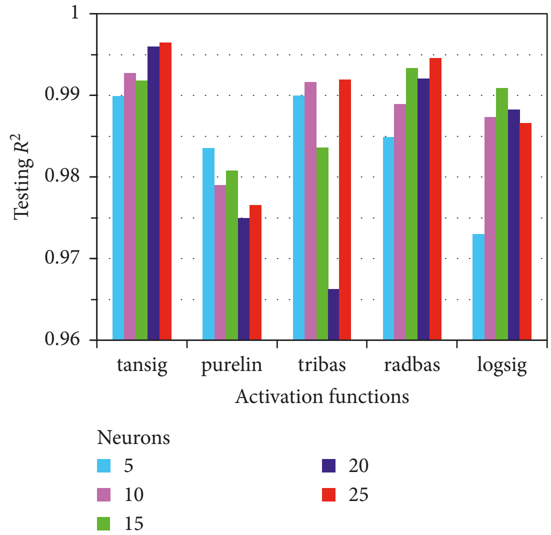
Figure 5 illustrates RMSE, MAE, and MAPE performance indices of the ANN in training and testing phases for the prediction of thermal conductivity, respectively. The results show that the RMSE values of the tansig activation function-based neural network with 25 neurons in training and testing phases are 0.001508 and 0.011086, respectively. MAE shows the average absolute error where the values are 0.012485 and 0.031103 in the training and testing phases for the tansig-based neural network with 25 neurons, respectively. When the MAPE performance indicator is examined, the best performances of the MAPE values in training and testing phases are 0.049987 and 0.141836 for the tansig-based neural network with 25 neurons, respectively.

Figure 6 shows the R^2 performance results of the ANN for the specific heat in training, validation, testing, and overall phases, respectively. When overall R^2 values are considered, the tansig activation function-based neural network with 25 neurons has the best R^2 performance with the value of 0.983.

Figure 7 illustrates RMSE, MAE, and MAPE performance indices of the ANN in training and testing phases for prediction of the specific heat, respectively. The results show that the RMSE value of tansig activation function-based ANN with 25 neurons in the training phase is 0.001787 and the RMSE value in the testing phase is 0.017423. The results for the MAE value of logsig-based ANN with 25 neurons in the training phase is 0.015459 and for the MAE value of tribas-based ANN with 15 neurons in the testing phase is 0.030337. When the MAPE performance indicator is considered, the best performances of the MAPE values in training and testing phases are 0.044071 and 0.088857 for the radbas-based ANN with 20 neurons



(a)



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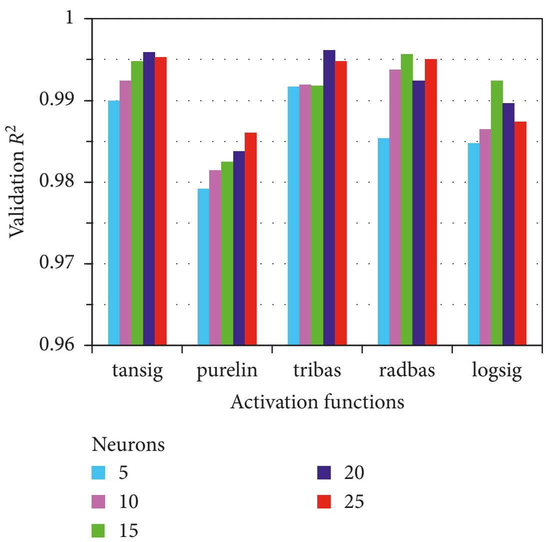

