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Predicting the effective thermal conductivity of dry granular media using artificial neural networks

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Abstract

Thermal conductivity of heterogeneous materials is a complex function of not only properties and amounts of constituents, but also of many structural factors. Experimental measurements are time-consuming processes, so it is justifiable to replace laboratory tests with prediction methods. An attempt to predict thermal conductivity of granular media using an Artificial Neural Network (ANN) model is undertaken in the paper. It was assumed that it is a function of a ratio of thermal conductivities of the constituents, medium porosity as well as coordination number describing the mean number of the nearest neighbours to each grain. Several configurations of the ANNs were tested while developing the optimal model. As a measure of prediction accuracy, the coefficient of linear regression and the mean squared error were used. The optimal model of ANN was found to consist of three hidden layers with eight neurons in each layer for both types of media. Some problems associated with application of ANN were discussed. The predicted values of thermal conductivity obtained with ANN were compared with values calculated from an analytical formula. It was found that the ANN predictions show identical trends and similar values to the analytical formula for all factors affecting thermal conductivities of the granular media. Since analytical formula work is suitable only for a narrow range of properties of granular materials, it is recommended to use ANN as a supplement for a wider range.

Keywords: Granular materials, Thermal conductivity, Prediction, Artificial neural network (ANN)

1. Introduction

Granular media are types of heterogeneous materials which appear in many engineering aspects. Granular media are here understood as heterogeneous materials made of loose grains that can touch fluids that fill the empty spaces between grains [1]. Sand, soil, agricultural products and thermal insulations serve as examples. Many other such materials are widely used in civil engineering, metallurgy, agriculture or the chemical industry. The thermal properties of such materials are very important in every task whenever heat transfer processes are considered. Thermal conductivity of heterogeneous materials is considered to be an effective, macroscopic value. This thermal property depends not only on thermal properties of constituents, their volume fractions and their microscopic properties but also on the way the constituents are distributed in the material. Therefore, heterogeneous materials made of the same con-

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stituents and in the same proportions usually have different thermal conductivity values. Experimental determination of thermal properties is very expensive, tedious and time-consuming, thus noting the dependence of thermal conductivity on the microstructure, predictions methods are of great interest. Two groups of prediction methods can be found in the literature. The first group assumes a simplified microstructure of the heterogeneous material with the most characteristic features of the original material retained [2, 3]. The simplified geometry is subsequently used to predict thermal conductivity of these materials using either analytical or numerical techniques. The second group of methods is based on an approximation of experimental results. Here too the main factors affecting thermal conductivity of the particular heterogeneous material should be selected and a relationship between thermal conductivity and these factors is sought to obtain the best fit with the experimental data. This group of methods encompasses predictions based on the Artificial Neural Network (ANN).

A review of the literature revealed that the ANN has been used to date for predicting the thermal conductivity of such heterogeneous materials as food, textiles and rocks [4–9]. Fayala [4] used ANN to predict the thermal conductivity of a knitting structure as a function of porosity, air permeability, yarn conductivity and weight per unit area. A suitable ANN was used to predict the thermal conductivity of pistachio [10]. ANN modelling has been successfully applied to the prediction of thermal conductivity of fruits and vegetables [11] and bakery products [6]. Finally the ANN was used to predict the thermal conductivity of sedimentary rocks from a set of geophysical well logs [12, 13]. The review showed that no considerable effort was directed toward prediction of thermal conductivity of granular materials. Therefore, this task was undertaken in the present paper.

