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# Modelling the effective thermal conductivity of an unidirectional composite by the use of artificial neural networks

Ignacio J. Turias [a,*], José M. Gutiérrez [b], Pedro L. Galindo [a]

[a] *Department of Computer Science – Research Group "Intelligent Systems", Escuela Politécnica Superior de Algeciras, University of Cádiz, Avda. Ramón Puyol, s/n 11202 Algeciras (Cádiz), Spain*

[b] *Department of Applied Physics – Research Group "Composite Materials", University of Cádiz, Spain*

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**Abstract**

This paper explores the application of pattern recognition and artificial intelligence techniques in the characterization of a multiphase realistic disordered composite and in the design of a multiple regression model to estimate effective thermal conductivity. An image database of computer simulated microstructures was generated. Some descriptors based on boundary and area shapes of Voronoi cells were extracted for each fiber distribution. Several approaches have been used to reduce the high original dimensionality. Selected features can be introduced as inputs in a multiple regression model. This procedure provides an alternative to the finite element method for the computation of effective thermal conductivity. Different regression models (classical and neural approaches) have been considered and a randomised resampling procedure has been designed in order to choose the best estimation model from a statistical point of view.


*Keywords:* B. Microstructure; B. Modelling; B. Thermal properties; Artificial neural networks

## 1. Introduction

The properties of unidirectional aligned fiber reinforced composites depend on: (i) properties of each phase (matrix and reinforcement conductivities), (ii) fiber volume fraction, (iii) geometrical arrangements. The spatial arrangement of fibers or microstructure is usually not uniform, and its nature is linked to the processing techniques used for making the composites. Understanding of the microstructure-property relationships is a necessary step in an effective component design and fabrication, and in the prediction of component behaviour and life.

The approaches in the literature either idealize the arrangements as being ordered arrays described by a repeating unit cell [1,2] or simulate disordered arrangements by statistical means and correlation functions [3,4].

Determination of the effective thermal properties of composites is crucial for a successful design and for the manufacture of materials. The effective thermal conductivity of a composite in normal direction to the fiber axes has been the specific objective to study. This paper focuses in (iii), specifically considering regular distributions of fibers (rectangular, squared, and hexagonal arrays), and exploring realistic composites microstructures generated through computer simulations adding "noise" to the positions of fibers centres of each regular array distribution.

In this work, the first step was the computer generation of simulated artificial microstructures. The ANSYS program (copyright by SAS IP, Inc.) was used to compute the transversal effective thermal conductivity by the finite element method (FEM).

* Corresponding author. Fax: +34 956 028 014.
*E-mail address:* ignacio.turias@uca.es (I.J. Turias).

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Application of Voronoi tessellation of a planar two-phase composite has been explored in order to quantify a composite microstructure. Several techniques based on automated image pattern recognition have recently been introduced for characterizing composites microstructures. Among them, it is necessary to underline the important contributions made by Brockenbrough et al. [5], Everett and Chu [6], Pyrz [7], and Ghosh et al. [8,9], where Dirichlet tessellation has been used as a tool in the characterization. This characterization it is based on a set of computed descriptors of the corresponding Voronoi cells. An alternative approach was proposed by Pitchumani [10] based on fractal geometry.

Firstly, in this paper the computed descriptors are used in order to distinguish or classify among different distributions. Secondly, they are used as inputs to a regression model which computes an estimation of the transverse effective thermal conductivity of a composite. In this way, it will be shown how it is possible to use a multiple regression approach based on artificial neural networks (ANNs) as an alternative method to FEM.

Two methods of dimensionality reduction are discussed: (1) Fisher's linear discriminant, which aims to achieve an optimal linear dimensionality reduction maximizing a criteria which is discussed in depth in Fukunaga [11] and, (2) principal components analysis (PCA), which extracts the most relevant features, leaving the redundant information behind, but trying to preserve as much of the relevant information as possible. PCA is also called Karhunen–Loéve transformation and is discussed at length in Jollife [12].

As well as this, it is necessary the multiple comparison of the different regression models proposed [13–15]. In order to make inferences about population means, a randomised data collecting procedure has been designed. Analysis of variance (ANOVA) test [16] allows to reject the null hypothesis that the means of the groups are all equal, but it does not pinpoint where the significant differences lie. Bonferroni method [17] has been used in order to compare the models while controlling the probability of making at least one Type I error (or null hypothesis false when it is true).

The different preprocessing methods have been combined with several topologies of backpropagation feed-forward neural networks [18] and together with classical multiple linear regression (MLR). Furthermore, in order to obtain the best possible results, a classification process has been applied previously to discriminate between realistic hexagonal samples and realistic rectangular/squared samples. Then, a separate regression model has been designed for each class, trying to improve the estimation done with only one regression model for the whole set of samples. Thermal conductivities obtained with FEM are referred to as the exact values, and serve as a benchmark for comparison with results of the proposed regression methods.

In the following section, the database creation procedure which will be used in this work, will be formulated. Section 3 discusses the methods used in order to characterize each composite sample. The primary objective of Section 4 is to present the feature selection algorithms used to achieve dimensionality reduction. Formulation of the estimation problem as a regression system is introduced in Section 5. The well-known regression model is briefly outlined in Section 5.1, and the artificial neural network approach is presented in Section 5.2. Section 6 discusses the experimental procedure developed to assure the best generalization performance of the models. These models will be analysed and compared by the way of statistical methods in Section 7. Finally, the conclusions are exposed in Section 8.

