CILAMCE 2017
Florianópolis - Santa Catarina - Brazil

PREDICTION OF THE TRANSVERSE ELASTICITY MODULUS OF UNIDIRECTIONAL COMPOSITES THROUGH NEURAL NETWORK ANALYSIS USING THE RPROP ALGORITHM

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Abstract. *The artificial neural networks (ANN) is a new computational tool which has been used in several areas of Engineering. In Mechanical Engineering, among its newest applications is the evaluation of mechanical properties of composite materials. This work aims to create an ANN capable of predicting the transverse elasticity modulus (E_2) of unidirectional composites, comparing two types of training algorithms of ANN, to verify which one has the best mathematical model. To achieve that, two groups of data will be analyzed using cross validation. Thus, two kinds of ANN architecture will be analyzed, one of them with three inputs, and a mixed model that combines a three input model with equations developed by Halpin-Tsai. These sorts of architecture were already evaluated using the backpropagation algorithm, on this work, another type was ascertained, called resilient backpropagation (Rprop). After the training, the results were compared and the ANN with Rprop training algorithm showed a high efficiency and relevance. The Halpin-Tsai model was utilized as a comparison parameter, thereby, higher correlation coefficients were observed as well as lower root mean square values.*

Keywords: *Neural Network, Mechanical Properties, Rprop Algorithm.*

1 INTRODUCTION

The laminas of unidirectional composites are constituted of two elements, the matrix and the reinforcement, which is composed of fibers in only one orientation. Composites are generally made of several of these stacked laminas, which makes the detailed characterization of such materials essential in the sectors that utilize these types of materials.

In projects of structural components, it is clear the need for a fast and accurate analysis of its mechanical properties, especially the ones made of composite material, due to its anisotropic behavior.

The ascertainment of mechanical properties of composite materials are made, practically, on estimation based on empirical, semi-empirical and computational models, which approach in a more precise way to reality, and thus, the experimental values. A pure experimental estimation can demand a larger time, which makes necessary severe capital investments to perform the tests. Mathematical models do not need this capital investment; however, they have the risk to possess a lower precision.

The mathematical models are destined to the obtainment of the mechanical properties of the lamina, which are denominated, micromechanical models. Simpler and purely analytical models, such as the rule of mixtures, can serve as an initial approach in the analysis of the mechanical behavior, since it considers several factors as negligible. In parallel to these models, others based on the elasticity theory arose, the semi-empiric models. Hill (1965) proposed a model called “Self consistent model”, which was utilized by Whitney and Riley (1966). Halpin and Tsai (1969) deepened the analysis on those models, developing their own, which had large acceptance in engineering projects (Câmara and Freire, 2011). Aboudi (1989) developed models which predicted transverse properties G_{23} (Shear Modulus in direction 23) and ν_{23} (Poisson coefficient in direction 23). Hopkins and Chamis (1988) proposed a multicellular model similar to the rule of mixtures. Adam and Doner (1967) utilized finite differences to obtain G_{12} (Shear Modulus in direction 12), and the E_2 (transverse elasticity modulus) through finite elements. Dezhsetan and Aghdam (2005) also performed a study to obtain the mechanical properties of composites, based on its components, however, their model involved a wide range of variables, making possible to apply it on particular cases.

Szabó (2015) proposed a homogenization modeling, so that, through numerical simulations based on the values for the composite constituents, it was possible to predict some properties of the unidirectional lamina. Based on the fracture mechanics, Lee and Palley (2012) comparing the values for elastic energy before and after the damage, were capable of determining the value of the shear modulus of unidirectional fiber composites of the polymeric matrix. Recently, there is still the application performed by Dong (2015) utilizing models in finite elements and analytical approaches to study the influence of the void content in the mechanical response of laminate composites.

It is possible to notice that several approaches were proposed to ascertain the mechanical properties of laminate composites, however, models which utilized artificial neural networks (ANN) were not widely explored in the area, making it a scientific gap in the literature. According to Lee *et al* (1999), the use of artificial neural networks represents a new computational paradigm, with respect to the composite materials, allowing an effective approach of complex data sets with totally non-linear relations. Friedrich and Zhang (2003) summarized the main applications of neural networks in the area of composite materials, such as fatigue, tribologic properties, dynamic properties, manufacturing processes, among others.

