PREDICTING WOOD THERMAL CONDUCTIVITY USING ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

An artificial neural network model that estimates wood thermal conductivity under a wide range of conditions of moisture content, temperature and apparent density was developed and tested with literature-obtained experimental data. The optimal network was determined to consist of an input layer, three hidden layers, and one output layer following the feed forward network structure and more specifically the back-propagation algorithm. Each of the three hidden layers of the ANN consisted of eleven neurons. The Neuralworks software package was used for the determination of the network structure and architecture, and for the training and testing phase. The evaluation produced an R^2 value equal to 0.9994 and a RMS Error equal to 0.0123, thus proving that the developed ANN model is a reliable approach with powerful predictive capacity towards the estimation of thermal conductivity and it can be used by researchers under a wide range of conditions.

Keywords: Artificial neural networks, density, moisture content, temperature, thermal conductivity coefficient, wood.

INTRODUCTION

The knowledge of wood thermal properties is essential when simulation and optimization of processes such as air-conditioning in timber buildings, heating of logs, and drying of timbers, veneers, chips, and fibers are attempted. In recent years, mathematical modeling and computer-based numerical analysis have become the main tools for understanding and predicting wood drying phenomena where heat and moisture diffusion coefficients are extensively used in the calculation of fluxes and profiles (Keey 2000; Koumoutsakos et al. 2003).

Thermal conductivity coefficients along with specific heat values are important parameters required to calculate thermal diffusivity. Of the first two properties, specific heat is simpler to measure than thermal conductivity from the experimental point of view since the latter usually requires very elegant arrangement to avoid the effect of internal moisture redistribution during testing and its effect on the measure heat flux. Thermal conductivity coefficients have been reported in the past for various wood species and as a function of density, temperature, moisture content, and fiber direction (Chia et al. 1985; Hendricks 1962; MacLean 1941; Maku 1954;

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Shida 1982; Steinhagen 1977; Suleiman et al. 1999; Wangaard 1943), with very little work done in the area of developing models based on wood anatomical and thermodynamic principles (Cai and Chang 1995; Khattabi and Steinhagen 1993; Siau 1970, 1984; Suleiman et al. 1999). Most of the models used nowadays are empirical equations developed for above and below the fiber saturation regimes as a function of moisture content, specific gravity, and porosity (Siau 1995). It is thus imperative as a first step to explore the modeling of wood thermal conductivity using theoretical rather than empirical means by implementing sophisticated modeling techniques like Artificial Neural Networks (ANN) that will not be species specific, but more universal such as depending on material properties including chemical and anatomical characteristics.

ANNs are highly complex nonlinear information-processing systems, operating in a parallel way and they consist of interconnected Processing Elements (PE). These elements are called neurons and they were inspired from biological nervous systems (Picton 2000). They are capable of training from examples through iteration without requiring a prior knowledge of the relationships between process parameters. ANNs learn to solve problems by adequately adjusting the strength of the interconnections according to the input data. They can also adapt easily to new environments by training and they can deal with noisy, vague, or probabilistic data (Leondes 1998). An extensive description of ANN background is given in Avramidis and Iliadis (2005). Figure 1 shows the general structure of an ANN.

In this study, neural networks were evaluated as predictors of thermal conductivity of wood by comparing them to existing literature data. Furthermore, MacLean's empirical thermal conductivity equation for above and below 40% moisture content (Siau 1995) and Siau's transverse model developed based on the analogy between thermal and electrical circuits and the structure of wood cells (Siau 1970, 1995) were also used merely for comparison purposes.