## 2. Database calculation of transverse effective thermal conductivity

The fundamental theory of transverse effective conductivity was given by Maxwell [19], in the frame of electrical properties. This classical model can be considered as a first-order approximation because it is assumed that the thermal interaction between fibers is negligible. This implies that the model is valid only for dilute volume fractions. In later publications, the prediction of the classical model was obtained from different points of view. In this context, the models of Hashin [20], based on the self consistent scheme (SCS), and Behrens [1], based on the method of long waves, are well known. The complexity of the models increases when high fiber volume fractions are considered. In these cases, interactions terms must be introduced [21,22].

Another possibility to determine the effective properties is based on the unit-cell approach. This approach assumes a regular arrangement of fibers, but it allows considerations of symmetry conditions and hence the analysis remains limited to unit-cell. In this scope, several formulas can be obtained from series-parallel or parallel-series configurations of thermal resistances. Considering that the flow of heat in the unit cell is perturbed by different properties, these unidimensional approximations are only valid in cases of weak perturbation [23]. Therefore, the solution of the boundary value problem using numerical methods is a more rigorous procedure. Different approximations can be found in the literature such as the ones based on the finite difference method [24], the finite element method [23,25], the boundary collocations points [2,26,27] and the boundary element method [28].

The output $K_{ey}$ can be found out for each composite microstructure from Fourier's law solution through MEF [29] setting a thermal gradient unity (see Fig. 1). Fourier's law establishes (where $A$ is the area, and $u$ is the temperature),

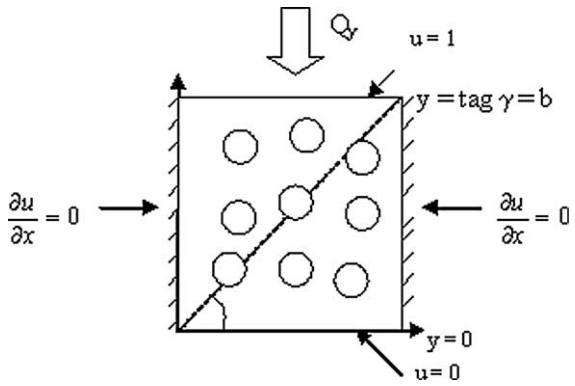


Fig. 1. $K_{ey}$ measurement based on Fourier's law, setting a thermal gradient unity in a composite microstructure ($u$ means temperature).

$$Q_y = -K_{ey} A \frac{\partial u}{\partial y}. \quad (1)$$

In order to generate the database of microstructures, the conductivity ratio fiber/matrix was fixed to 10 and the volume fraction fiber/matrix was considered equal to 25%. Each composite microstructure was limited to a $256 \times 256$ pixel resolution. Three different patterns of regular periodic arrangements were considered: squared array (five samples), rectangular array (20 samples) and hexagonal array (25 samples). For each sample, a set of 10 additional disordered microstructures has been obtained by addition of random noise to the coordinates $(x, y)$ of each fiber centre, resulting a set of 500 artificial (but realistic) disordered microstructures (see Table 1). The value of the introduced random noise was 10% at maximum of the inter-fiber distance in the original regular array. This randomness was applied to the 100% of the fibers in the distribution. Microstructures with overlapping in fiber locations were discarded. This database of artificial microstructures can be considered coherent [30] with the universe of the realistic microstructures which can be found in practice (see Fig. 2).

Table 1
Number of samples in each class of arrangements

| Samples | Type of fiber distribution |
|---|---|
| 1–5 | Regular square arrangement |
| 6–25 | Regular rectangular arrangement |
| 26–50 | Regular hexagonal arrangement |
| 51–100 | Disordered square arrangement |
| 101–300 | Disordered rectangular arrangement |
| 301–550 | Disordered hexagonal arrangement |

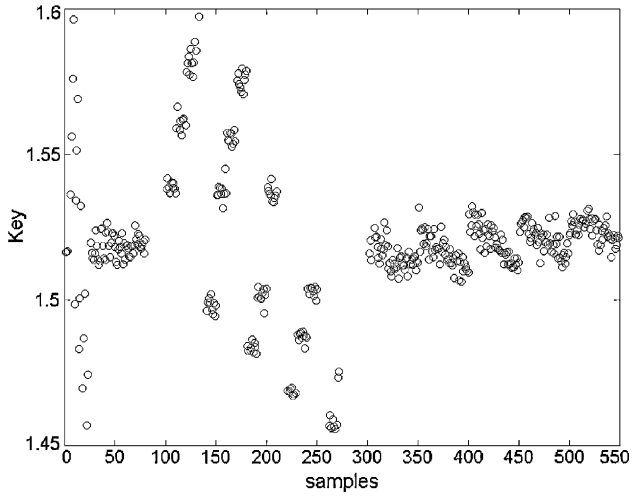


Fig. 2. $K_{ey}$ values for the database samples.