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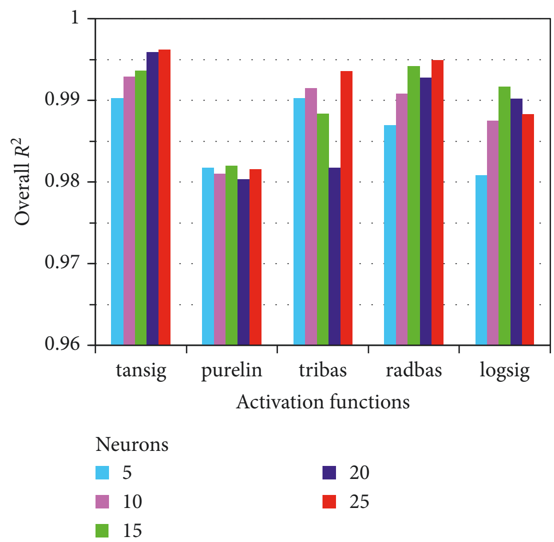
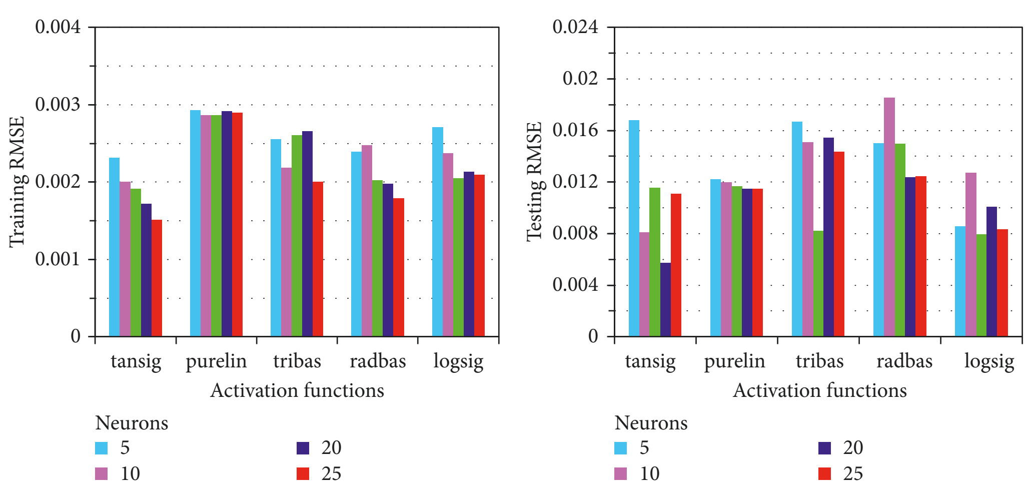


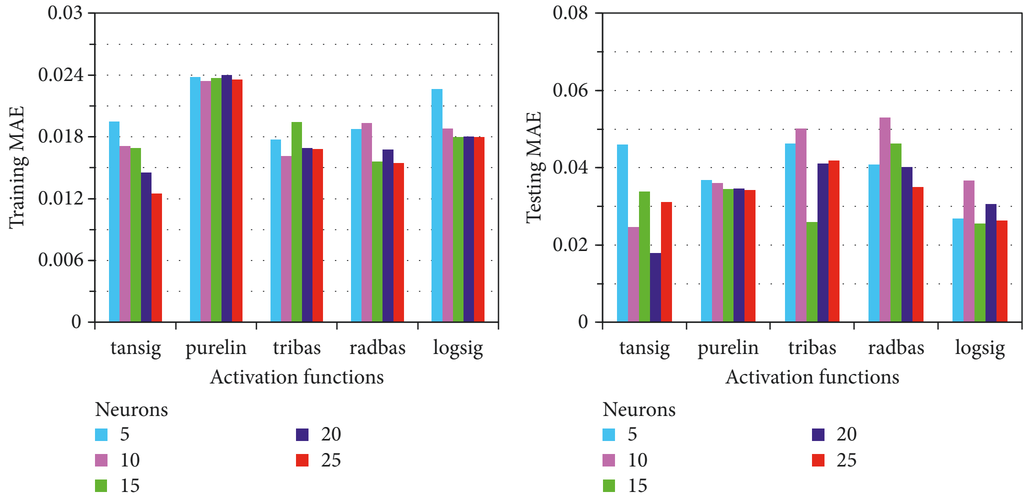
(d)

Figure 4: The coefficient of determination (R^2) values for the prediction of thermal conductivity.



(a)

Figure 5: Continued.