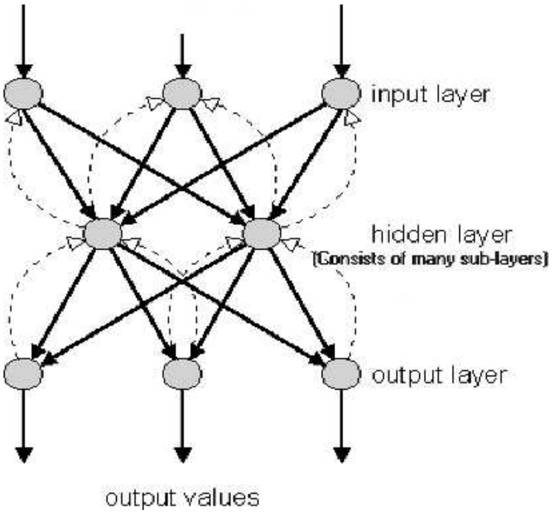

FIG. 1. General architecture of an artificial neural network. The dashed lines show that data may flow to both directions.

METHODOLOGY

The experimental thermal conductivity (K_q) data for wood used in this work were obtained from published work by other researchers in the field. The steady-state method was used to measure the K_q coefficients at various temperatures (T), moisture contents (M), and with a variety of wood species resulting in assorted densities (ρ) and in the transverse direction. Experimental data and reference sources can be found in Table 1. The strong dependency of K_q on the independent variables is quite evident.

The MacLean empirical equations for the calculation of K_q are the following:

$$K_q = G(0.2 + 0.0038M) + 0.024 \quad \text{for } M < 40\% \tag{1}$$

$$K_q = G(0.2 + 0.0052M) + 0.024 \quad \text{for } M > 40\% \tag{2}$$

where K_q is the transverse wood thermal conductivity (W/m K), M is the moisture content (%), and G is the specific gravity of wood [$= \rho/(1 + 0.01M)$] where ρ is the apparent wood density (kg/m^3).

Another accepted method for the estimation of K_q is Siau (1970) equation derived from the

TABLE 1. *Experimental data and outputs from the ANN and the two empirical equations.*

Wood species	T (°C)	M (%)	— (kg/m^3)	Exp K_q (W/m K)	ANN (W/m K)	MacLean (W/m K)	Siau (W/m K)	Reference
Ash, white	***29***	***15.6***	***647***	***0.1742***	0.2820	0.2180	0.1571	MacLean
Ash, white	***29***	***91.1***	***917***	***0.3744***	0.3834	0.3128	—	MacLean
Aspen, bigtooth	***29***	***12.1***	***460***	***0.1181***	0.1180	0.1507	0.1163	MacLean
Birch, yellow	29	10.8	709	0.1714	—	0.2134	0.1685	MacLean
Douglas-fir	29	18.4	545	0.1397	—	0.1981	0.1357	MacLean
Hemlock, west	29	23.0	541	0.2736	—	0.2153	0.1368	MacLean
Maple, sugar	29	11.7	737	0.1397	—	0.2253	0.1760	MacLean
Maple, sugar	29	50.0	930	0.3110	—	0.3970	—	MacLean
Oak, red	***29***	***12.4***	***697***	***0.1944***	0.2148	0.2176	0.1667	MacLean
Oak, red	***29***	***60.3***	***898***	***0.3211***	0.3507	0.3609	—	MacLean
Oak, white	29	11.1	689	0.1973	—	0.2093	0.1640	MacLean
Oak, white	29	57.6	914	0.3729	—	0.3730	—	MacLean
Pine, white	29	9.8	395	0.1109	—	0.1270	0.1037	MacLean
Cedar, west red	29	13.3	363	0.1051	—	0.1269	0.0988	MacLean
Redwood	29	11.7	436	0.1195	—	0.1430	0.1117	MacLean
Redwood	29	80.2	649	0.2722	—	0.2406	—	MacLean
Spruce, engelman	29	13.0	396	0.1109	—	0.1355	0.1047	MacLean
Cedar, Japanese	0	0	294	0.0731	—	0.0828	0.0841	Shida
Cedar, Japanese	20	0	294	0.0778	—	0.0828	0.0841	Shida
Cedar, Japanese	***40***	***0***	***294***	***0.0824***	0.0680	0.0828	0.0841	Shida
Cedar, Japanese	60	0	294	0.0882	—	0.0828	0.0841	Shida
Cedar, Japanese	25	50.0	420	0.1219	—	0.2184		Shida
Cedar, Japanese	25	70.0	500	0.1567	—	0.2554		Shida
Beech, Japanese	***0***	***0***	***622***	***0.1091***	0.1025	0.1484	0.1422	Shida
Beech, Japanese	20	0	622	0.1149	—	0.1484	0.1422	Shida
Beech, Japanese	40	0	622	0.1219	—	0.1484	0.1422	Shida
Beech, Japanese	60	0	622	0.1283	—	0.1484	0.1422	Shida
Beech, Japanese	***25***	***50.0***	***800***	***0.2032***	0.1896	0.3942	—	Shida
Beech, Japanese	25	70.0	920	0.2554	—	0.4498		Shida
Birch, silver	21	0	680	0.2140	—	0.1600	0.1542	Suleiman et al.
Birch, silver	21	0	473	0.1960	—	0.1186	0.1140	Suleiman et al.
Birch, silver	***21***	***0***	***443***	***0.1770***	0.1473	0.1126	0.1087	Suleiman et al.
Birch, silver	100	0	680	0.2500	—	0.1600	0.1542	Suleiman et al.
Birch, silver	***100***	***0***	***473***	***0.2440***	0.1979	0.1186	0.1140	Suleiman et al.
Birch, silver	100	0	443	0.2070	—	0.1126	0.1087	Suleiman et al.