## 3. Quantitative characterization

The Dirichlet tessellation allows finding out the "natural regions" of immediate influence of each fiber as

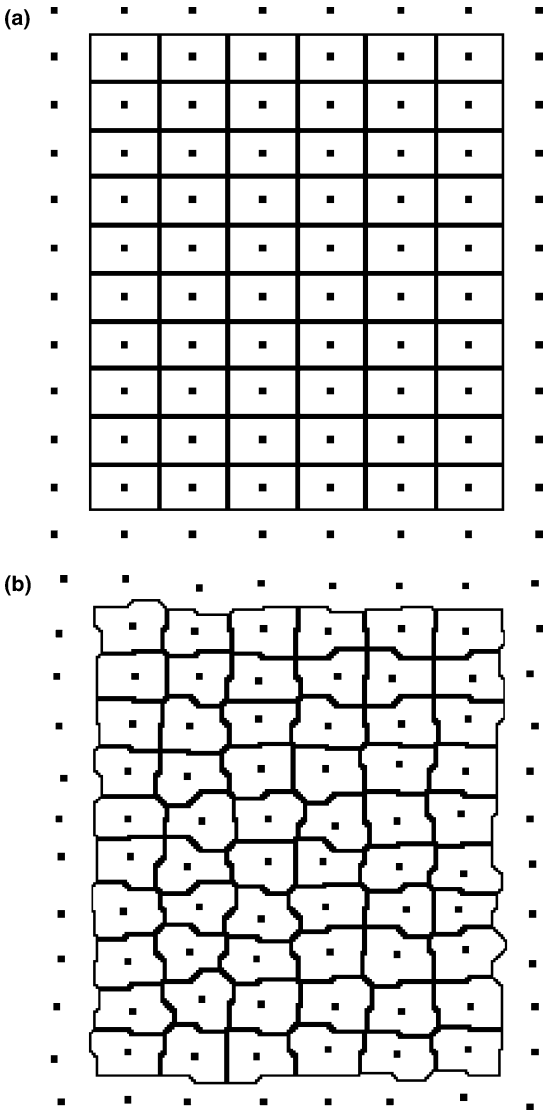


Fig. 3. Voronoi cells for two different microstructures: (a) regular, (b) disordered. The database contains 550 microstructures (50 regulars + 500 disordered samples).

shown by Ghosh et al. [8,9]. This facilitates characterization of an arrangement of fibers, computing some descriptors of the resulting Voronoi cells.

In order to perform Dirichlet tesellation, an original algorithm has been built, based on a rhomboidal region-growing of the centres [31]. Fig. 3 shows how different are the Voronoi cells corresponding to regular and disordered microstructure samples, respectively.

Dirichlet tessellation techniques have been used in composite materials literature [6–9]. In these papers, the main contributions relate to the characterization of fiber clustering. The present paper focuses on how to distinguish and characterize different kinds of arrangements of real non-ordered microstructures.

Pattern Recognition techniques categorize or analyse objects based on some measurements or features made on those objects, which in this application are the Voronoi cells of each microstructure. Each realistic disordered sample includes several fibers in a representative window or macrocell. A critical step in the estimation of the composite properties is the description of the dis-

