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The use of ANN technique to model the mechanical behavior of nanocomposites

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Abstract – Composite materials make possible the increase of strength by the incorporation of fibers and particles into polymers. The use of nanometric sized particles has enhanced the variation of properties with a smaller load of fillers. In this work, we attempt to approximate the experimental behavior of nanocomposites by using an artificial neural network. This technique allowed the modeling of Young's modulus of nanocomposites. A good approximation was obtained, as the correlation between the data and the response of the network was high, and the error percentage was low.

Composite materials became very popular due to improvements on certain properties achieved by the mixture of two different components. Initially, these materials were made, mainly, of E-glass and carbon fibers dispersed in a polymeric material. Fiber reinforced materials provide great improvement on material's mechanical properties, when used on concentrations beyond 30%. Nowadays, a new class of composites is being studied where at least one of its filler dimensions is on the nanometric scale. These nanocomposites evidence a property enhancement with lower concentration of filler (below 10%). Numerical and analytical models are essential tools for studying the controlling parameters of composites as well as nanocomposites' properties. The Young's modulus is one of the most studied properties of materials, once it measures the stiffness of the material. Although fiber reinforced composites have already several models to predict their behavior, nanocomposites don't have any good analytical model yet. Several models were proposed [1], but they either have some restrictions or the results get worse as the relationship stop being linear.

In this work we use a computational intelligence technique called Artificial Neural Network (ANN) to model the Young's modulus in terms of the matrix modulus and filler's characteristics: material, weight fraction, diameter and aspect ratio. ANN is a technique which mimics the behavior of a biological neuron and has been widely used in problems of series prediction, recognition of standards and function approximation [2]. It is a non-linear mathematical model used to find complex relationships between inputs and targets of a function. Each of the processing elements (PE) or neurons is represented as a nonlinear function, and is related through the pounded sum of the PEs output and the weights (coefficients). In order to achieve this approximation, it's necessary to collect enough data and divide them in three sets: training, validation and test. The first one is used to obtain the parameters of the network, the second one avoids the over-fitting of the training data, and the test set is used to verify the generalization of the network, presenting values that haven't been used yet.

The data used in this work was collected from experimental essays available on the literature. It consists of 13 matrices and 8 nanofillers, summing up 151 experimental elements. This data was randomly divided in the following way, 75% was used to the training set, 15% to the validation set and 10% to the test set. The topology used was the Multi-Layer Perceptron [2], with two hidden layers. The network acquisition was made using the Levenberg-Marquardt algorithm [3], varying the number of PEs and choosing the network with lower Mean Average Percentage Error (MAPE) of the validation set. In the first layer, the number of PE's was varied from 2 to 10 neurons, while in the second one, from 0 to 4. The input data was normalized from 0 to 1 to all variables, except for the filler concentration, which was normalized in the range [0, 9], enabling the user to increase the maximum load of nanofillers.

The resultant network presented MAPE values of 8.31, 4.96 and 7.82% for the training, validation and test sets, respectively. This means that the achieved approximation got close to the experimental data. Other useful metric used was the correlation, which was 0.951, 0.974 and 0.997, for the training, validation and test sets, respectively. This result shows that the network output follows the trend of the experimental data. The results presented above enables the use of this proxy to decrease the costs of synthesis of new nanocomposite materials, as they give a very good indication of best input set to obtain the desired elastic modulus.

References

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