Data "***bold italics***" were used in ANN testing whereas the other were used for ANN training.

analogy between cell wall and electrical circuit resistance,

$$1/K_q = (1-\alpha)/(0.651 - 0.609\alpha) + \alpha/(0.44(1-\alpha) + 0.042\alpha \qquad (3)$$

Equation (3) is applicable only for values of M below the fiber saturation point where $\alpha = \sqrt{V_a}$ and V_a is the wood porosity calculated from,

$$V_a = 1 - G(0.653 + 0.01M) \qquad (4)$$

The performance of an ANN is critically dependent on the training data that must be representative of the task to learn (Callan 1999). Thus, the first task was the accumulation of data that are necessary for its training and testing. Since the objective of this work was to model steady-state thermal conductivity coefficients as a function of temperature, moisture content, and density, experimental data required were obtained from past research reported in the literature. The experimental thermal conductivity (K_q) data for wood used in this work were obtained from published work by other researchers in the field. The steady-state method was used to measure the K_q coefficients at various temperatures (T), moisture contents (M), and with a variety of wood species resulting in assorted densities (ρ) and in the transverse direction. The dataset with the thirty-five experimental cases was divided randomly in two subsets. Twenty-five cases were used for the ANN training whereas ten cases were chosen randomly to be used for its testing. Experimental data of the two subsets and reference sources can be found in Table 1.

Once the experimental data were gathered, and the pertinent values were calculated from MacLean's and Siau's equations, the next step involved the selection of an optimal configuration for the ANN. The designer of an ANN needs to choose an appropriate network model and to specify a network topology. In order to design and develop the proper ANN, the Neuralworks Professional II/Plus (NeuralWare Inc, PA) software was used. The Neuralworks System allows the user to easily generate over two dozen of well-known network types and models, or to design a custom one. It also provides the designer with an extensive instrumentation package that allows monitoring of the network's performance. The coefficient of determination R^2 of the linear regression line between the predicted values from the ANN model and the desired output was used as a measure of performance. Additionally two ANN instruments, the Root Mean Square Error (RMS Error) and the Confusion Matrix (a graphical instrument of Neuralworks), were used to check its validity.