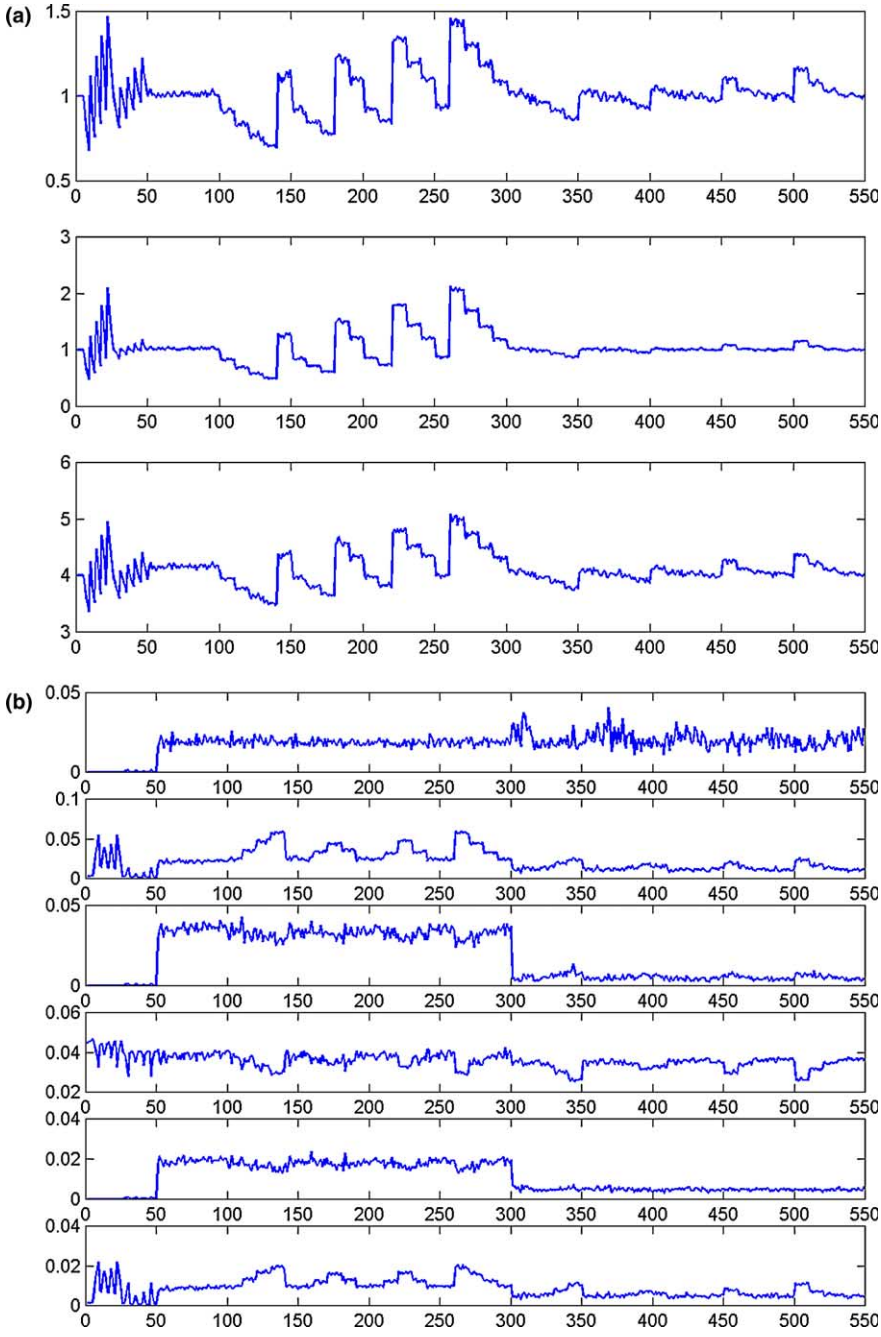


Fig. 4. Values of the features for the database of microstructures (550 samples). (a) BGFs, (b) FDs and (c) IMs.

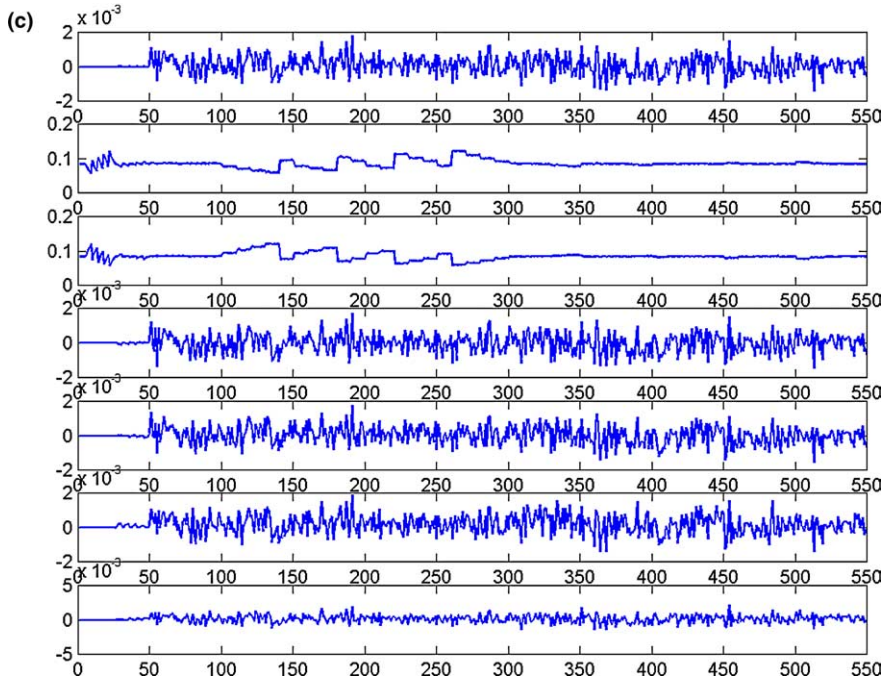


Fig. 4. (*continued*)

tribution of the disordered reinforcement [32]. This description must be invariant to scale, since two microstructures with different number and diameters of fibers can share the same volume fraction fiber/matrix. Besides, it must be invariant to location, but it can not be invariant to rotation because the final goal will be the prediction of a directional property of the composite material.

In this paper, the following quantitative descriptors based on geometric properties of Voronoi cells were computed [32,33]:

(1) Basic geometric features (BGFs). The ratios given by height/width, $ix/iy$, and perimeter/width have been considered (Fig. 4(a)).
(2) Fourier's descriptors (FDs) are widely used to identify objects with the aid of the boundary points. The best and most complete introduction can be found in the paper by Wallace [34]. Discrete Fourier Transform of a function $f(x)$, $x = 0, 1, 2, \ldots, N-1$ is defined as (where $u = 0, 1, 2, \ldots, N-1$),

$$F(u) = \frac{1}{N}\sum_{x=0}^{N-1} f(x)\mathrm{e}^{-\mathrm{j}2\pi ux/N}. \quad (2)$$

Firstly, the boundary must be stored in a counter clockwise direction. Each boundary point will be addressed as a complex number and the sequence of $N$ numbers as a complex function $f(z)$. The resulting transform $F(u)$ gives a set of $N$ Fourier descriptors. These values need to be normalized for location and size. Normalization for size is achieved by dividing all Fourier descriptors by the descriptor number 1 ($u = 1$). A further normalization is not necessary and only eight Fourier coefficients were used, where the first and second coefficients were rejected after the normalization (Fig. 4(b)).
(3) Invariant moments (IMs) are based on moments of a multidimensional function $f(x,y)$, which in this application represents a microstructure image [35,36]. Central discrete moments of order $pq$ ($\mu_{pq}$) and normalized central moments $\eta_{pq}$ were used to get scale invariance selecting the set of values for $pq = \{11, 20, 02, 12, 21, 30, 03\}$ (Fig. 4(c)). The central moments ($\mu_{pq}$) can be easily calculated in their discrete form with the following equation:

$$\mu_{pq} = \sum_x \sum_y (x-\bar{x})^p (y-\bar{y})^q f(x,y). \quad (3)$$

The central moments can be normalised for size as follows:

$$\eta_{pq} = \frac{\mu_{pq}}{\mu_{00}^{\gamma}}; \quad \text{where } \gamma = \frac{p+q}{2} + 1,$$
$$\text{for } (p+q) = 2, 3, \ldots \quad (4)$$

Figs. 4(a)–(c) show the BGFs, FDs, and IMs features, respectively, computed onto the database of composite microstructures.