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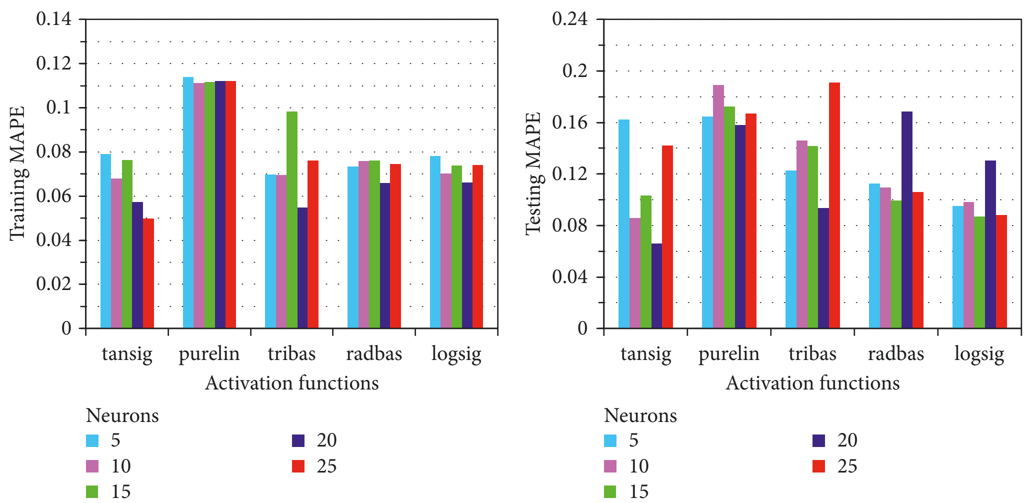
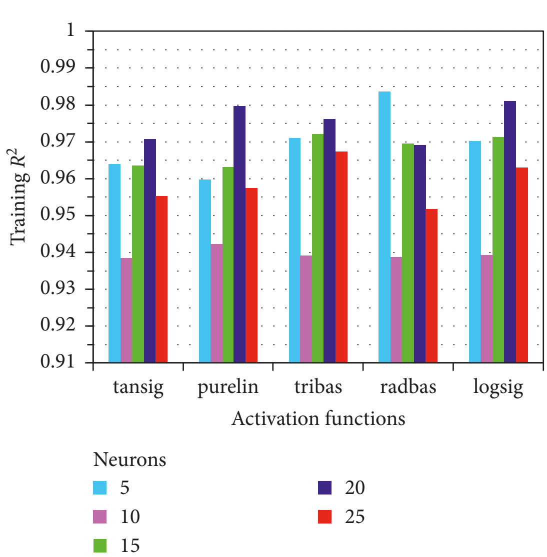
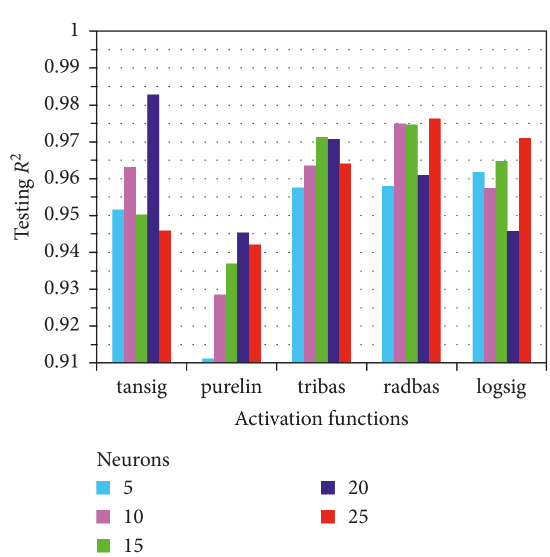


(c)

FIGURE 5: (a) RMSE, (b) MAE, and (c) MAPE performances of training and testing phases for thermal conductivity.

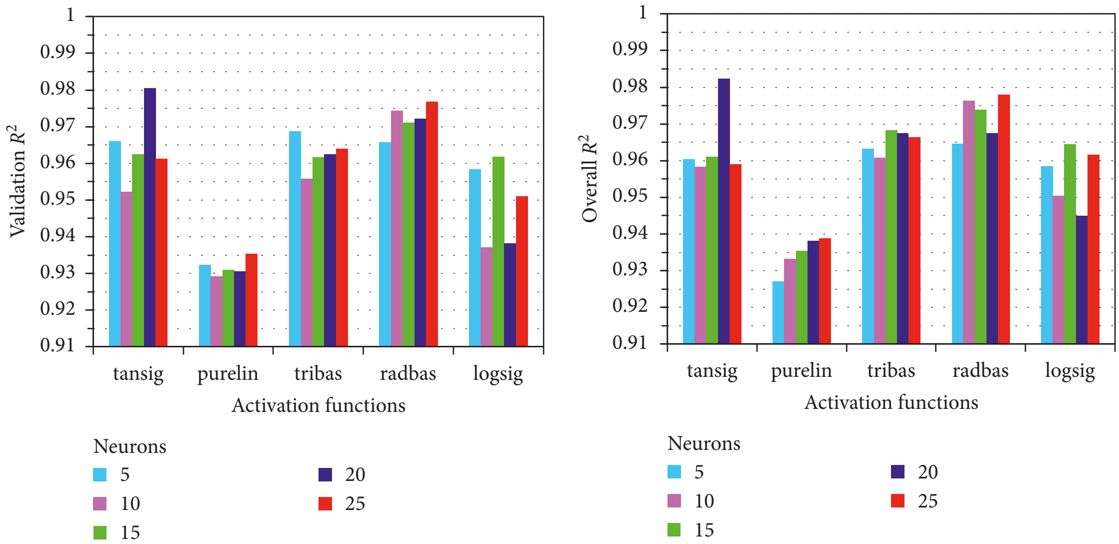


(a)