Applications related to the mathematical models of ANN were also observed in similar areas, such as, for instance, in the prediction of the bending resistance and mechanical hardness of particulate composites with polymeric matrix (Koker, Altinkok and Demir, 2007).

Câmara and Freire Junior (2011) utilized ANNs to predict the elasticity transverse modulus of unidirectional laminas. In the present work, it is proposed to investigate the influence of the training algorithm *Rprop* in an ANN which predicts the Elasticity Transverse Modulus (E_2), comparing it with other models in literature (Câmara and Freire, 2011). Based on the presented the main objective is to obtain this mechanical property in a fast and precise way. The results are validated through the root mean square error and the correlation coefficient.

2 USED DATA SET

In the development of the present work, it was necessary to perform a data collection which served to the test and training of the developed networks. The data set was obtained from bibliographic references such as scientific papers and subject related websites, all of them related to composites (Koker; Altinkok and Demir, 2007; Benedikt; Rupnowski and Kumosa, 2003; Teng, 2007; Benedikt et al., 2001; Shan and Chou, 1995; Berthelot and Sefrani, 2007; Zheng-Mind, 2001; Wacker; Bledzki and Chateb, 1998; Huang, 1999; Herakovich, 1988; Medonça, 2005; www.about.com; www.matweb.com). The Table 1 shows the values for elasticity modulus for each type of fiber and matrix collected in literature.

In the implementation of the ANN, 106 unidirectional composites were utilized, from these 92 were chosen for training and 14 for validation and network test. Each data contains different values for the transverse elasticity modulus of the matrix, fiber, and fiber volume fraction, needed for the effective mathematical modelling.

From the collected data, the materials used as reinforcement were carbon fibers (AS- 4, AS, IM6, MOD I, GRAFITE, T-300), glass fibers (GLASS- S, GLASS- E), boron, aramid. The resins, which served as matrices for the laminas were: Peek APC2, Epoxy, Polyester, DX210, and SR1500. The values obtained for the percentage variation of the fiber were in the range from 15% to 70%, in all of the unidirectional laminas. The Table 2 shows data from the transverse elasticity modulus of the composite lamina.

Table 1. Values for the elasticity modulus of the matrix and fiber.

Fiber	E_f (GPa)	Matrix	E_m (GPa)
Carbon	15-23	Epoxy	2.8-4.6
Aramid	5.1	Polyester	2
Glass	61-81	DX210	3.21
Boron	61.77	SR1500	2.8

		PEEK APC2	3.66

Table 2. Tranverse elasticity modulus of the lamina.

Lamina	E_2 (GPa)	Lamina	E_2 (GPa)
Carbon/Epoxy	6.4-17.84	Glass/Polypropylene	3.09
Carbon/PEEK ACP2	8.7-9.8	Glass/Polyester	2.96-4.29
Carbon/Polyester	5	Aramid/Epoxy	4-5.5
Carbon/DX210	7.2	Aramid/SR1500	3.66
Glass/DX210	5.85	Boron/Polyester	14.87
Glass/SR1500	10.9	Boron/Epoxy	18.5
Glass/Epoxy	3.12-29.7	-	

3 MATHEMATICAL MODELLING

The mathematical modelling was based on two types of ANN architectures, with both having multi-layers perceptron networks, however, analyzing two different training algorithms, the *backpropagation* and the *resilient backpropagation* (*Rprop*). The ANNs will have three entries for the modelling of the mechanical property (E_2). One of the models is based on the results of the Halpin-Tsai equations, which is considered as a mixed model. During the training a stop criterion of cross validation was adopted, so that the data were divided into training data (85%) and test data (15%), for both modulus, so that the network is capable to have an optimum capacity of generalization.

The artificial neural network has only one hidden layer, ranging from 40 to 120 neurons, to analyse and observe in which architecture has the best results. All the layers have the bias; the hidden layer has neurons with a sigmoid activation function while the outer layer will have the linear activation function. The ANNs were trained with a maximum number of 15000 epochs. It is important to point out that all the input and output data were standardized with the objective of improving the learning rate of the network.