## 4. Feature selection

In order to avoid the tendency to sparseness, it is necessary to consider a feature selection procedure. In this paper, the following techniques have been used:

### 4.1. Principal component analysis

The objective of principal component analysis (PCA) is to reduce the dimension, preserving as much of the relevant information as possible, finding out those directions which maximise the variance. The transformation maps vectors $x^n$ in a $d$-dimensional space onto vectors $z^n$ in another $M$-dimensional space, where $M < d$. The set of $n$ patterns can be represented as a linear combination of the original $d$ orthonormal vectors $u_i$ [12],

$$x_n = \sum_{i=1}^{d} z_i^n \cdot u_i. \tag{5}$$

$M$ basis vectors $u_i$ can be retained, and therefore only $M$ coefficients $z_i$ must be used and the remaining coefficients replaced by constants $b_i$,

$$\tilde{x}^n = \sum_{i=1}^{M} z_i^n \cdot u_i + \sum_{i=M+1}^{d} b_i \cdot u_i. \tag{6}$$

The vectors $u_i$ and the constants $b_i$ must be selected to achieve the minimization of $E_M$,

$$E_M = \frac{1}{2} \sum_{n=1}^{N} \|x^n - \tilde{x}^n\|^2. \tag{7}$$

The minimum error satisfies $\Sigma u_i = \lambda_i u_i$ and can be obtained by choosing the $d$–$M$ smallest eigenvalues of covariance matrix ($\Sigma$) of the set of vectors [16]. Fig. 5 shows PCA reduction onto the database of samples, where only two final features are used in the PCA transformed space ($u_1$ and $u_2$). These new components are linear combination of the original features ($x_i$, where $i = 1, 2, 3, \ldots, 16$ computed features).

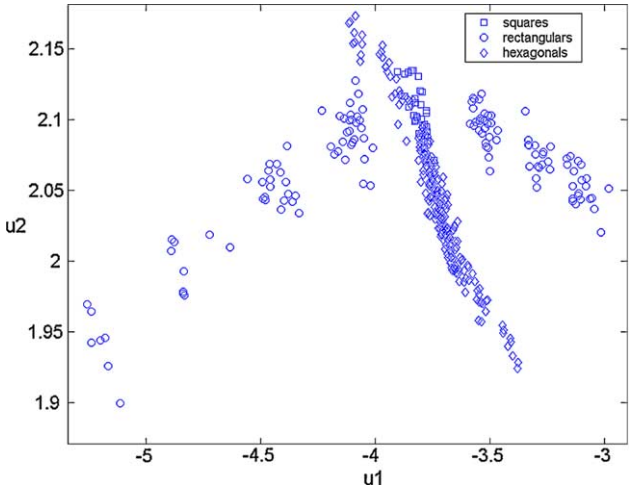


Fig. 5. Results of the principal component analysis. Realistic squared arrangements are represented by squares, rectangulars patterns by circles and hexagonals by diamonds. Axes correspond to the basis of a new PCA 2D transformed space.

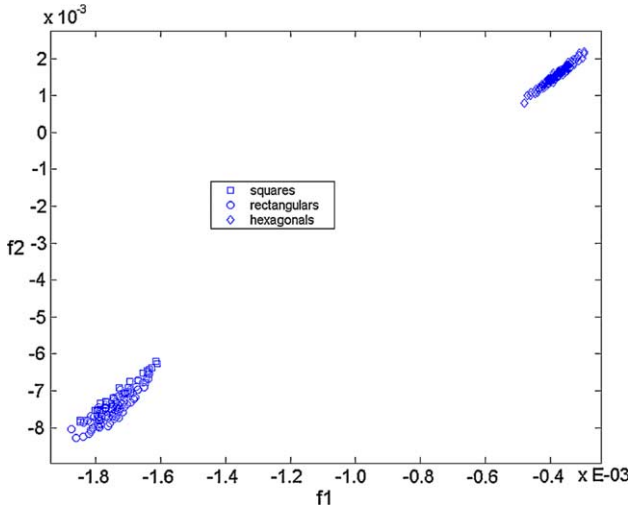


Fig. 6. Results of Fisher method. Realistic squared arrangements are represented by squares, rectangulars patterns by circles and hexagonals by diamonds. Axes correspond to the basis of a new Fisher 2D transformed space.

### 4.2. Fisher analysis

Fisher discriminant method achieves an optimal linear dimensionality reduction for classification problems [36,37,38]. Fisher criterion is derived by requiring maximum class separation in the output space, and seeks a linear combination of the variables which maximizes the ratio of its between-group variance to its within-group variance [18]. In this way, the method calculates the between-group covariance matrix ($B$) and the within-group covariance matrix ($W$). Then, the Fisher variables can be found as in PCA algorithm as the highest eigenvalues of the matrix ratio $B*W^{-1}$. Fig. 6 shows how the microstructures classes are separated with the Fisher 2D transformation, where $f_1$ and $f_2$ are the new basis (linear combination of the original basis $x_i$), and the database is projected using the Fisher transformation matrix.