Heat transfer in granular media is a complex phenomenon with many heat transfer modes involved simultaneously. Heat conduction occurs in the grains and gas-filled pores (also water-filled pores, but in this paper only dry granular media was discussed). Heat is also directly transferred through points of contact between adjacent grains. Moreover, it may also be conducted through a fluid filling the space in surface roughness zones of the contact area between particles. The heat flow lines are here mainly constricted to the contact spots due to the higher conductivity of grains than of the gas filling the pores. In fluid filled pores convection can be present if the pores are large enough. If the gas in the pores is transparent then radiation heat transfer can also arise (appearing by increased effective thermal conductivity). The effective thermal conductivity of dry granular media therefore depends on:

- thermal conductivity of medium components
- volume fraction of each component
- way of distribution of particles (configuration), size of contact area between particles and their diameter
- pressure of fluid phase
- surface roughness of particles affecting contact resistance between particles
- active external loads affecting the contact area
- radiative properties of particle surface
- temperature level

As the list of factors affecting thermal conductivity of dry granular media is a long one, finding the universal correlation seems difficult. However if a large enough set of experimental data exists, the ANN approach may prove very efficient.

2. Neural network for dry granular media

An artificial neural network is an algorithm mathematically modelling the learning process from examples through iteration, without requiring a prior knowledge of the relationships between process parameters [14]. It is, therefore, based on concepts inherent in the learning processes of brains [15]. Neural network modelling is becoming an interesting and effective method in the estimation and prediction of thermal properties. Major advantages of the ANN are efficient management of uncertainties, noisy data and highly non-linear relationships in data [16]. The process of developing a neural network model involves:

- generation of (or compilation of available) experimental data on thermal properties and forming a database. The database should also contain all available information about properties of constituents, their way of distribution and other factors listed above that affect thermal properties,
- training of a neutral network,
- finding neural network architecture to enable selection of an optimal configuration,
- validation of the optimal ANN model with a data set which was not used in training.

Many experimental data on thermal conductivity of heterogeneous media presented in the literature did not include details on material characteristics (e.g., thermal properties of constituents, full characteristics of their microstructure). Therefore, selection and compilation of the respective data which can be used for the ANN is a very complicated process. In the present paper the experimental data for dry granular materials were taken only from the paper by Crane and Vachon [12], because the provided data set was sufficient. They gathered and verified copious data taken from literature on the thermal conductivity of this type of material. Their paper was used to form a database suitable for ANN training. As many factors affect the thermal conductivity of granular materials, the major difficulty in creating a prediction model for these materials was making a wise choice of factors that influence it significantly and disregarding those whose impact on thermal conductivity can be ignored. Before creating the ANN model for dry, granular media some simplifications were made, namely that the medium was two-component with grains distributed in a fluid, all grains had the same, spherical shape of equal diameter and did not overlap. Thus it was assumed that the general relationship between effective thermal conductivity takes the following form:

$$k_{ef}/k_f = f\left(\varepsilon, \ln\left(k_s/k_f\right), N_c\right) \tag{1}$$

with k_s thermal conductivity of discontinuous phase (solid grains), k_f thermal conductivity of the continuous phase filling the pores, ε porosity and N_c – the mean coordination number of grains being the input parameters. The mean coordination number is in general an independent element of the microstructure description, but some attempts have been made to correlate it to the porosity of the medium and to show this relationship in an analytical form. One of the formulae which depict this relation is known as Jeremiejev's formula:

$$N_c = \frac{2 + \varepsilon + \sqrt{(1-\varepsilon)(9-\varepsilon)}}{2\varepsilon} \tag{2}$$

Comparison of this formula with experimental data was carried out in [6]. Using the mean coordination number as an independent variable in eq. (1) helped the ANN to find a more accurate approximation of the relationship between the effective thermal conductivity and porosity of the material. This smoothed the progress of learning by the network, because the additional, known coupling between input parameters made it simpler for the ANN to find its optimal configuration [17, 18]. Application of the natural logarithm of the thermal conductivity ratio of material constituents instead of simply the respective ratio allowed one to decrease the scope of variation in this input variable and helped in predictions.