The networks that use the *backpropagation* algorithm are based on the *momentum* rule (Haykin and Engel, 2001). The adopted learning rate was 0.1, alongside with a momentum constant of 0.7. For more details see reference (Câmara and Freire, 2011).

The networks which utilized the *Rprop* algorithm are different from the classical *backpropagation* ones, in which for every interaction, having specific sample size, the weights are updated in the most predisposed direction. The *Rprop* determines the size of the step in the individual weights interaction, based on the sign of the partial derivative, whether is the same of the previous step or not (Riedmiller and Braun, 1993). The greatest advantage of this algorithm is that its learning rates adapt to the topology of the error. (Bailey, 2015). In this model, learning rates ranging between 0.1 and 0.2 were utilized. The networks with *Rprop* will have a learning rate larger than 1.2.

To make a comparison and analyse the results, the correlation coefficient, as well as the root mean sqaure error were estimated. The mathematical equation for the root mean square erro is given by equation 1.

$$RMS = \frac{\sum e^2}{2N} . \tag{1}$$

Where N is the number of samples that are being used to calculate the error (e).

To implement the neural networks the software MATLAB was used.

3.1 ANN Rprop with three inputs

The first ANN has three inputs and one output, on the input neurons there are the values of E_f (transverse elasticity modulus of the fiber), E_m (transverse elasticity modulus of the matrix), as well as the value of V_f (volume fraction of the fiber). On the output, there is the value of E_2 (transverse elasticity modulus of the unidirectional laminate).

Thus, the equation 2 is that will rule this ANN. As follow:

$$E_2 = f(E_f, E_m, V_f) . \tag{2}$$

Figure 1 shows the scheme for the neural network model. The Fig. 2 shows the architecture of the ANN and how the training algorithm works.

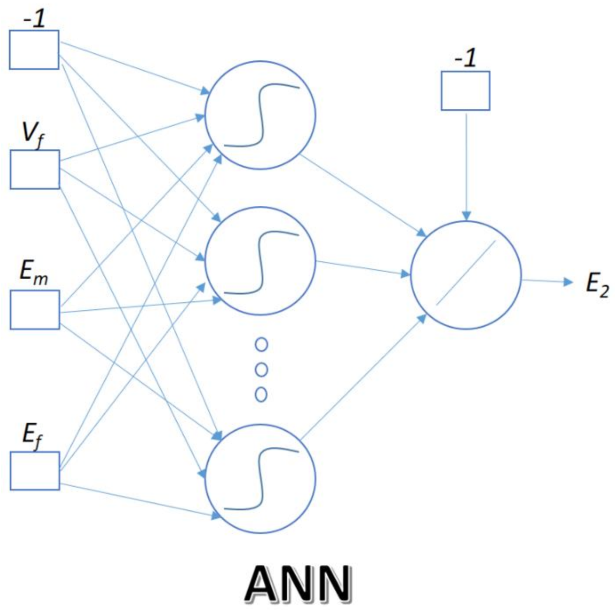

Figure 1. Architecture of the ANN

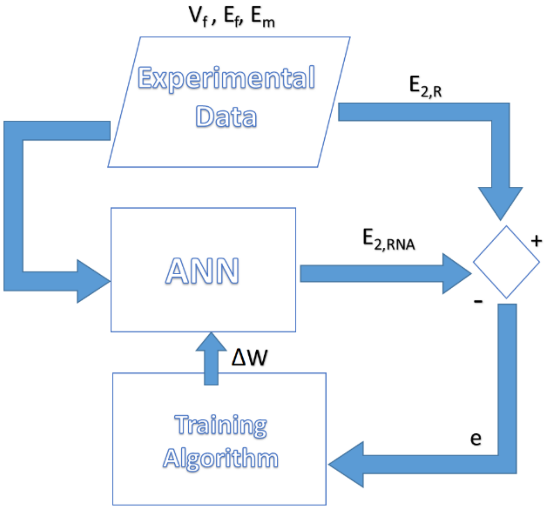

Figure 2. Training scheme of the ANN

It is possible to see from Fig 1 that in all the layers the same input bias was adopted (-1). In figure 2 the training algorithm that will be modeled is presented, according to the value of the difference (e) of the experimental data ($E_{2,R}$) and the output of the network ($E_{2,RNA}$), updating the network with new weights in every interaction (dW).