The RMS Error adds up the squares of the errors for each PE in the output layer, divides by the number of PEs in the output layer to obtain an average, and then takes the square root of that average hence the name "root square." The Confusion Matrix (CM) provides an advanced way of measuring ANN performance during the "learn" and "recall" phase. It allows the correlation of the actual results of the ANN to the desired results in a visual display (Neuralware 2001). It provides the user a visual indication of how well the ANN is doing. The CM is roughly akin to a scatter diagram, with the x-axis representing the desired output and the y-axis representing the actual output. The major difference from a scatter diagram, however, is that the CM breaks that diagram into a grid. Each grid square is called a bin (Neuralworks 2001). Each output from the probe points produces a count within one of the bins. For example, if the probe points produce an output of 0.7 and the desired output is 0.5, the bin around the intersection of 0.7 from the y-axis and 0.5 from the x-axis receives a count. Counts are displayed by a bar within the bin, and the bar grows as counts are received. The bin that received the most counts is shown at full height, while all other bins are scales in relation to it. The CM instrument is also equipped with a pair of histograms. The histogram running across the top of the instrument shows the distribution of the desired outputs. The histogram along the right shows the distribution of the actual outputs. Any actual outputs lying outside the range of the instrument graph are added to the top or the bottom bins along the right. The network with the optimal configuration must have the bins (the cells in each matrix) on the diagonal from the lower left to the upper right. Also the value of the vertical axis of the produced histogram is the Common Mean Correlation (CMC) coefficient of the desired (d) and the actual (predicted) output (y) across the Epoch. The CMC is calculated by

$$CMC = \frac{\sum (d_i - \bar{d})(y_i - \bar{y})}{\sqrt{\sum (d_i - \bar{d})^2 \sum (y_i - \bar{y})^2}} \qquad (5)$$

$$\text{where } \bar{d} = \frac{1}{E}\sum d_i \text{ and } \bar{y} = \frac{1}{E}\sum y_i \qquad (6)$$

It should be clarified that *d* stands for the desired values, *y* for the predicted values, and *i* ranges from 1 to *n* (the number of cases in the data training set), and *E* is the Epoch size which is the number of sets of training data presented to the ANN training cycles between weight updates.

RESULTS AND DISCUSSION

The determination of the ANN structure and the selection of the appropriate models to be used constituted the first task to be carried out. Three variables were employed as inputs concerning the wood *T*, *M*, and ρ and only one variable as output, namely, the transverse K_q coefficient of wood. After performing several model tests, the Feed Forward Network Structure (FFNS) with input, output, and hidden layers varying from 1 to 3 was used in this work (Gaupe 1997). In a FFNS, the flow of information is all in one direction. In such networks there are no feedback loops from a PE to a previous one (Bishop 1994; Hornik et. al. 1989). Standard Back-Propagation Algorithm (BPA) and Tangent Hyperbolic function (mapping into the range −1.0 to 1.0) with the Extended Delta Bar Delta (Ext DBD) training rule (Jacobs 1988; Minai and Williams 1990) were utilized for network training. More specifically, the DBD algorithm is an attempt to address the speed of convergence issue, via the heuristic route. By using past values of the gradient, heuristics can be applied to infer the curvature of the local error surface. With this type of information, intelligent steps can be taken in the weight space using a number of straightforward rules. Minai and Williams (1990) recognized that the DBD algorithm is an excellent technique for decreasing the training time for ANN. A more detailed description of the Extended DBD network architecture can be found in Neural Computing (2001). The Epoch value of the ANN was kept stable and equal to 16 which is the default value of the Neuralworks package.

The BPA is the most popular local algorithm for adjusting the weights of a multilayer neural network (Rummelhart et al. 1985). The BPA uses the supervised training technique where the network weight and biases are initialized randomly at the beginning of the training phase. For each given set of inputs to the ANN, the response to each neuron in the output layer is calculated and compared with the corresponding desired output response. The errors produced are adjusted in such a way that the errors in each neuron are reduced. This process is performed from the output to the input Layer (Hornik et. al. 1989). The random number seed was kept constant before each training round and the training coefficient ratio was kept at 1. The Delta Rule Training is a type of training where weights are modified in order to reduce the difference between the desired output and the actual output of a PE. The Ext DBD is a heuristic technique that has been successfully used in a number of application areas and that uses termed momentum. A term is added to the standard weight change, which is proportional to the previous weight change. In this way, good general trends are reinforced and oscillations are damped.