For dry granular materials several neural networks models with different structures were developed. Their input layer consisted of three neurons which corresponded to: logarithm of continuous to dis-

Table 1: Summary of ANN tested architecture effects for dry granular materials

Number of hidden layers	Number of neurons on each hidden layer	MSE, 10^{-3}	R
2	4	0.185	0.58
2	6	0.773	0.74
2	8	0.191	0.68
2	10	0.389	0.72
2	12	0.827	0.61
3	2	0.855	0.45
3	4	0.732	0.32
3	6	0.269	0.77
3	8	0.621	0.89
4	2	0.868	0.82

continuous thermal conductivity ratio of the constituents, porosity and the mean coordination number. The number of hidden layers was varied between 2 and 4 with an increment of 1, while the number of neurons within each hidden layer was varied between 2 and 8 with an increment of 2 – see Table 1. This resulted in a total of 12 networks. The authors' concept was that if the number of inputs is odd then the number of neurons should be even to better blur responsibility in the ANN between layers and neurons and to make the network resistant to fault. The subsequently mentioned ANN models were trained for 200 epochs (increasing the number of training epochs to almost 1000 showed that the ANN start to memorize instead of learn) using approximately 70% of the given thermal conductivity data [12]. All of them were fed-forward and the back-propagation algorithm was utilized in the learning process [5]. The back-propagation algorithm uses the supervised learning technique, where the network weights and biases are initialized randomly at the beginning of the training phase (which leaves room for further improvement [19]). As the activation function, the hyperbolic tangent function was used for all of the hidden layers. This structure enables the network to achieve better results in less time. The output layer had one neuron representing the ratio of the effective thermal conductivity of the granular medium to the fluid thermal conductivity. For a given set of inputs to the network, the response of the output layer was calculated and compared with the corresponding desired output response. Design and training of the networks was carried out using the MatLab programming environment 7.10.0 (version R2010a) with Neural Networks Toolbox.

Selection of the optimal ANN configuration was carried out by determination of the hidden neuron number. When the neural network had too few hidden neurons, the model complexity was not sufficient to extract the deterministic relationship between the input variables and the outputs. On the other hand, a neural network with excessive hidden neurons could precisely adjust the training data and fit the noise present in the data, but gave the ANN predictions deprived of physical connotation. Therefore, its performance depended largely on the particular training set.

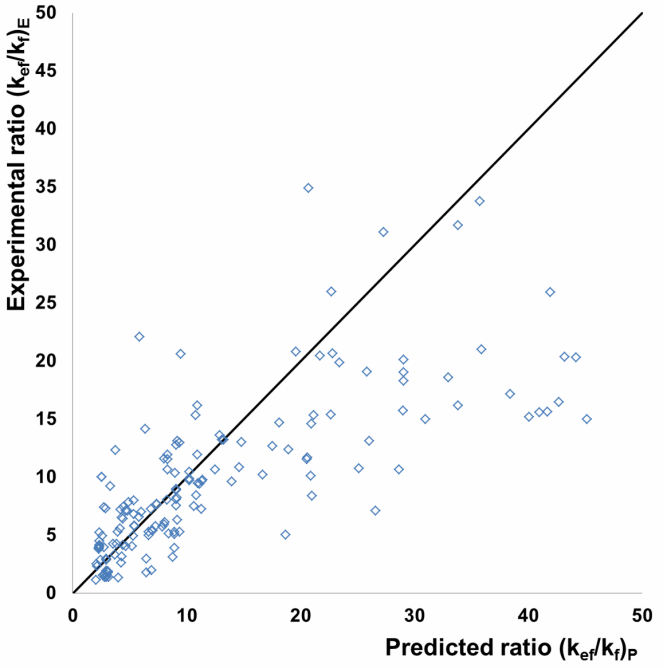

Figure 1: Illustration of ANN training effects for dry granular materials built from 3 hidden layers with 8 neurons in each layer

Two parameters were used to compare network usefulness in prediction of thermal conductivity after training. The first one was the Mean Squared Error (MSE). It is defined as the arithmetic mean of the squared differences between outcome (predicted effective thermal conductivity – index P) and the expected values (experimental effective thermal conductivity – index E).

$$MSE = \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=0}^{m}\left(\left(\frac{k_{ef}}{k_f}\right)_E - \left(\frac{k_{ef}}{k_f}\right)_P\right)^2 \qquad (3)$$

The smaller the value of this parameter the more accurate the network is in predicting the effective thermal conductivity of the granular medium. The second chosen parameter was R which describes the linear regression line between the predicted values from the ANN model. When the parameter R is equal to 1, this means that the accurate relationship is obtained. Similarly, when it is close to zero this denotes that no clear relationship was obtained. This parameter can also be understood as the tangent of the linear function that approximates the correlation between the outcome and expected values.