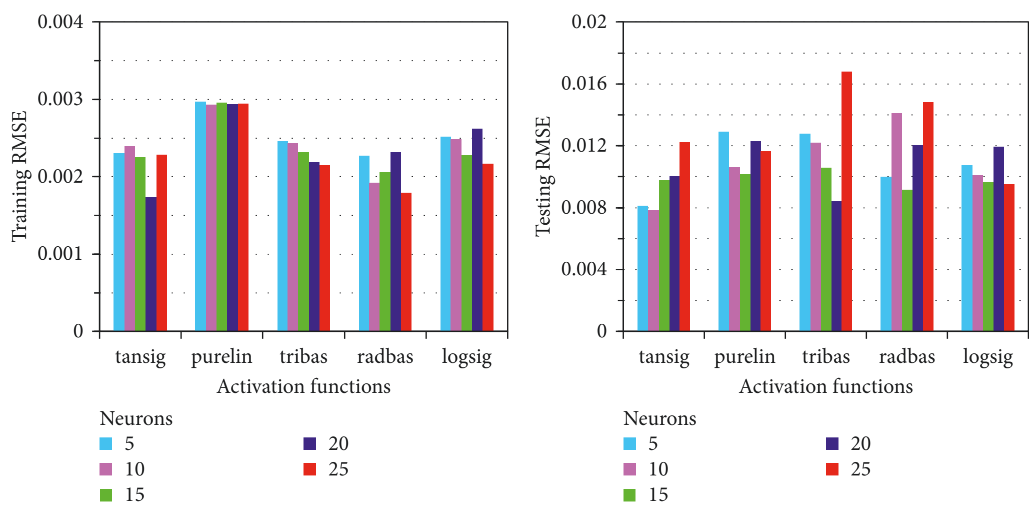
(b)

FIGURE 6: Continued.

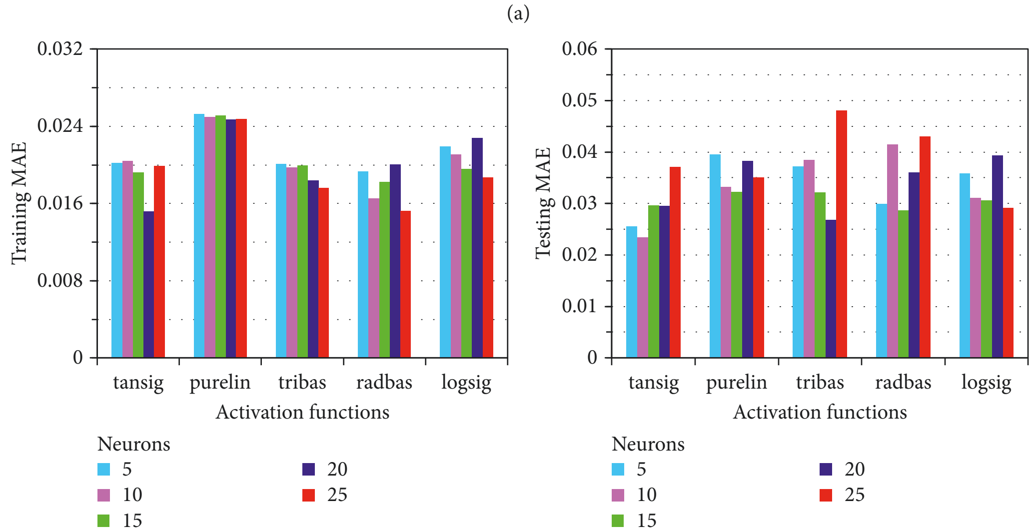


(c) (d)

FIGURE 6: The coefficient of determination (R^2) values for the prediction of specific heat.

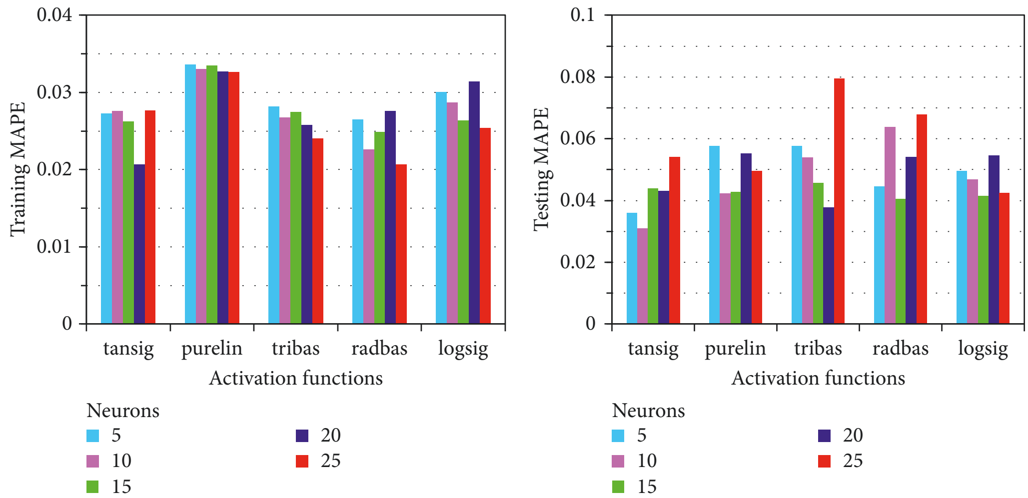


(a)



(b)

FIGURE 7: Continued.



