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Towards smart modeling of mechanical properties of a bio composite based on a machine learning

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ABSTRACT

The main interest in many research problems in polymer bio composites and machine learning (ML) is the development of predictive models to one or several variables of interest by the use of suitable independent inputs or variables. Nevertheless, these fields have generally adopted several approaches, while bio composite behavior modeling is usually based on phenomenological theories and physical models. These latter are more robust and precise, but they are generally under the restricted predictive ability due to the particular set of conditions. On the other hand, Machine learning models can be highly efficient in the modeling phase by allowing the management of high and massive dimensional sets of data to predict the best behavior of bio composites. In this situation, biomaterial scientists would like to benefit from the comprehension and implementation of the powerful ML models to characterize or predict the bio composites. In this study, we implement a smart methodology employing supervised neural network models to predict the bio composites properties presenting more significant environmental and economic advantages than composites reinforced by synthetic fibers.

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1. INTRODUCTION

The prediction of the bio composites behavior is a critical problem both in bio composites research, design, and development. Several research were conducted to model bio composites based on natural loads [1]–[7] physical and mathematical-based models were the standard key to predict bio composites properties. However, these models are more idealistic because they are restricted to unbroken interfacial conditions and perfect microstructures. Other numerical models describing several physical scenarios of bio composites were studied. Nevertheless, these phenomenological methods usually use complicated analytical expressions challenging to resolve computationally demanding. As well, these models often depended on different empirical parameters obtained from experimentation. This limits using the phenomenological models because the parameters obtained are limited to the studied bio composite [8]. From a simulating standpoint, the desired goal of these models is facilitating the simulating design process of bio composites. In other hand, the predictive methods are studied to help in choosing the best appropriate bio composite constituents (matrix type, fiber type architecture, sizing, and content) so that resulting bio composite part will be able to carry the anticipated loads to specific applications.

The importance of predicting and characterizing the bio composites behavior has conducted to several published research in the subject [9]–[12]. However, these investigations are usually assigned to a

specific combination of process parameters, manufacturing process and materials constituent or life conditions. A lot of studies are focused on the optimization of particular manufacturing process by using the effects of process parameters in the behavior of bio composites, with keeping matrix type, fiber type architecture, sizing, and content constant. On the other hand, studying the manufacturing processes effect on the resulting bio composite [13]. Other research focus on life conditions effects, like environmental history and loading, on the studied bio composites behavior [14], [15]. Each of these researches will help to understand and predict a specific bio composite behavior. However, they are not utilized far away a specific application, limiting their wider utility. When modeling a bio composite, researchers generally mention their own tests and experiences and are based on predefined methods in selection, property predictions and materials classification. Practicing engineers would rarely study outside their zone of comfort to experiment new processes or constituents, as the introduction of a new process will imply a rigorous effort of trial and error with a high cost prior to reaching the maturity and profitability process. We can avoid this problem of expensive experiments trial and error during the modeling of bio composites through using the appropriate collective knowledge in bio composite field. The several studies investigating these materials behavior could be manipulated by machine learning to select the suitable manufacturing process and components materials for any particular bio composite application.

Unlike physical methods, during the modeling of bio composites, machine learning (ML) models could be highly efficient as they enable managing large and high dimension of data sets in order to obtain the best desired behavior [16], [17]. Nowadays, these intelligent methods are used to create predictive approach for biomaterial modeling. For example, these techniques are successfully applied to predict some metals properties, like microstructure [18] and plastic behavior [19]. They are also studied for atomistic modeling [20], electronic component [21] and predictions of chemical similarity [22]. In these conditions, biomaterial scientists want to benefit from the comprehension and implementation of some powerful machine learning methods, to characterize or predict the behavior of bio composites. In this study, we will present a systematic methodology to predict the young modulus of polypropylene reinforced with horn powder using supervised ML models.

2. PROPOSED METHOD

The method proposed for using ML techniques to predict targeted properties of the bio composite includes three phases: i) preparation of data, ii) ML model building, and iii) evaluation. As described previously, each phase is divided to several steps. The main ingredients of the method proposed are illustrated schematically in Figure 1.

2.1. First phase: data preparation

The first stage includes gathering all data available pertinent to the bio composites behavior. The objective is to assemble an understood data base which can be used to build a predictive machine learning model. As presented in Figure 2, this stage consists itself of 3 steps: data structuring, compilation, and cleaning.