## 5. Multiple regression models

The final objective of this study is the estimation of effective thermal conductivity of an unidirectional composite. The overall system can be viewed as a mapping from a set of input features to an output variable. In general, it is not possible to determine a suitable form for the mapping and it is necessary to work with a set

of examples, which are called the "training set". Therefore, effective transverse thermal conductivity estimation can be solved as a regression problem over the database of samples using two different regression approaches: the first approach is the classical MLR. The second approach is based on ANNs.

### 5.1. Multiple linear regression

The purpose of MLR is to establish a quantitative relationship between a group of independent variables, $X$ (features), and a response, $y$ (transverse effective thermal conductivities $K_{ey}$). The linear model can be expressed using matrix notation, as $y = X\beta + \varepsilon$. However, computing $\beta$ by inverting $X$ is really dangerous. In most of real situations, $X$ will often be either totally singular or ill-conditioned. It is very interesting to emphasize that PCA results are independent and uncorrelated. Therefore, in this study MLR is solved with a QR method when PCA method is used before, otherwise MLR is solved with singular value decomposition (SVD) algorithm [39,40]. MLR approach generally produces suitable estimations for the design samples (training set) and inadequate estimations for the samples in the test set (see Table 3).

### 5.2. Backpropagation neural networks

Neural networks have been applied to composites materials area [41] and many ANN-based models were developed for very different composites analyses purposes [42–47].

In some cases, MLR may not be the best model available. In such cases, a nonlinear regression method such as neural networks (ANN) may provide a better analysis. The most widely used ANN model is known as *multilayer perceptron (also multilayer feedforward neural network)*. This neural approach models the relationship between $X$ and $Y$ in the form (through a weighted structure of layers, usually *input-hidden(s)-output*),

$$Y = g\left(\sum_{j=0}^{M} w_{kj} \cdot f\left(\sum_{i=0}^{D} w_{ij} \cdot X_i\right)\right). \tag{8}$$

Neural networks, where $g(x) = x$ and $f(x) = \tanh(x)$, have been proved to be universal approximators. Such networks can, therefore, approximate arbitrarily well any general function, which makes them highly interesting for regression purposes.

The backpropagation learning rule [48] is based on an error function that has a particular surface over the weight space and therefore, an iterative process such as gradient descent method [18] can be used for its minimisation. There are many other algorithms [18,39,40] for training feedforward neural networks: conjugate gradients, quasi-Newton, Levenberg–Marquardt and others. Standard backpropagation learning rule has slow convergence. In practice, the Levenberg–Marquardt algorithm finds better optima and faster solutions for networks up to several hundred weights [49]. This study uses Levenberg–Marquardt optimization method.

Capabilities of feedforward neural networks with one hidden layer can be iluminated by Kolmogorov's theorem [50,51], and Vapnik and Chervonenkis dimension [52], but there is no way to determine an optimal network topology just from the numbers of inputs and outputs. A simple choice, would be to train many networks with different number of hidden units and layers, then to estimate the generalization error for each one, and finally to select the network with the smallest one [13–15]. However, this process depends critically on the training/test set and the initial weights, so it is necessary to compute the mean generalization error over a design resampling experiment.

## 6. Experimental procedure

Several multiple regression models have been proposed in this study by combinations of above explained preprocessing methods, and also according to the type of regression system and the topology of the ANN models (the number of layers and hidden units). A group of previous experiments were developed in order to reduce the number of neural networks topologies [53]. The models can be found in Table 2.

Once the models were developed, it must be considered the problem of determining the best model on a previous set. Statistical methods analyze how the models

Table 2
Regression models

| Model | Preprocessing | Regression |
|---|---|---|
| 1–9 | PCA-2 | RML, 3 layers BPNN (nhiddens = 1:4), 4 layers BPNN (nhid1 = 1:2) (nhid2 = 1:2) |
| 10–18 | PCA-4 | RML, 3 layers BPNN (nhiddens = 1:4), 4 layers BPNN (nhid1 = 1:2) (nhid2 = 1:2) |
| 19–27 | PCA-8 | RML, 3 layers BPNN (nhiddens = 1:4), 4 layers BPNN (nhid1 = 1:2) (nhid2 = 1:2) |
| 28–36 | PCA-12 | RML, 3 layers BPNN (nhiddens = 1:4), 4 layers BPNN (nhid1 = 1:2) (nhid2 = 1:2) |
| 37–45 | No preprocessing | RML, 3 layers BPNN (nhiddens = 1:4), 4 layers BPNN (nhid1 = 1:2) (nhid2 = 1:2) |

Table 3
MLR versus BPNN best models (RMSE in 30-times resampling procedure)

| | MLR | BPNN |
|---|---|---|
| Fisher Class 1 | 8.2 E − 03 | 3.1 E − 06 |
| Fisher Class 2 | 3.3 E − 04 | 6.6 E − 06 |

behave on average. As well as, it is necessary to consider the performance of a model over all the training sets that might be drawn from the underlying distribution. Analysis of variance (ANOVA) [54] has been used to test the null hypothesis taking into account certain assumptions, i.e., all populations are approximately normal and the samples from each population should be random and independent. Besides, the population variances should be equal. However, this assumption is not meaningful when all the models have the same number of error measures. In this paper, the first assumption has been verified using the Kolmogorov–Smirnov test.