(c)

Figure 7: (a) RMSE, (b) MAE, and (c) MAPE performances of training and testing phases for specific heat.

and for the logsig activation function-based ANN with 15 neurons, respectively.

Figure 8 shows the R^2 performance results of the ANN for thermal diffusivity in training, validation, testing, and overall phases, respectively. When overall R^2 values are examined, the tansig-based neural network with 20 neurons has the best R^2 performance with the value of 0.983. Although the best R^2 performance results were obtained in those function-based networks, other network results are also successful to predict the thermal diffusivity values.

Figure 9 illustrates RMSE, MAE, and MAPE performance indices of the ANN in training and testing phases for the prediction of thermal diffusivity, respectively. The results show that the RMSE values of tansig-based neural network with 20 neurons in training and training phases are 0.001733 and 0.01001, respectively. The best performance results for the MAE value of the tansig-based neural network with 20 neurons in the training phase is 0.015156 and for the MAE value of the tansig-based neural network with 10 neurons in the training phase is 0.023443. When the MAPE performance indicator is examined, the best performances of MAPE values in training and testing phases are 0.020641 and 0.043037 for the tansig-based neural network with 20 neurons, respectively.

There are a few studies in the literature to estimate the thermal properties of concrete through mechanical properties such as density. In the studies [34–37], regression analyses were performed to obtain some correlations from experimental results of those properties. The comparison results of experimental and tansig-based ANN with 25 neuron with a correlation obtained in Reference [37] for thermal conductivity is shown in Figure 10.

There is a significant difference between the experimental and correlation results when the density values are between 1600 and 2500 kg/m^3. The difference is due to both the correlation range, which gives better results with densities from 320 to 1600 kg/m^3 as stated in Reference [37], and the nature of linear regression. It is shown that, while linear regression modeling approach is deficient to predict the thermal conductivity values, more accurate results are obtained with the usage of ANN which perfectly represents the features of the thermal conductivity values. This is due to the fact that ANN can approximate nonlinear relationships between mechanical and thermal properties without any presumptions, while the linear regression model is performed between one input and output that leads to less accuracy and also requires more assumptions.

4. Conclusions

In this study, a single hidden layer ANN model with five different activation functions and five different neuron numbers was designed to perform the prediction of thermal properties of concrete through its mechanical properties. The Levenberg–Marquardt training algorithm-based neural network was designed to predict the thermal properties of building materials. In order to evaluate the predictions, the normalization and the cross-validation processes were performed at first. Then, R^2, RMSE, MAE, and MAPE performance indicators were investigated for five different numbers of neurons and activation functions. For each thermal property, various transfer functions are used to examine the best solution performance in the ANN. Due to the fact that the best performance results were obtained in the ANNs with single hidden layer, in this study, it was not required to design a multilayered ANN. The ANN results showed that the best overall R^2 performances for predicting thermal conductivity, specific heat, and thermal diffusivity were obtained as 0.996, 0.983, and 0.995 for tansig activation function-based ANN with 25, 25, and 20 neurons, respectively. Although the best R^2 performance results have been obtained in these function-based networks, other network results are also successful to predict the thermal properties of concrete structures. The performance results indicated that there was a great consistency between the predicted and the tested results. Moreover, the experimental