3.2 Mixed Rprop ANN

In this ANN the Halpin-Tsai equations will be used as a learning parameter, in order to approximate the values of the semi-empiric model to the experimental values. The Halpin-Tsai model is expressed through the equations 3 and 4:

$$P_c = \left(\frac{1+\xi\eta V_f}{1-\eta V_f} \right) P_m \,. \tag{3}$$

$$\eta = \frac{P_f / P_f - 1}{P_f / P_m + \xi} \,. \tag{4}$$

So that P_c is the analysed composite property (E_2), P_m is the matrix property (E_m) and P_f is the fiber property (E_f). The parameter is a number that depends on the geometry of the fibers, the arrangement of the fibers and the loading. The value of 2 was adopted for, as recommended by Halpin-Tsai.

Figures 3 and 4 shows the schematics of the neural network architecture. Three input parameters will also be used: volume fraction of the fiber, elasticity modulus of the fiber and elasticity modulus of the matrix. In this case, the training has the objective of reducing as much as possible the output value of the network, which is the error between the Halpin-Tsai model and the experimental values.

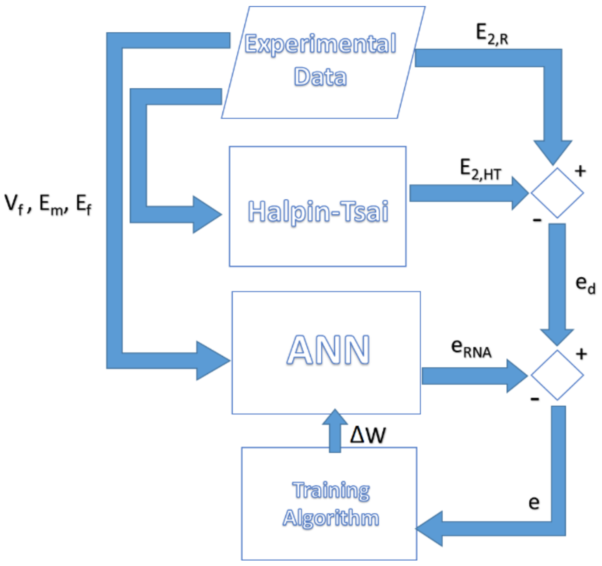

Figure 3. Training schematics of the ANN

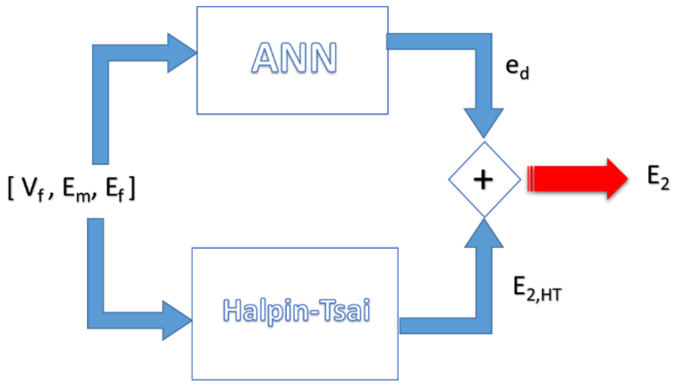

Figure 4. Architecture of the mixed network.

3.3 ANN Momentum

These models were already evaluated by Câmara and Freire Jr (2011), utilizing them only as a comparative element, since they had already been validated.

An ANN with three inputs was used, in the same manner as the previous ANNs, with fiber and matrix modulus and volume fraction of the fiber. The scheme of architecture and training is the same as the one presented in Fig. 1 and Fig. 2, respectively. It is known that the alteration occurs in the training mode which is given by the *backpropagation* method with the *momentum* rule. It is also possible to consider the same equation 2 for this ANN.