Only a limited sample of data is available and a complete strategy of experiments must be described to guarantee the independence of the results. In accordance with the works of Galindo, Pizarro et al. [13–15], a randomised procedure has been designed to control the different sources of variation in order to compare the different models. The averaged performance of the models over resampled training sets has been considered. In order to carry out this procedure, the database must be divided into a training set and a test set. The complete strategy is repeated 30 times using the well-known two-fold cross-validation method [18,39] for the estimation of the root mean squared error (RMSE) for the $M$ models.

Bonferroni multiple comparison procedure [55] has been used to decrease the probability of making at least one Type I error. This approach is a follow-up method to ANOVA based on the following: if $n$ comparisons are to be made, each one with confidence coefficient $(1-\alpha/n)$, then the maximum value of overall probability of making one or more Type I errors is $\alpha$. If the difference between the sample means exceeds a critical threshold, there is sufficient evidence to conclude that the population means differ. Bonferroni method adjusts the observed significance level based on the number of pair comparisons.

## 7. Results and discussion

Figs. 5 and 6 show results from PCA and Fisher preprocessing methods. Different final features were tested in the experiments (see Table 2). With this dimensional reduction the data can be shown in a planar graph which is another advantage of these methods. Fisher method produces a perfect discrimination in 2D transformation, therefore two classes of real-disordered samples should be considered (class of squared and rectangular disordered arrangements and class of hexagonal disordered patterns).

Two regression models (one for each class) have been built in order to improve the results obtained using only one regression model. Regression results obtained using PCA transformation versus the performance obtained by using all of the original features are compared in the experiments, computing the RMSE (for 30 simulations).

Comparing the classical MLR and ANN analyses, it becomes clear that the predictions from neural networks models follow the experimental data much more closely than those obtained from multiple regression analysis (Table 3). Neural networks models are highly robust with respect to underlying data distributions (non-parametric). Thus, neural networks models are well-suited to modelling estimation of transverse conductivities.

The RMSE means (for the 45 models considered in Table 2) have been compared by using the ANOVA Test (Table 4). In any case, ANOVA $F$-test is significant and therefore the null hypothesis is rejected. This fact is due to the intergroup variability of the different models (see second column of Table 4). Therefore, Bonferroni method was used in order to pinpoint which the best model is (Table 5 summarizes the best models obtained). When these strategies are adequately applied to the obtained error rates in a well designed experiment, and the needed assumptions are verified, it is possible to determine the optimal complexity, or even, to determine which model fits better the samples. Results are shown in Table 5, where d$t$ is the threshold difference between groups, and statistical significance $\alpha$ is fixed at 0.1. Results are shown for the models explained above: one separate

Table 4
ANOVA test results

| | Intergroup variance | Residual variance | $F$ |
|---|---|---|---|
| Class 1 model | 4.10 E − 010 | 9.03 E − 012 | 45.45 |
| Class 2 model | 2.24 E − 08 | 3.98 E − 09 | 5.73 |
| C12 model – error C1 | 6.02 E − 09 | 4.65 E − 10 | 12.94 |
| C12 model – error C2 | 8.45 E − 09 | 4.16 E − 10 | 20.29 |

C12 model means only one model for the two classes 1 and 2, where 1 is the class of squared-rectangular disordered arrangements and 2 is the class of hexagonal realistic distributions of fibers.

Table 5
Selected models obtained with Bonferroni method in the resampling procedure

| | d$t$ | Model number | Model type | Preprocessing | RMSE test mean |
|---|---|---|---|---|---|
| Class 1 model | 0.311 | 15 | BP1x1 | PCA-4 | 3.1E − 06 |
| Class 2 model | 0.646 | 8 | BP2x1 | PCA-2 | 6.6E − 06 |
| C12 model – error C1 | 0.222 | 12 | BP2 | PCA-4 | 9.3E − 06 |
| C12 model – error C2 | 0.211 | 12 | BP2 | PCA-4 | 7.5E − 06 |

model for class 1 (squared-rectangular arrangements), another model for class 2 (only hexagonal arrangements), and finally, one model for the whole database. In this three models scenario using Bonferroni method, the groups are overlapped and therefore, the model with the smallest error should be selected. In Table 5, data are collected from a training/test set size of 100. For class 1, the best model is a backpropagation neural network with two hidden layers (each one with one hidden unit) and PCA preprocessing method with four final features. In a similar way, for hexagonal samples (class 2) the best model is obtained with PCA-2 preprocessing and a four layer backpropagation neural network $2 \times 1$. In both classes, the magnitude order of RMSE is E − 06.

Furthermore, different sizes of the sets (training/test) in the resampling procedure have been tried showing that the error means do not sensibly change. It is worth emphasizing that RMSE is better when separate neural regression models are built for each class, and also that in general, the results obtained with this approach are more accurate since standard variations are smaller. The procedure of resampling simulation has been designed to avoid variation proceeding from different sources, thus independence and randomness are guaranteed. Therefore, the generalization obtained is sufficiently adequate. These results show how statistical methods can be successfully employed for the topology determination of neural networks architectures applied to the problem of effective thermal conductivity estimation.