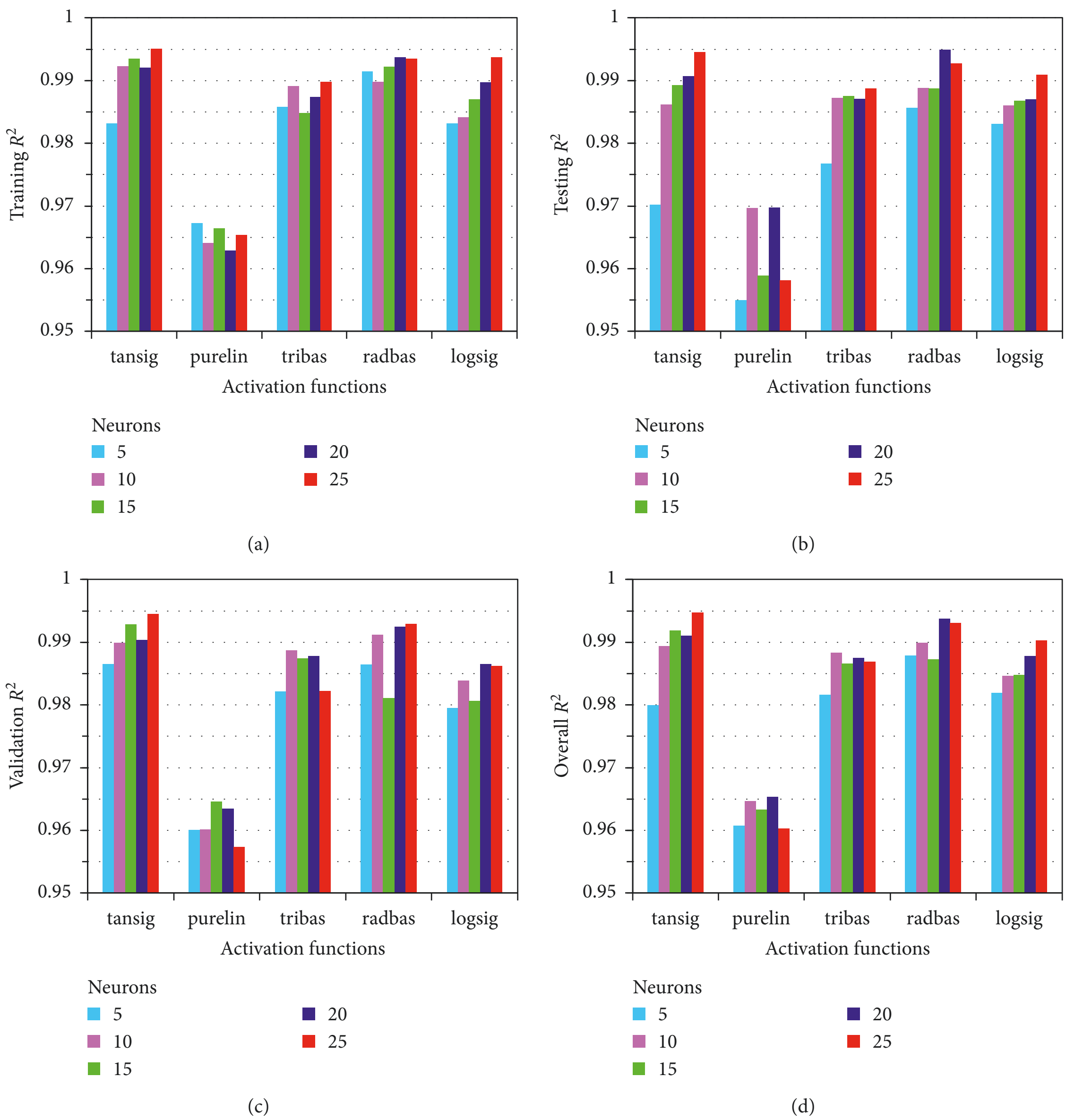


Figure 8: The coefficient of determination (R^2) values for prediction of thermal diffusivity.