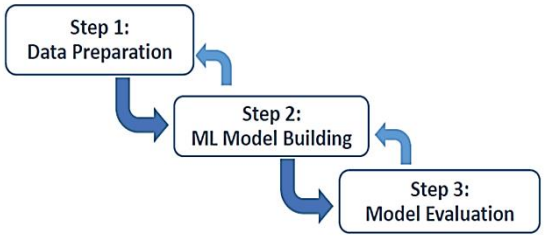

Figure 1. The steps of predicting bio composites behavior with machine learning

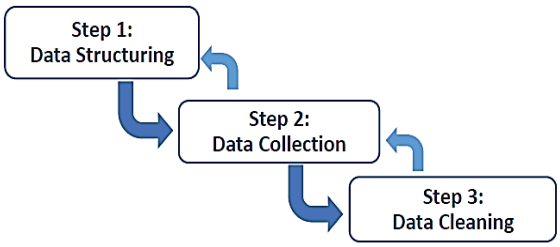

Figure 2. The data preparation steps of the ML Methodology

2.1.1. Data structuring

In this stage, it is important to carefully decide process variable and appropriate material relevant influencing the modeled bio composite. For instance, all parameters known or suspected of influencing the rigidity in polymer bio composites need to be used throughout this stage to stop the duplicating process. The relative significance of these parameters, often referred to explanatory variables in ML context by respecting the output behavior could usually be calculated once the machine learning model is constructed. Certainly,

natural fibers parameters like the content, type and architecture have to be considered. Likewise, it is important to consider the matrix type, filler, and content of filler in addition to the processing temperature. The processing processes used to produce the polymer bio composites may also influence their behavior and have to be considered. Furthermore, parameters that reflect the conditions of the life span or other essential variables, as they are known to influence the bio composites behavior, component thickness and void content (or a typical dimension) must be considered. Most articles published and sources data will not document all variables considered.

Additional attractive property of a lot of ML methods is the probability of building models with missing values in the constructed database. A distinction of every explanatory variable is needed in most instances. For example, natural fibers architecture could be categorized into hybrid, random, multidirectional, and unidirectional architectures. The type of matrix can be classified into the main resins known and so on. This step is crucial as a careful classification of explanatory variables, and a good-defined distinction for each one of them is necessary for any learning method algorithm to be used successfully.

2.1.2. Data collection

In this phase, extensive bio composite data relative to the predicted behavior needed to be generated from scientific publications, industrial data technical reports of all phases implied in the method proposed, this phase is the most consuming and tedious time. However, it is the constructed bloc upon which the model is constructed. The ML predictive model accuracy would depend on the diversity and size of the analyzed database. Consequently, an evolving database could be built progressively. In the process, several published materials focusing on the behavior needed to be checked before the data could be retrieved. This phase is ideally performed after structuring data to avoid the duplicating collection data.

2.1.3. Data cleaning

In this stage, to ensure quality of data, the accuracy of all recovered values needs to be evaluated. The accuracy of machine learning predictive models could be immensely harmed by incorrect data. These inaccurate data could occur during recovering data from literature and inserting the data into the database. All inserted values have to be double tested to ensure that no incorrect value was wrongly included in database. In situation of doubt, same author's publisher research has to be evaluated to verify the value reported.

2.2. Second phase: building the machine learning model

Second phase also involves 3 steps as presented in Figure 3. An efficient machine learning method needs to be chosen. After, the trained data have to be selected from the dataset collected in order to apply the chosen ML algorithm for constructing the model. The final step involves constructing a predictive ML model that could imply a relation between a possible explanatory set of variables (as well as independent variables) and a particular property of material (dependent response or variable). The model prediction performance could be evaluated to check the input variable's ability to explain the difference in the targeted bio composite behavior.

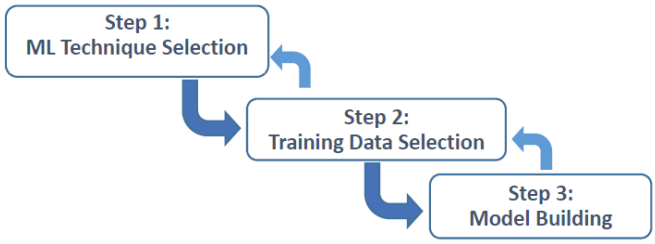

Figure 3. The model building steps of the ML methodology

2.2.1. Machine learning method selection

A wide variety of sophisticated learning algorithms are accessible, using neural networks, decision trees, Bayesian networks, and among others. This step implies a careful choice of the most supervised appropriate technique for simulating the predicted behavior. For example, in case of missed values. The random-forests algorithm could be chosen as it deals well with ignored values and mixed data. Other forms of the database compiled have to be taken in consideration like the nonlinearity handling and robustness to outliers.