For this training algorithm, it was also proposed a mixed model. Such model utilized the same architecture as the mixed *Rprop* ANN (figures 3 and 4), the mixed momentum ANN will use the *backpropagation* method with *momentum* rule in the network training.

4 RESULTS

The results were displayed in three graphic analysis. The first shows the root mean square error as a function of the first training epochs, for the training and test data set. The second shows a selective analysis, so that the data were divided into groups, considering the value of the ration between the fiber and matrix modulus (E_f/E_m), and also the amount of data in a determined range. The range of values considered were: “3 and 7”, “13 and 22”, “22 and 30” e “30 and 50”. The curves obtained with these models were plotted with values for E_f/E_m of 5, 21, 25 and 40. The data were divided in such way to facilitate the understanding, the curves were divided according to the amount of data in each range. The third analysis shows the result of the values coming from the ANN, compared with the real values. The data utilized for test validation will be the test and training data.

4.1 ANN Rprop with three inputs

The first result of this model comes from the training stop criterion, which was adopted through cross validation as shown in Fig. 5, for the training and test data set. Then, it is possible to see the characteristics of the algorithm with stochastic learning, with a lot of disturbances in all epochs. It is also noticed that different from the *backprogation* training algorithms, the models that utilized the *Rprop* reach the critical values in the cross validation, soon and in the first epochs. The values for the error were in the range of 0.0018 and 0.003, with this model presenting the best values.

The Fig. 6 shows a comparative analysis for a range of values. It is perceived that the curves presented an initial fluctuation, however, end up adjusting to the data. This might have occurred due to the absence of data in the initial region. Another factor is the type of *Rprop* algorithm, which tends to converge more rapidly than the common *backpropagation* (Riedmiller and Braun, 1993), alongside with a learning rate of 0.2, this resulted in an initial undulatory behavior which rapidly adjusted when reached the range that includes the experimental data. The blue curve (35 to 50) since it is the region with the smaller amount of data (three), probably could not reach a good generalization.