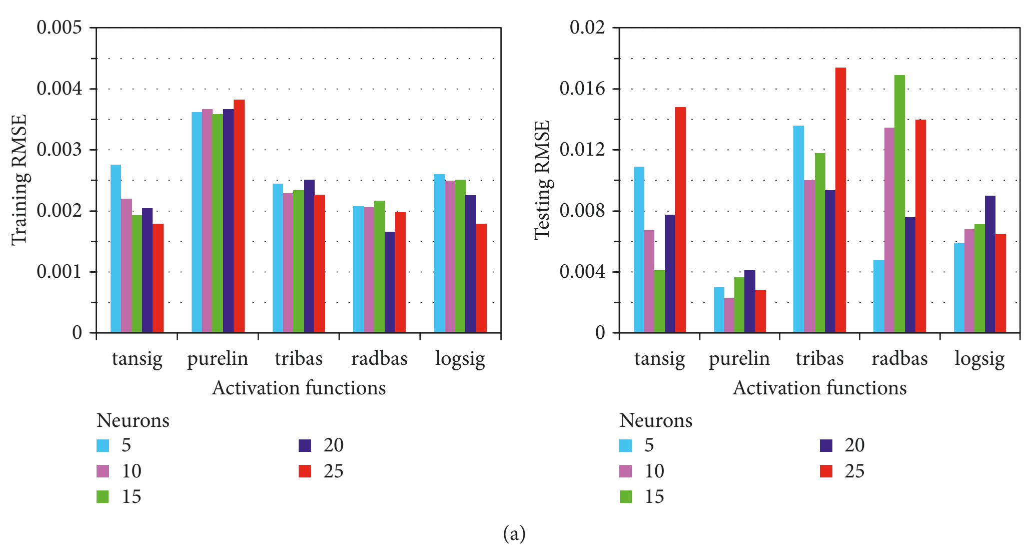
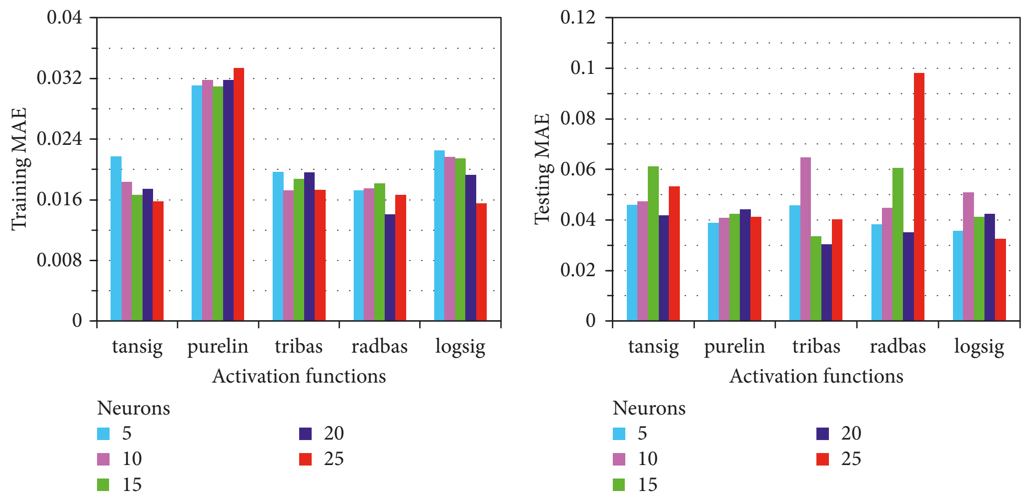
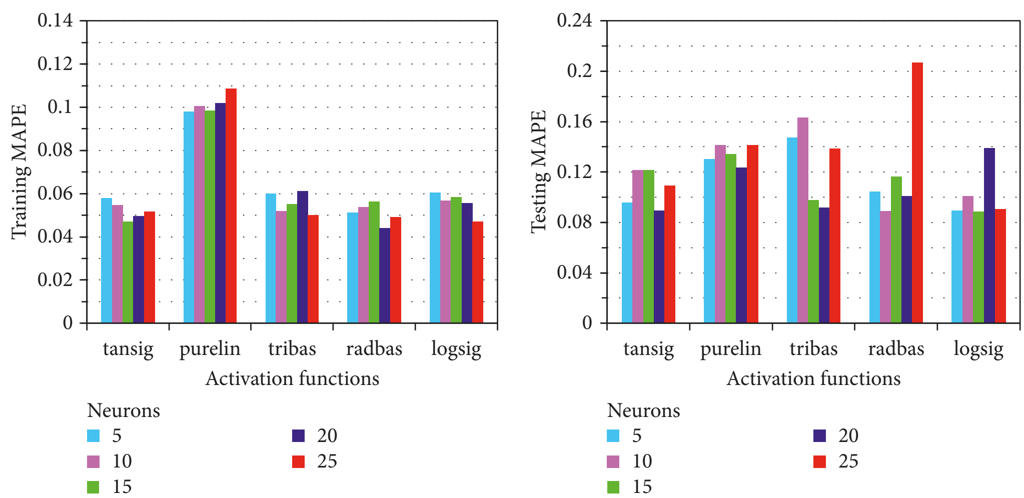


Figure 9: Continued.



(b)



(c)

FIGURE 9: (a) RMSE, (b) MAE, and (c) MAPE performances of training and testing phases for thermal diffusivity.

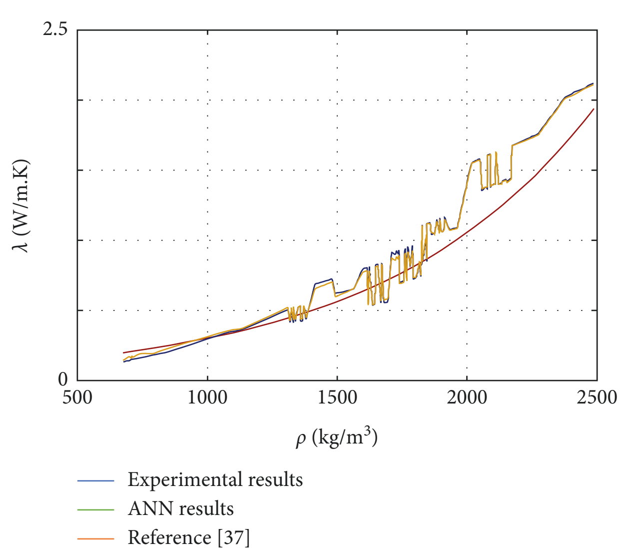


FIGURE 10: The comparison of the experimental, ANN, and a correlation to Reference [37] results for thermal conductivity.

and the ANN results of thermal conductivity values have been compared with the literature studies. More accurate results are obtained with the usage of ANN instead of regression models. Consequently, the study is a major contribution to the neural network literature, demonstrating the feasibility and practicability of the proposed ANN models for predicting the thermal property of concrete structures.