It was found out that the best ANN architecture for predicting the effective thermal conductivity of dry

granular materials was built from three hidden layers with eight neurons in each layer – Table 1. Training and selection of the optimal ANN make it possible to obtain a list of weights, describing the connections between neurons. That list can be applied in a spreadsheet to obtain a very accurate tool for predicting the thermal conductivity of granular materials.

The rest of the experimental data set of thermal conductivity (circa 30% per cent of the whole database values) was used for validation of the chosen network model. Fig. 1 presents a graph of convergence. It shows how close these network responses were to the expected values. The more experimental the data in Fig. 1, the closer to the solid line, the more predictive the ANN model is. Although it may seem that there is a lot of scattering in the data set, the value of MSE and parameter R suggest that ANN performs well.

3. Analytical formula to predict thermal conductivity

Several analytical formulae were proposed in the past to predict the effective thermal conductivity of heterogeneous materials consisting of spherical inclusions distributed in the matrix. They may roughly be divided into three groups. The first group contains exact formulae for regular or random arrangement of spheres, which are valid either for a small fraction of inclusions or when the inclusions are not touching, i.e., for the so-called "well-separated" case. The second group is formed by formulae in which inclusions are ordered in space and touching but the assumed or calculated temperature distribution in the medium used for prediction is approximate. In the last, third group the spherical inclusions appear in a regular arrangement, but they may be close to each other. The prediction of temperature distribution can essentially be achieved to any degree of accuracy, but major problems appear for touching and highly conductive inclusions. A different formula for random and touching spherical inclusions was proposed by Furmanski et al. [20]. The formula is derived from the general expression linking the mean, statistically averaged heat flux in the medium with the heat flux distribution on the part of inclusion surface close to the neighbour inclusion:

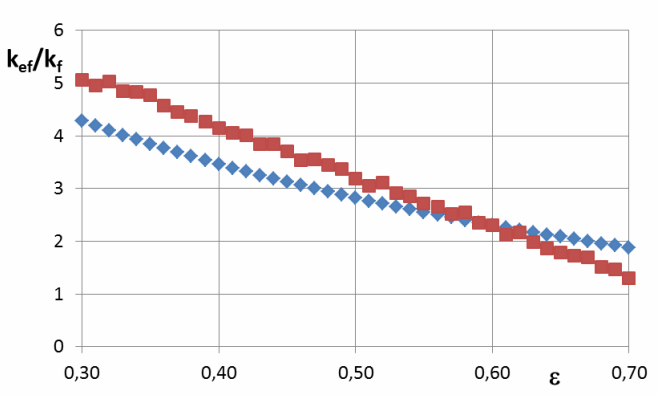

Figure 2: Ratio of effective thermal conductivity to conductivity of continuous phase versus porosity (ε): □ – ANN predictions, ◊ – from eq. (6)

$$-\{q\} = k_{ef} \cdot \nabla\{T\} = k_f \nabla\{T\} \\ -\frac{(k_s - k_f)}{k_s} \tilde{n}_s N_c \left\{ \int_{A_k} (q \cdot n)(r \cdot n_k)\, dA\, n_k \right\}^* \tag{4}$$

where $\tilde{n}_s$ is the inclusions density, i.e., number of inclusions per unit volume of the medium; n_k – unit vector along the line joining two neighbour inclusions while n is the unit vector normal to the inclusion surface. The statistical averaging $\{\}^*$ is carried out over all possible location of inclusions in the medium when location of the considered "selected" inclusion is fixed. In order to obtain formula for the effective thermal conductivity of the granular medium the heat flux distribution on part A_k of the surface of this inclusion should be known – see eq. (4).