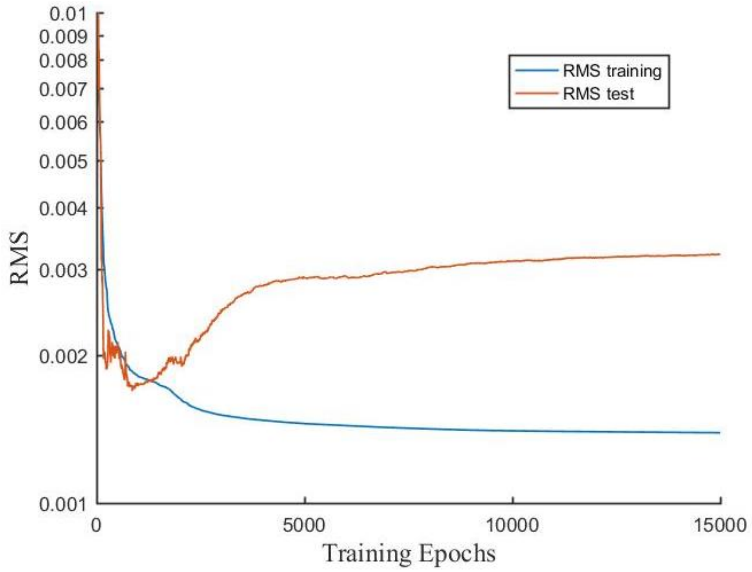

Figure 5. RMS in function of the training epochs

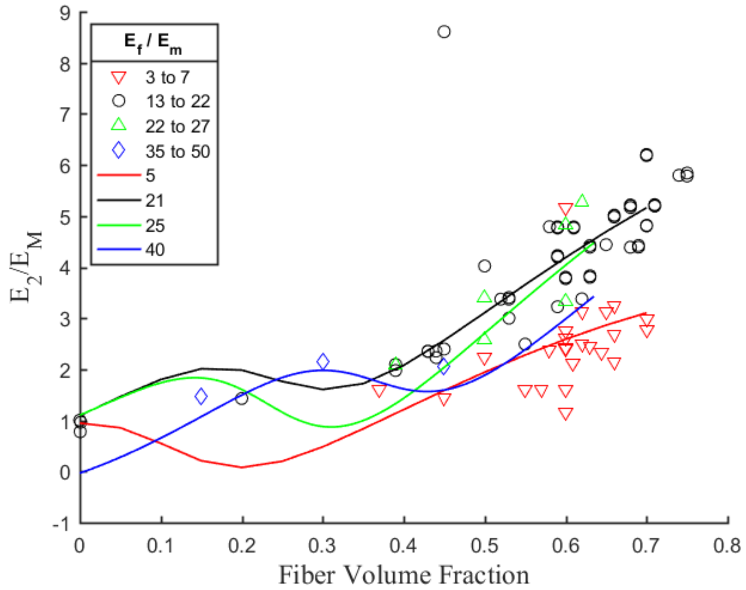

Figure 6. Comparison curves with the experimental data, divided in bands.

Figure 7 shows another comparative approach focusing only on the values of E_2 coming from the ANN. An Analysis of the training data and the test data was performed, in a graphic of the real values in function of the ANN values, in a way that as closest to the blue line, there will be a linearity with the experimental values, thus, the values of the ANN would be the same as the real values.

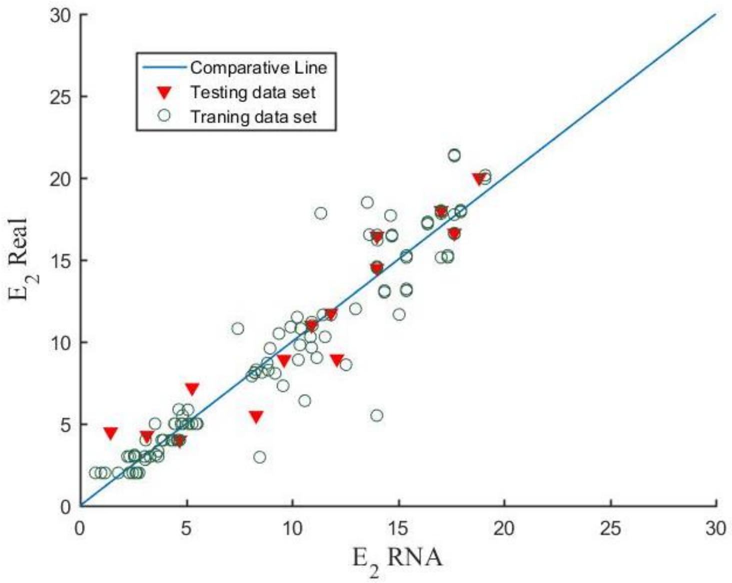

Figure 7. Alternative analysis, comparison between the real and the ANN values.

An alignment between most of the data is observed, for the training and test data. Only a few training data had very distinct values from the real ones. Such analysis proves that a good performance of the network using the *Rprop* algorithm was reached, as shown through the results in Table 3.

Despite the great performance presente by the ANN, for a general use, it is needed a larger amount of data, due to the increase in precision and trustworthiness for all bands of values for E_2. Hence, it is proposed a mixed model very similar to the one utilized by Câmara and Freire Jr (2011), combining the ANN results with the Halpin-Tsai equations, being possible then to have a higher generalization of the network, obtaining satisfactory values with or without the presence of a large number of experimental data.

4.2 Mixed Rprop ANN

Following the same principle as the previous model, the cross validation was adopted as stop criterion for the ANN. Fig. 8 shows the values for root mean square error for the training and test data in function of the number of epochs. It is noticed that, as previously, in the first epochs the errors presented were high, however, they rapidly tend to stabilize with characteristic fluctuations of the model. The ANN exhibited values, approximately in the same order of magnitude as the previous network (between 0.002 and 0.003), which are better values than the own Halpin-Tsai model. Therefore, this ANN also has the capacity to generalize the micromechanic behavior, in a more satisfactory way when compared to the previous model, since it is based in the Halpin-Tsai equations.