Data Availability

All the data used to support the findings of this study have been deposited in the Dropbox repository (https://www.dropbox.com/sh/aqj7elcvjmb6376/AADvAV5QodxDQeWmUsIFJoM2a?dl=0).

Conflicts of Interest

The authors declare no conflicts of interest.

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Supplementary Materials

The pdf file titled as "The experimental data" includes the experimental test results for the produced concrete samples. The file titled as "Specific heat" contains the raw ANN data (excel files), and the figures of ANN results for specific heat values of concrete samples. The file titled as "Thermal conductivity" contains the raw ANN data (excel files), and the figures of ANN results for thermal conductivity values of concrete samples. The file titled as "Thermal diffusivity" contains the raw ANN data (excel files), and the figures of ANN results for thermal diffusivity values of concrete samples. (*Supplementary Materials*)

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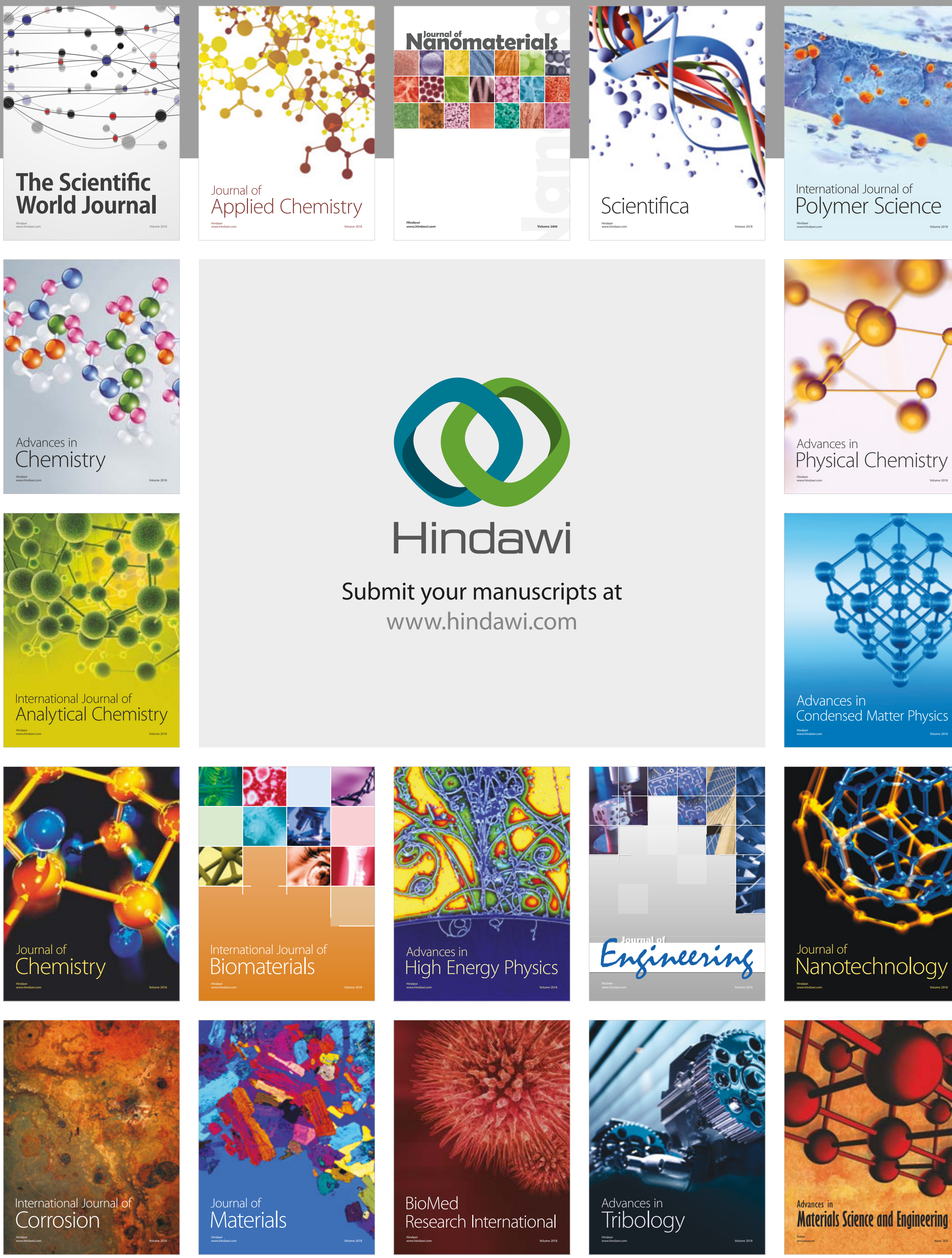
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