The solid grains usually have greater thermal conductivity than the surrounding fluid and therefore the heat flow lines are concentrated in the place where the inclusions surface is the closest.

An approximate formula for the sought heat flux on the inclusion surface may be found by assuming unidirectional heat flow between two neighboring inclusions according to the method presented in [20]. This allows the following formula to be written for the effective thermal conductivity of the granular medium:

$$\frac{k_{ef}}{k_f} = 1 + \frac{(\sigma_s - 1)(1 - \varepsilon) N_c D_c}{\sigma_s [3N_c\eta - 2(N_c - 2) - N_c\eta^3]} \tag{5}$$

where the symbol η denotes consolidation factor describing a degree of particle merging [6]. For no

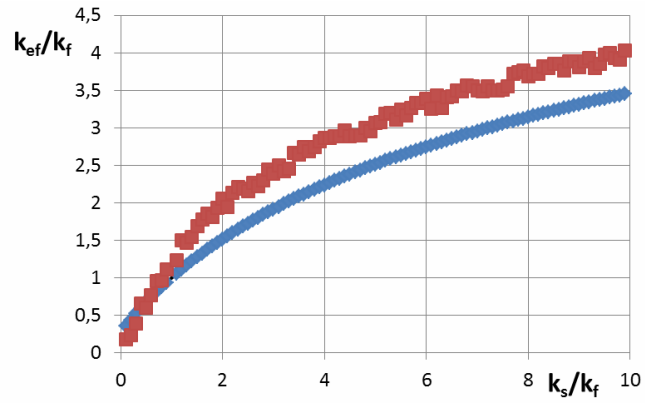

Figure 3: Ratio of effective thermal conductivity to conductivity of continuous phase versus ratio of conductivities of discontinuous and continuous phase ($\varepsilon = 0.4$ $k_s/k_f < 10$): □ – ANN predictions, ◊ – from eq. (6)

merging of particle, i.e., $\eta = 1$, the formula can be simplified to:

$$\frac{k_{ef}}{k_f} = 1 + \frac{(\sigma_s - 1)(1-\varepsilon) N_c D_c}{4\sigma_s} \qquad (6)$$

where:

$$\sigma_s = \frac{k_s}{k_f}, \quad C_c = \frac{\sigma_s}{(1-\sigma_s)},$$

$$D_c = 2C_c \ln\left(\frac{C_c + 1}{C_c + 1 - \frac{2}{N_c}}\right).$$

4. Results

The effective thermal conductivity of the heterogeneous medium should satisfy some physical conditions. First of all for the same values of thermal conductivity of constituents the ratio we have to deal with a homogeneous medium, i.e., $k_{ef}/k_f = 1$while for $\sigma_s > 1$ the effective thermal conductivity should be smaller than the thermal conductivity of solid grains, i.e., for $k_{ef}/k_f < \sigma_s$. As the artificial neural network does not know anything about these physical limitations, if the experimental data set is not dense enough close to $k_s/k_f = \sigma_s = 1$ it can show wrong predictions in the region. In order to better adjust to the available data, the set was additionally split into subsets corresponding to $k_s/k_f = \sigma_s < 10$ – Fig. 3 and $k_s/k_f = \sigma_s > 10$ – Fig. 4, respectively.

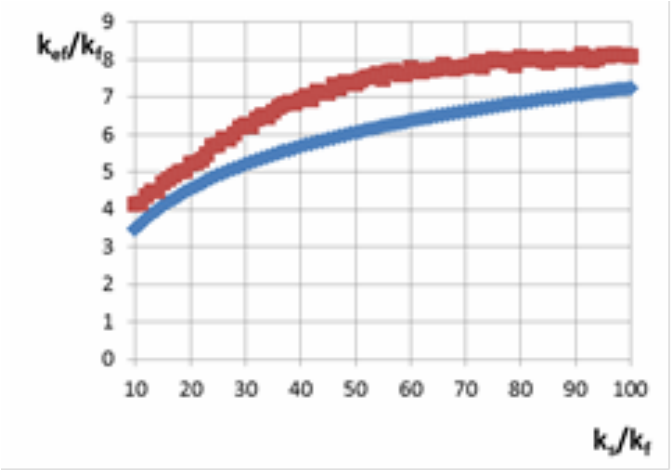

Figure 4: Ratio of effective thermal conductivity to conductivity of continuous phase versus ratio of conductivities of discontinuous and continuous phase ($\varepsilon = 0.4$ $k_s/k_f > 10$): □ – ANN predictions, ◊ – from eq. (6)