One of the problems of a gradient descent algorithm is setting an appropriate training rate. It is not advisable to change the weight in a linear way and make the assumption that the error surface is locally linear, where "locally" is defined by the size of the training coefficient. At point of high curvature, this linearity assumption does not hold, and divergent behavior might occur near such points. It is therefore important to keep the training coefficient low to avoid such behavior. On the other hand, a small training coefficient can lead to very slow training. The concept of "term momentum" was introduced to solve this dichotomy. The delta weight equation is modified so that a portion of the previous delta weight is fed through to the current delta weight. This acts as a low-pass filter on the delta weight terms, since general trends are reinforced whereas oscillatory behavior cancels itself out. This allows a low training coefficient but faster training (Neural Computing 2001).

Some really important aspects that have to be clarified initially are the amount of data required, the number of layers and neurons per layer and the number of iterations performed, in order to avoid problems like overfitting or overtraining (where the ANN memorizes more and learns less). It is a fact that for fully connected feed-forward networks (like the one developed here) there are some general guidelines for deciding how many neurons should be placed in the hidden layer. The data volume and the number of hidden neurons depend primarily on the nature of the data. More specifically, there are two main categories of data, the physical and the behavioral ones. For example, temperature, thermal conductivity, and pressure are physical data. ANN models of physical data need not be as constrained as behavioral models and do not require so much data or equivalently they can use more hidden neurons. This is certainly the case here, where the large number of hidden neurons can solve the problem of the small training data set (Neuralware 2001).

Various independent experiments were performed in this study in order to find out if overtraining has been caused due to the large number of iterations (200,000 times). Various independent ANNs (having the same structure) were developed that learn using much smaller numbers of iterations varying from 50,000 to 200,000. All these attempts resulted in various ANNs with R^2 always greater than 0.899, whereas the RMS error was always very low. These results can be seen in Table 2, thus proving that the high R^2 value and the low RMS error value are not proportional to the number of iterations. For example, in the 70,000 iterations, we have much better R^2 than the one with the 90,000 iterations. Thus the ANN performance would still be very high even if 50,000 or 70,000 cycles had been used. It should be mentioned that the default number of iterations is 50,000 for the Neuralworks package.

After formatting the ANN model, its topology had to be decided and thereafter, several tests were executed. Various ANN configurations were trained performing 200,000 iterations each time, using the same input data sets for all of them. The instruments measures (R^2 and RMS Error values) associated with the different ANN architectures that were applied in this phase are presented in Table 3, in order to indicate the superiority of the selected topology.

The selected ANN with the optimal performance had an input layer consisting of three processing elements (neurons) that correspond to the three input variables, the hidden layer consisted of three sub-layers and each sub-layer consisted of eleven neurons, whereas the output layer had only one neuron representing K_q. Figure 2 shows the architecture of the developed ANN.

TABLE 2. *The performance of the ANN for various numbers of iterations.*

Number of training cycles	R^2	RMS error
50,000	0.8997	0.0876
70,000	0.9976	0.0834
90,000	0.9722	0.0405
100,000	0.9761	0.0663
150,000	0.9966	0.0111
170,000	0.9996	0.0079
200,000	0.9994	0.0123

TABLE 3. *Instruments values for various ANN architectures tried in training phase with 200,000 iterations performed.*

Number of hidden layers	Number of neurons in each hidden layer	R^2	RMS error
1	6	0.9507	0.2092
1	10	0.9745	0.1215
1	11	0.9892	0.0678
1	15	0.9130	0.1289
2	6	0.98570	0.795
2	10	0.9822	0.0649
2	15	0.9557	0.1256
3	6	0.9842	0.1041
3	10	0.9871	0.0949
3	11	0.9994	0.0123
3	15	0.9970	0.0682

The optimal configuration was decided based on minimizing the difference between the ANN predicted values and the actual experimental data. The ANN behaved very well, giving a $R^2 = 0.9994$ in the training phase. The RMS Error of the ANN had a very low value that was equal to 0.0123. In the Confusion Matrix, all of the cells are located in the diagonal from the lower left to the upper right and also the CMC coefficient of the desired and actual output is 0.9994. This means that the results of the ANN and the experimental data are very close to each other and there exists a very good agreement between the predicted and the desired values of thermal conductivity. It should be clarified that if CMC was equal to 1 we would have a perfect match.