2.2.2. Training selection data

In order to determine the predictive ability of the ML algorithm chosen, the processed dataset requires being separate into 2 subsets: i) a trained dataset containing most of the data collected and ii) remaining data, called unknown or validation data. The training data size have to be a balance between how training the model, and how evaluating its predictive ability. The chosen ML algorithm would be used to the trained data to construct a predictive model explaining the analyzed bio composite behavior variations based on a large variety of process and material variables (explanatory or independent variables).

2.2.3. Model building

In this phase, the chosen algorithm is now run on the trained data. The obtained predictive model will provide a correlation between the bio composite properties and the explanatory variables with a quantitative predictive precision. Several algorithms may determine each independent variables contribution the interpretation of the response variability in the resulted predictive model.

2.3. Model evaluation

Phase 3's objective is the predictive performance evaluation of the model. Consequently, the ML predictive performance model requires to be checked using the ignored data, also related to as data test. The chosen algorithm has to be used for predicting the unseen dataset response, and the responses predicted have to be compared to the actual responses. The accuracy obtained can be a best indicator of the bio composites behavior predictive model to be designed.

Another important characteristic of most ML method is their capacity to discern the explanatory variables effect on the behavior predicted. Explanatory variables can therefore be categorized to their effect on the targeted bio composite behavior. This could be more helpful when extending the database by trying to redefine the explanatory variables to be collected in the first phase.

3. RESULTS AND DISCUSSION

3.1. Predicting Young modulus of polypropylene reinforced by horn fibers with the finite element method

In order to test the performance of the machine learning model constructed, we used the finite element method widely known by its efficiency in determining the properties of complex structures but with a large time of computing [20]–[25]. The number of elements and nodes is respectively 170,152 and 290,352. The Figures 4 and 5 show respectively the geometry created and the mesh obtained by the FEM [24]–[28].

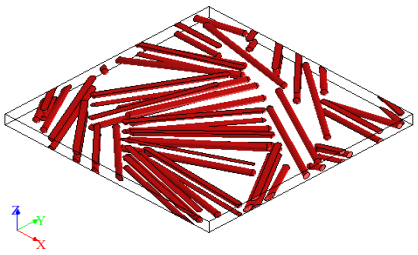

Figure 4. Geometry created for the bio composite

Figure 5. Mesh obtained for the bio composite

3.2. Predicting the Young modulus of polypropylene reinforced by horn fibers with machine learning model

Using the analyzed methodology, we studied the predicted Young modulus of polypropylene reinforced by horn fibers. The Figure 6 presents the machine learning model. The Tables 1 and 2 present the machine learning algorithms and progress parameters. The evaluation of machine learning neural network performance could be performed by two indicators. They are the correlation-coefficient (R) and mean square-error (MSE). Figures 7, 8, and 9 present the MSE, training network and correlation-coefficient at 6 epochs. The more R value is nearest to 1 and the more the MSE is smaller, the better NN is efficient. Smaller value of MSE (0.827) is determined for the bio composite Young modulus prediction (1229.0963 MPa) in comparison with the finite element method (1229.2 MPa). The best performance is also observed in terms of the correlation-coefficient, with an R closest to 0.99999 for training and validation and 0.97503 for test which validate the performance of the machine learning neural network model selected.

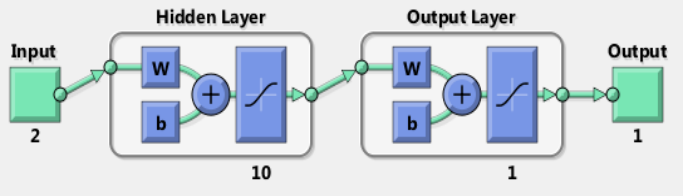

Figure 6. Machine learning model

Table 1. Machine learning algorithms parameters

Parameters	Type
Data division algorithm	Random
Training algorithm	Levenberg-Marquardt
Performance algorithm	Mean-Squared Error
Calculation's algorithm	MEX

Table 2. Machine learning progress

Parameters	Values
Iterations	6
Performance	0.679
Gradient	11.2
Mu	0.1
Validation Checks	6