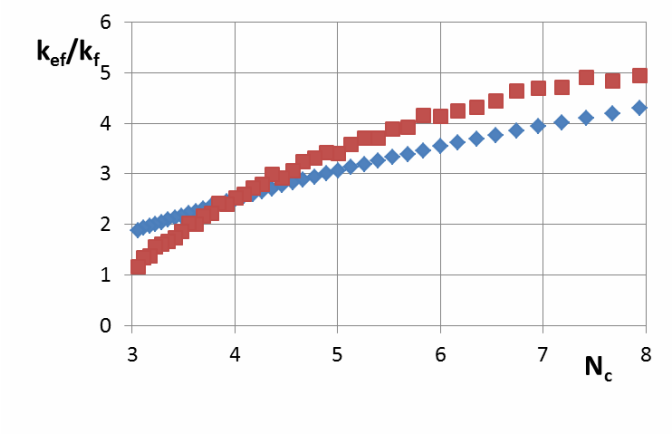

Figure 5: Ratio of effective thermal conductivity to conductivity of discontinuous phase versus mean coordination number of grains ($k_s/k_f = 10$): □ – ANN predictions, ◊ – from eq. (6)

The effective thermal conductivity increases alongside the increase in the ratio of the thermal conductivity of grains to the thermal conductivity of the fluid. For $k_s/k_f > 10$ the ANN results are more divergent from the analytical formula than for $k_s/k_f < 10$– see Fig. 3 and 4.

Fig. 5 shows variation of the effective thermal conductivity with the coordination number. For a two-phase composite with regularly arranged spherical inclusions the coordination number is independent of the inclusion volume fraction and the effective thermal conductivity is greater if the value is lower. For granular material with touching grains the reverse is

true, as can be observed in Fig. 5. Moreover, for approximately for the ANN predictions give higher values for the effective thermal conductivity than the values following from equation (6).

5. Conclusions

Predicting the thermal conductivity of heterogeneous materials is difficult primarily due to the many, complex structural factors affecting its value and the different properties of their constituents. The main objective of this paper is to verify how the ANN copes with this task in the case of dry granular materials. Once trained and optimized, the ANN can serve as a complete tool for finding correlations between various factors of the material and its thermal conductivity. However, some problems can arise with finding the proper correlation due to the ANN not adjusting to the physical limitations imposed on the effective thermal conductivity. The ANN predictions need a sufficiently dense experimental data set supplemented with information on properties and the manner of distribution of their constituent parts. Any additional correlations between factors affecting effective thermal conductivity, e.g., between the mean coordination number and porosity, can contribute to better accuracy of the ANN approximation. The predicted values of thermal conductivity obtained with the ANN were compared with values calculated from an analytical formula proposed earlier in the literature for granular media. It was found that the ANN predictions and results following from the analytical formula are qualitatively consistent and show similar values for all factors influencing thermal conductivities of the granular media.

The main advantage of the ANN model is that it may be used to provide an excellent tool for prediction of thermal properties, regardless of the number of factors.

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References

[1] W. Gogół, A. Próchniak, Thermal conductivity of granular materials, Bulletin of Institute of Heat Engineering 50 (1977) 1–42.

[2] A. Gemant, The thermal conductivity of soils, Journal of Applied Physics 21 (1950) 750–752.

[3] F. Gori, S. Corasaniti, Theoretical prediction of the soil thermal conductivity at moderately high temperatures, ASME Journal of Heat Transfer 124 (2002) 1001–1008.