Fig. 7 shows $R$ correlation coefficient (for each class) for the best neural models (over test sets). It can be noticed that the $R$ correlation coefficient for the rectangular arrangements (Fig. 7(a)) is greater than the one obtained for hexagonal class (Fig. 7(b)). As it is expected, the effective thermal conductivity corresponding to the hexagonal class is less sensitive to the added noise (with respect to the regular array distribution) than the showed by the rectangular class. Finally, the neural estimations (over the test set), once trained the network are showed in Fig. 8. The effective thermal conductivities obtained by ANN models provide estimations very close to those obtained by a rigorous FEM analysis. On the other hand, considering the computing times required by the proposed analysis ($t_{\text{mean}} = 13.17$ s, SD = 1.73 s) and the corresponding to FEM analysis ($t_{\text{mean}} = 31.54$ s,

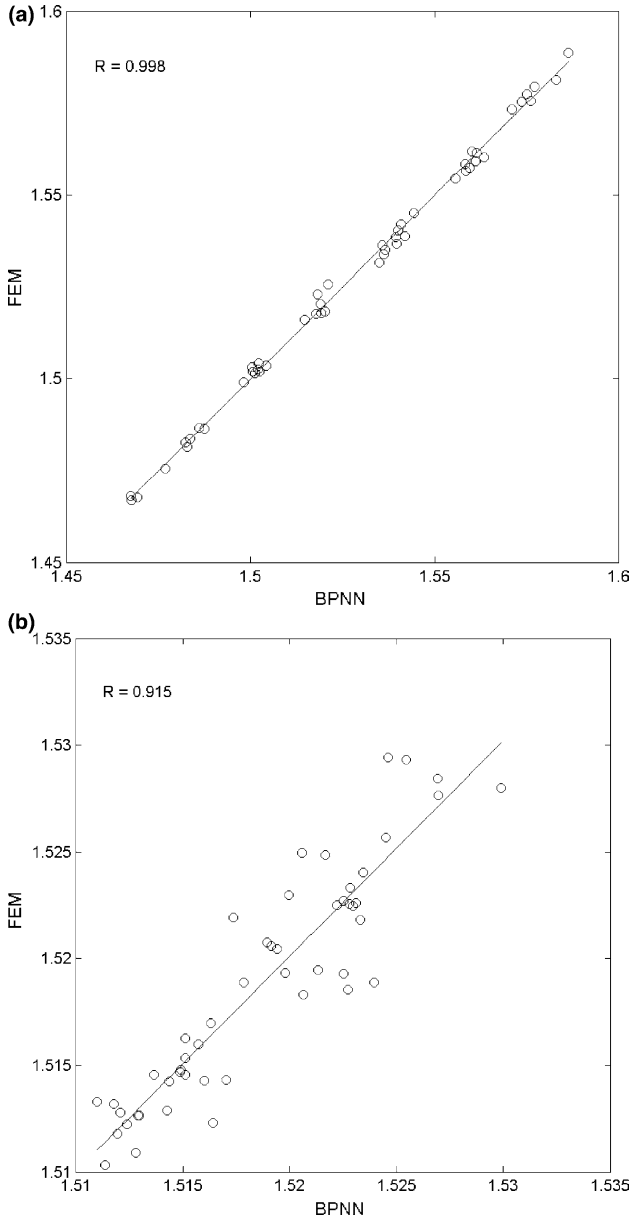


Fig. 7. FEM versus neural regression models. Results for the best models in one of the 30 simulations in the resampling procedure. Class Model 15 (Topology BP1x1, Preprocessing PCA-4). (a) Test RMSE-06, $R$ correlation coefficient (test set) = 0.998 Class 2:Model 8 (Topology BP2x1, Preprocessing PCA-2). (b) Test RMSE-5.55E-06, $R$ correlation coefficient (test set) = 0.915.

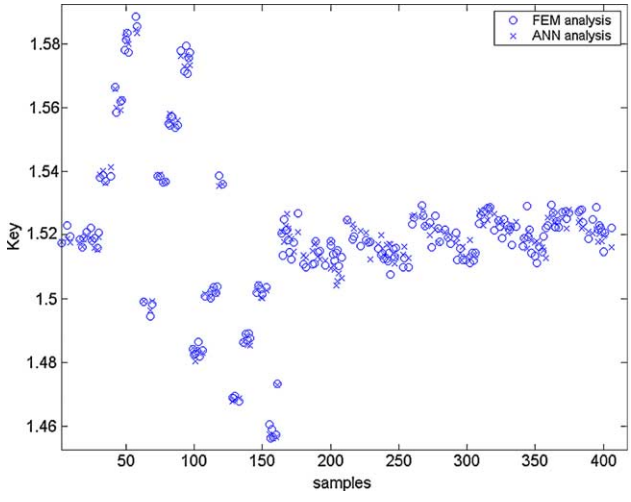


Fig. 8. $K_{ey}$ neural estimation. FEM conductivities are represented by circles and ANN estimations are represented by $X$.

SD = 6.44 s), it is evident that this procedure based on ANN is more computationally efficient.

## 8. Conclusions

The following concluding remarks can be made from the results discussed above:

- PCA method prevents problems arising from "the curse of dimensionality" and although there is a loss of information, the overall performance of the selected models has increased.
- Fisher method allows a perfect classification of the database, suggesting that square-rectangular and hexagonal disordered arrangements should be considered in different classes. Therefore, each class must be modelled with a specific regression system.
- ANN models, once trained, are fast at predicting the desired values, so that the computing time required by this procedure is noticeable smaller than the required to perform the FEM calculations. The main advantage is that the accuracy of generalization of the neural models is higher than standard MLR models over test sets.
- In the experiments carried out for the selected models, the values of $R$ correlation coefficient (over test sets) yields close estimations to conductivities calculated with FEM. These results suggest that the selected neural models provide a properly and alternative procedure to compute effective thermal conductivities on real unidirectional composite materials.

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