Figure 3 is a graphical representation of the instruments used in this project and it proves the high performance of the ANN and its credibility of prediction.

Table 1 lists (along with the experimental) the calculated K_q values by the MacLean and Siau equations and by the developed artificial neural network, during the testing phase. It is very important that in the testing phase, R^2 becomes

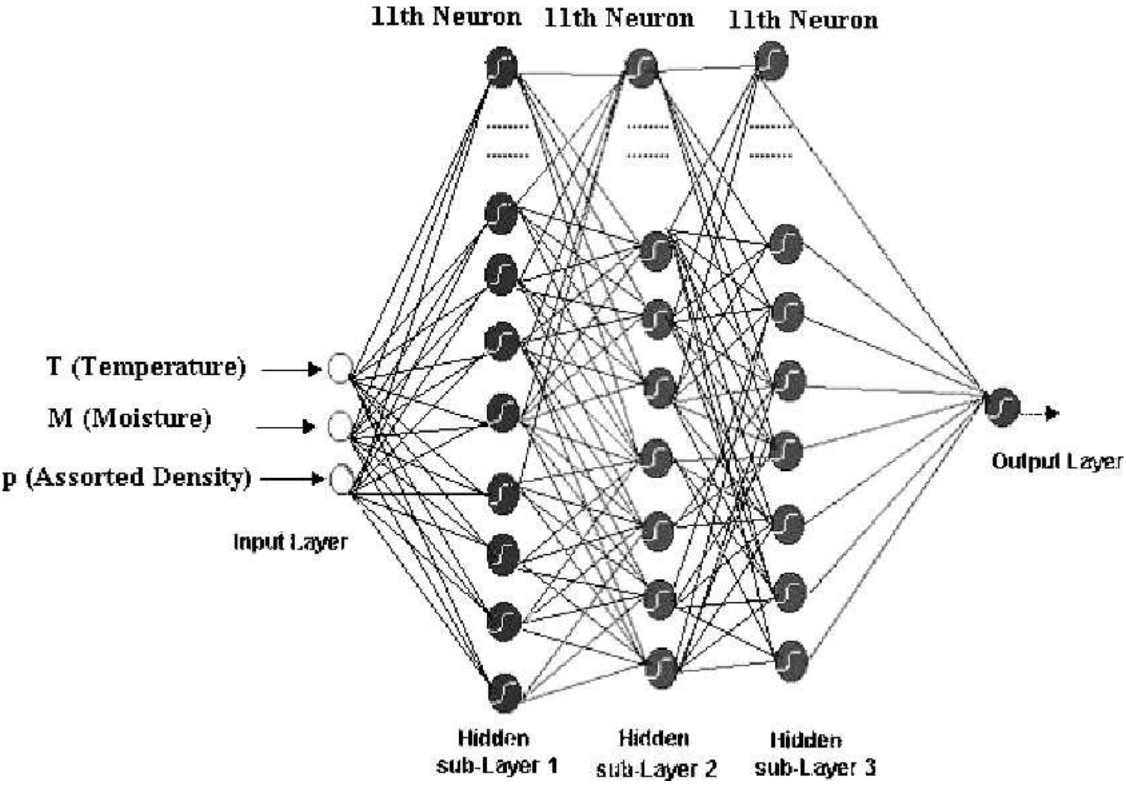

FIG. 2. Architecture of the developed wood thermal conductivity artificial neural network.