[4] F. Fayala, H. Alibi, S. Benltoufa, A. Jemni, Neural network for predicting thermal conductivity of knit materials, Journal of Engineered Fibers and Fabrics 3 (4) (2008) 53–60.

[5] K. Hornik, M. Stinchcombe, H. White, Multilayer feedforward networks are universal approximators, Neural Networks Comput. 2 (5) (1989) 359–366.

[6] S. S. Sablani, O.-D. Baik, M. Marcotte, Neural networks for predicting thermal conductivity of bakery products, Journal of Food Science 52 (2002) 299–304.

[7] T. N. Singh, S. Sinha, V. Singh, Prediction of thermal conductivity of rock through physico-mechanical properties, Building and Environment 42 (1) (2007) 146–155.

[8] D. J. Scott, P. V. Coveney, J. A. Kilner, J. C. H. Rossiny, N. M. N. Alford, Prediction of the functional properties of ceramic materials from composition using artificial neural networks, Journal of the European Society.

[9] S. S. Sablani, M. S. Rahman, Using neural networks to predict thermal conductivity of food as a function of moisture content, temperature and apparent porosity, Food Research International.

[10] R. A. Chayjan, G. A. Montazer, T. T. Hashjin, M. H. Khoshtaghaza, B. Ghobadian, Prediction of pistachio thermal conductivity using artificial neural network approach, International Journal of Agriculture & Biology 9 (2007) 816–820.

[11] A. M. Hussain, M. Rahman, Thermal conductivity prediction of fruits and vegetables using neutral networks, International Journal of Food Properties 2 (1999) 121–138.

[12] R. A. Crane, R. I. Vachon, A prediction of the bounds on the effective thermal conductivity of granular materials, International Journal of Heat & Mass Transfer 20 (1977) 711–723.

[13] B. Goutorbe, F. Lucazeau, A. Bonneville, Using neural networks to predict thermal conductivity from geophysical well logs, Geophysical Journal International 166 (1) (2006) 115–125.

[14] M. C. Bishop, Neutral network and their applications, Review in Scientific Instruments 64 (1994) 1803–1831.

[15] J. E. Dayhoff, Neural Networks Principles, Prentice-Hall International, 1990.

[16] T. Khanna, Foundations of Neural Networks, Addison-Wesley Publishing Company, 1990.

[17] T. N. Singh, Artificial neural network approach for prediction and control of ground vibrations in mines, Mining Technology (Trans. Inst. Min. Metall. A) 113 (2004) A251–A257.

[18] T. N. Singh, A. K. Verma, Prediction of creep characteristics of rock under varying environment, Environmental Geology 48 (2005) 559–568.
[19] S. Sinha, T. Singh, V. Singh, A. K. Verma, Epoch determination for neural network by self organized map, Computational Geosciences 14 (2010) 199–207.
[20] P. Furmański, T. Wisniewski, P. Łapka, Study on a degree of degradation of design materials under different ambient interactions, in: W. Kurnik (Ed.), Nonconventional materials in diagnostics and active reduction of vibration, Scientific Publications of Institute of Exploitation Technology, Warsaw–Radom, 2008, pp. 207–233, in Polish.
[21] S. Azizi, C. Moyane, A. Degiovanni, Approche experimentale et theorique de la conductiveite thermique des milieux poreux humides, International Journal of Heat & Mass Transfer.
[22] K. W. Jackson, W. Z. Black, A unit cell model for predicting the thermal conductivity of a granular medium containing an adhesive binder, International Journal of Heat and Mass Transfer.
[23] R. N. Pande, F. Gori, Effective media formation and conduction through unsaturated granular materials, International Journal of Heat and Mass Transfer.
[24] A. Stefański, Thermal conductivity of civil engineering materials, Polish Scientific Publisher PWN, 1975, in Polish.
[25] V. R. Tarnawski, W. H. Leong, Thermal conductivity of soils at very low moisture content and moderate temperatures, Transport in Porous Media 41 (2) (2000) 137–147. doi:10.1023/A:1006738727206.