Figure 9 shows a comparative graphic of the test data, comparing the experimental data from the ANN, through a range of values of E_f / E_m. The behavior of the points close to the line indicates a good adjustment of the network, which on this occasion served to approximate the valyes from the Halpin-Tsai model for the experimental values. In this model, the initial undulation was not severe, when compared to the *Rprop* with three inputs model. However, an abrupt variation is still presented at the beginning of the curves, which is a characteristic of the *Rprop* algorithm. In the absence of data in the initial region, the curves presented that abnormal behavior; nevertheless, they rapidly adjusted with the experimental data after this region.

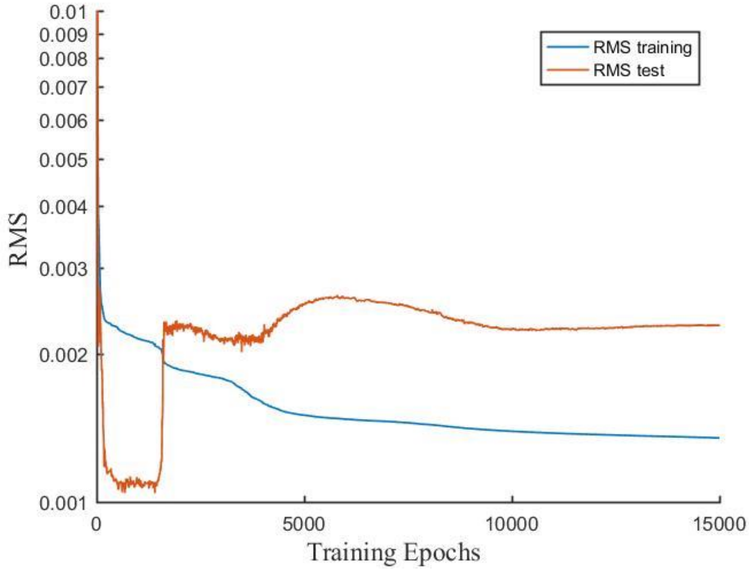

Figure 8. RMS in function of the training epochs

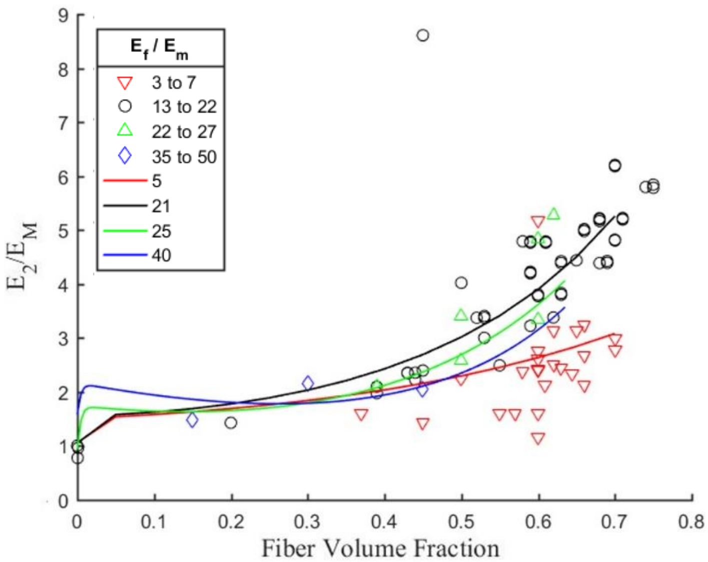

Figure 9. Comparison curves with the experimental data, divided in bands

In Fig 10 the mixed model with three inputs alongside with the Halpin-Tsai is presented, showing that using the *Rprop* training algorithm obtained great results, with most of the data aligned with the comparative line, for the training as well as for the test data. In spite of having a higher dispersion of the values, compared to the previous model, for being associated with the Halpin-Tsai equations, this model has a higher capacity of generalization.

In the next item, it is observed a comparative analysis obtained from the networks with *Rprop* training algorithm with the Halpin-Tsai model and the validated models in literature (Câmara and Freire, 2011).