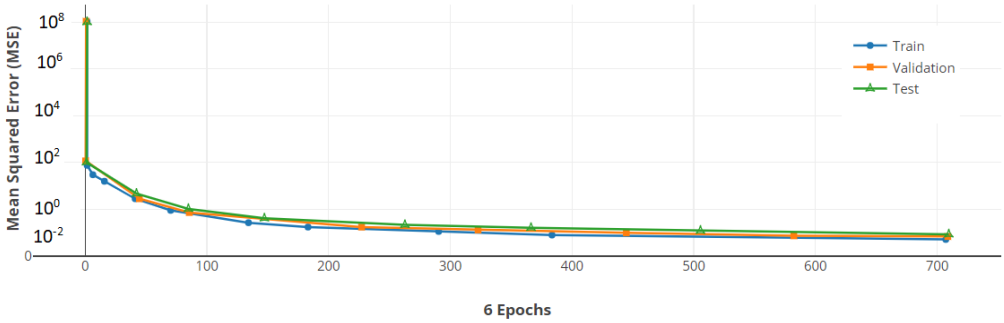

Figure 7. Machine learning model

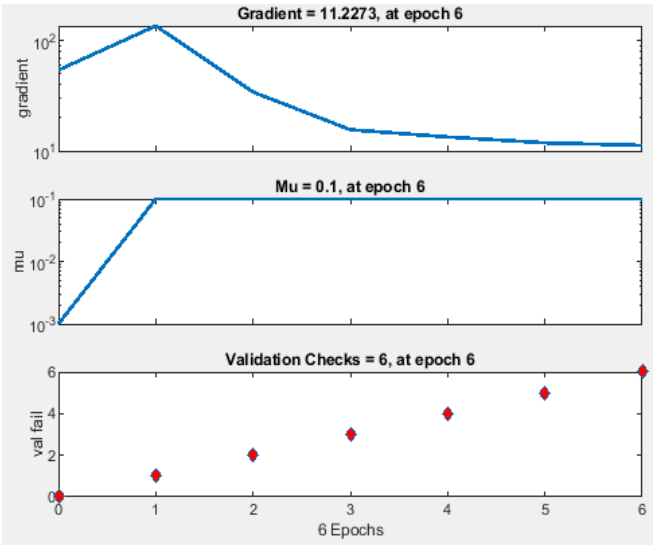

Figure 8. Machine learning training state

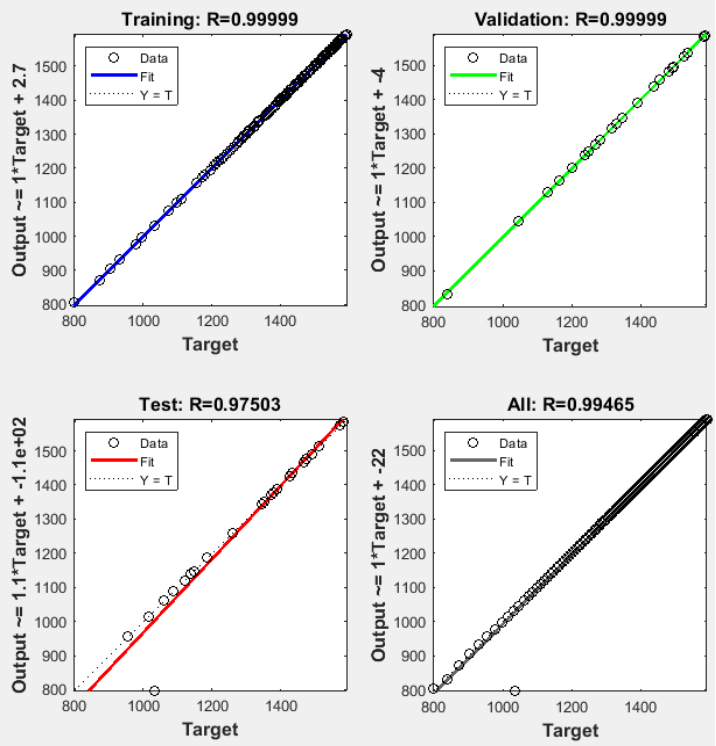

Figure 9. Machine learning correlation coefficient

4. CONCLUSION

A general methodology is studied for predicting the bio composites behavior by using supervised ML models. The machine learning method will predict particular bio composite properties by taking into account their manufacturing processes constituents, expected life span and process parameters. The chosen methodology, based on the application of ML methods to the all knowledge in the bio composite materials field, implies three stages. First, a database is compiled from technical reports, industrial data, and research articles. Second, the best appropriate supervised statistical learning is utilized to construct a predictive method that explains the investigated behavior based on a best process variables and selected material. Third, the built model predictive performance is assessed, and the used explanatory variables importance is evaluated. This anticipated approach offers the efficiency to significantly get better the design process for bio composite materials. It will improve the trial-error iterations by the refinement of the primary selection of bio composite manufacturing process parameters and constituents for any particular application. In this paper, we studied the mechanical behavior of polypropylene reinforced by horn fibers. It will be attractive to study the thermo mechanical behavior and perform other tests on this bio composite like aging and fatigue tests. Additional bio loads of plant or animal source can be analyzed for the reinforcement of this polymer using digital modeling and experimental tests.

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