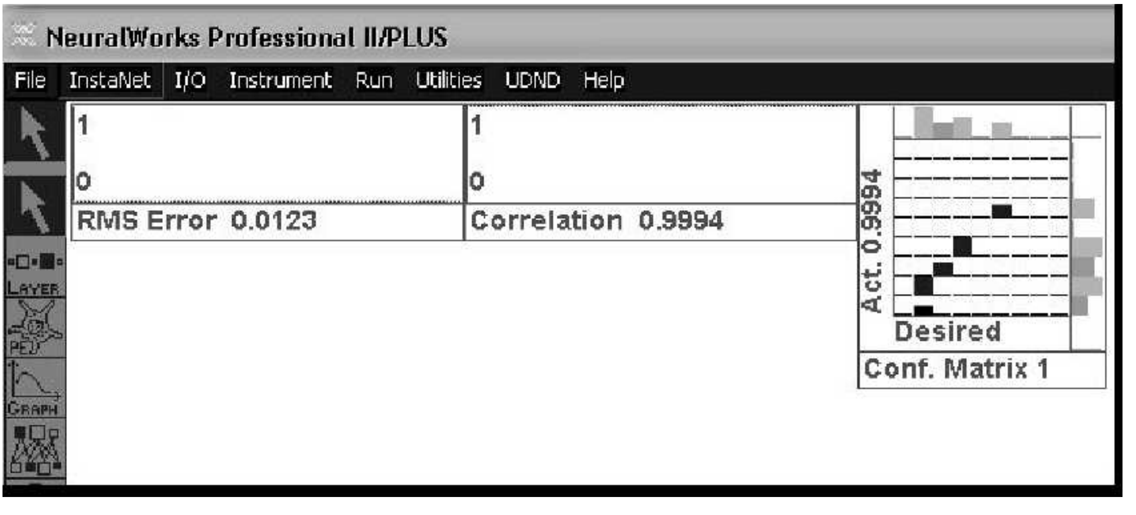

FIG. 3. The values and shape of the performance evaluation instruments of the artificial neural network in the training phase.

equal to 0.9070, which means that the predicted values by the ANN are very close to the actual ones. It is clear from the table that the calculated values by the three models, i.e., ANN, MacLean, and Siau, did exhibit anticipated trends as related to the three independent variables tested.

However, the deviation of the last two models from the experimental values is quite apparent in Table 1 and more pronounced in Fig. 4. In the latter, only at low K_q values from the MacLean and Siau models are close to the experimental and ANN ones, whereas at K_q of about 0.15 W/m K and thereafter the former two equations predictions spread out. However, the ANN predictions continue to remain close to the experimental ones with minor deviation at experimental K_q values above 0.32 W/m K.

CONCLUSIONS

In this exploratory work, an original artificial neural network is proposed that could be used in predicting the thermal conductivity in wood as a function of density, moisture content, and temperature. The optimal network was determined to consist of an input layer, three hidden layers, and one output layer following the feed forward network structure and more specifically the back-propagation algorithm. Each of the three hidden layers of the ANN consisted of eleven neurons.

The development of the ANN was described and its powerful predictive capacity was demonstrated by comparing it to steady-state thermal conductivity data for various wood species obtained from the literature and calculated values from two empirical equations. A Neuralworks software package was used for the determination of the ANN's structure and architecture and for the training and testing phase. In the training phase the instruments of the software have produced a value of R^2 equal to 0.9994 and the RMS Error was equal to 0.0123, whereas in the testing phase the R^2 value remained still very high and it was equal to 0.9070. The developed ANN model has proven to be a reliable approach towards the estimation of thermal conductivity and it can be used by researchers under a wide range of conditions.

It is well understood that this is a first major step in exploring neural networks as possible predictors of the thermo-physical wood properties. A need for further testing with a wider experimental database is paramount. More work toward this objective is under way.

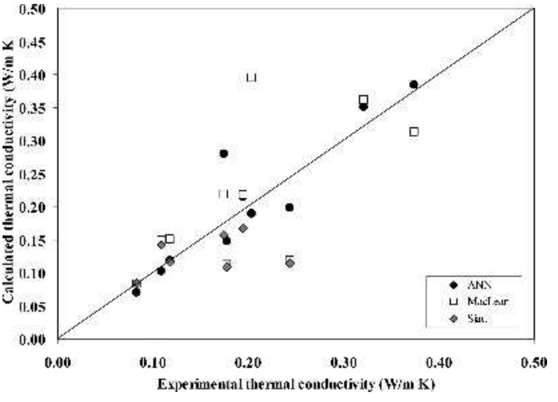

FIG. 4. Comparison of the experimental to the calculated thermal conductivity data by the ANN ($R^2 = 0.9994$) and the two equations.

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