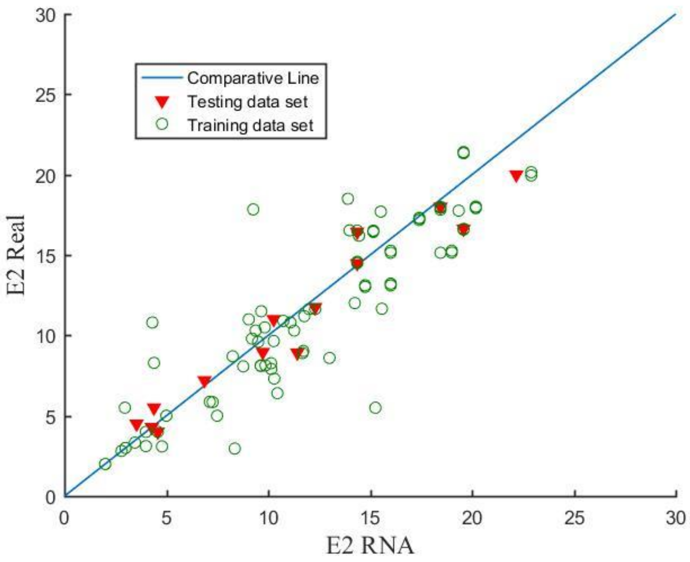

Figure 10. Alternative analysis, comparative between the experimental values and the values presented by the ANN.

5 DICUSSIONS

In this topic, an evaluation of the obtained results will be performed, based on a comparative analysis with models that have already been validated. The main parameter will be the Halpin-Tsai model; the two models based on ANN with Momentum rule in section 3.3, will also serve as comparative elements.

5.1 Comparative analysis of the models

At Table 3, there is a comparative analysis of the three following models, the mixed model (M. Mixed) that has the same architecture as the mixed *Rprop* model, but with a training algorithm based on the momentum rule. There is also the three inputs model (M. 3I) which has the same architecture as the *Rprop* 3I model, however, it uses the momentum rule for the network training. At last, there is also the Halpin-Tsai model.

The table shows the best values for root mean square error (RMS), as well as the correlation coefficient (r), in terms of the number of epochs and the number of neurons for the models mentioned above. It is possible to realize that the ANNs with *Rprop* algorithm obtained the best performance, when compared to the other models, despite the curves in Fig. 6 and Fig. 9 presenting distortions in the initial region, which does not seem to characterize the behavior of the mechanical property in the materials, the values presented are highlighted in the table.

It is observed that the RMS values obtained by the ANN with the *Rprop* training algorithm were lower, as well as the number of epochs in which the lower error is reached. These parameters are all lower than the ones in the Halpin-Tsai model, demonstrating one of the characteristics of the *Rprop* that is its fast convergence, being four times larger than the common *backpropagation* (Riedmiller and Braun, 1993).

Table 3. Comparison between the model with Rprop, Momentum (Câmara and Freire, 2011) and the Halpin-Tsai model.

Model	RMS	*r*	Epochs	Number of neurons
Rprop Mixed	0.00208	0.944	1407	71
Rprop 3I	0.00185	0.950	864	68
M. Mixed	0.00216	0.942	14122	48
M. 3I	0.00320	0.923	14581	79
Halpin-Tsai	0.00364	0.917	-	-

Due to the lack of robustness of the algorithms that utilize *Rprop* (Freire Júnior, Doria Neto and Aquino, 2005), in comparison to the model that use the moment rule, at the moment of training, a large variation in results was observed, so that it was necessary a large amount of training to reach the ideal values. Notwithstanding the best models, in terms of the correlation coefficient values and RMS were the models with the *Rprop* algorithm, as shown in Table 3.

6 CONCLUSIONS

According to the approached in this work, it is possible to assert that:

- The model with the best values of RMS and correlation coefficient was the ANN Rprop with three inputs.
- The mixed Rprop ANN model presented excellent results, being the most recommended for utilization than the mixed Rprop ANN with three inputs, due to its generalization capability, since it is associated with the Halpin-Tsai model.
- It was shown the capacity of the *Rprop* algorithm in the prediction of the transverse elasticity modulus (E_2), serving as a new tool to determine this mechanical property.

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