Available online at www.eccomasproceedia.org
Eccomas Proceedia SMART (2023) 911-922

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X ECCOMAS Thematic Conference on Smart Structures and Materials
SMART 2023
D.A. Saravanos, A. Benjeddou, N. Chrysochoidis and T. Theodosiou (Eds)

RIGHT-FIRST-TIME MANUFACTURE OF SUSTAINABLE COMPOSITE LAMINATES USING STATISTICAL AND MACHINE LEARNING MODELLING

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Abstract. The design and behaviour of advanced composite material systems have been investigated and studied for several decades now. A huge amount of time-consuming experimental tests supported by analytical and numerical models have been used extensively to gain a better understanding of the material's behaviour and, ideally, predict the performance of a composite structure under specific loading conditions. Composite materials, being an inherently complex structure with more than one constituent, require extremely intensive computational effort to maintain sufficient accuracy of the numerical models in the behavioural prediction, with a highly time-consuming solution process. For the above reasons, this paper uses a set of statistical and machine learning modelling methodologies to optimise the design and manufacture of sustainable composite laminates made of flax and basalt fibres. A preliminary Design-of-Experiments (DoE) was constructed which included manufacturing parameters, such as temperature, pressure, and time of the curing cycle as well as variations in the material layers of the laminate. A series of laminates were manufactured using a hot press compression moulding process and experimental tests were performed to characterise the behaviour of each laminate. Machine Learning (ML) models, including Gaussian Process Regression (GPR) and Bayesian Regularized Artificial Neural Network (BRANN) models, were then developed, capable of predicting the mechanical properties of the laminate so that extensive experimental testing can be minimised.

Keywords: composites manufacturing, machine learning, AI, sustainable composites, sustainability

1 INTRODUCTION

Fibre-reinforced polymer composites are an important structural material in many advanced applications, including aerospace, automotive, space and marine sectors, owing to their excellent mechanical properties. Their use in highly demanding applications means that their structural integrity is of utmost importance, with efforts on the prediction of remaining life or their sudden failure being at the forefront of the composites' scientific community. Over the

Peer-review under responsibility of the organizing committee of SMART 2023.
doi: 10.7712/150123.9843.451122

past two decades, more sustainable lightweight materials have been adopted in various non-load-bearing engineering applications as an environmentally friendly alternative to synthetic fibre-reinforced materials. Over the years, several labour-intensive experimental procedures and time-consuming analytical/numerical analyses have been performed to achieve the design optimisation of composite structures, following international testing standards as well as various non-destructive testing (NDT) to determine the residual properties and critical remaining life of composite structures [1],[2]. With the advancements of technology and computing power, more accurate methods have been developed to facilitate the nano/microstructural observations and measurements in composite materials, including Scanning Electron Microscopy (SEM), X-ray micro-Computed Tomography (mCT), Differential Scanning Calorimetry (DSC) and Fourier-transform infrared spectroscopy. Machine Learning (ML) has become increasingly valuable to enable right-first-time manufacture of materials and reduce the volume of non-added value processes such as inspection [3; 4; 5]. The application of deep learning in the optimisation and prediction of the properties of composite materials is mainly focused on training datasets, algorithms and output data [6]. In the traditional design processes of composites, several manufacturing attempts are required, due to the large number of design variables available, to achieve the desired final product's properties and performance. Additionally, several analytical and numerical tools, detailed finite element (FE) models and simulations have assisted these processes, however, their accuracy is not always aligned with their time and cost efficiency. These limitations have driven research into more efficient methods for the properties prediction of composite materials using deep learning techniques.

Researchers have used neural networks in forward propagation processes, where they map from input to output space, by running iterations until the optimal topology is obtained. The use of neural networks to predict the strength of glass/epoxy composite laminates was implemented by Kumar et al. [7] using data collected from acoustic emission measurements of the flexural behaviour of the material after being submerged in seawater. Altarazi et al. [8] built a detailed Artificial Neural Network (ANN) model to predict and optimise the tensile strength, ductility and density of composites, based on weight measurements of the constituents. The use of SEM images for the training of the model was proposed by Li et al. [9] to predict the effective modulus of a complex heterogeneous composite sample consisting of multiple mineral constituents. The model used SEM images to generate a large number of stochastic samples and the FE method to create the labels on the dataset, which represent the modulus of the samples. Alongside SEM images, which contain a great amount of information about the microstructure of the materials, X-ray images have also been used in the work from Tong et al. [10] to assist the characterisation of the tested samples in an attempt to use a deep learning method to characterise carbon fibre reinforced cement-based composites in terms of the carbon fibre distribution in the composites and predict the properties of the material. Computational modelling and other analytical methods are critical to analyse and understand the behaviour of materials and structures, having increased drastically their accuracy with the advancements in the computational power available. However, the time required for high-accuracy analyses remains high, whereas the use of deep learning methods can become beneficial, significantly reducing the calculation time. Yang et al. [11] proposed a deep learning model that combines datasets produced by FE simulations and information localised from macro-scale to micro-scale material level, in order to efficiently predict the microscale elastic strain field of 3D composites. This localisation method is critical in assessing and predicting failure-related properties of composite materials. In another work, Gong et al. [12] trained a deep transfer learning model to obtain domain-invariant features and used a label classifier to identify and detect inclusion defects in aerospace composite materials. The results are a strong indication that a high accuracy of above 96% can be achieved in a real-time detection system that can be applied efficiently for health monitoring of composite structures. Furthermore, using data and images from thermography, an NDT imaging method used widely to detect defects on materials by observing heat patterns. Bang et al. [13] prepared carbon fibre composite samples with artificial defects and evaluated the damage identification process using a Convolution Neural Network (CNN)-based model. The lack of data, however, was concluded in this study as the main source of low overall accuracy of the methodology, suggesting further improvement by enlarging the obtained data set.

Another aspect that research on optimisation of composite structures can be applied is the Topology Optimisation (TO) of structures, which is widely used in the automotive and aerospace industries to design lightweight structures. TO is a valuable tool in the early design stages to find the best materials distribution and patterns to maximise the structure's performance while adhering to design specifications and constraints. A promising application of a deep learning model for TO has been proposed by Kollmann et al. [14], which used three input images and produced an output image, and the predictions were very close to the ground-truth image. Other researchers [15],[16] have also developed CNN models to predict optimised designs, when a set of operating conditions is required (e.g. loads, boundary conditions, etc.) or to design the manufacturing processes of composite structures for the optimisation of the textiles' formation, to avoid flaws due to manufacturing. The benefit of such ML models was provided to the designers to explore alternative designs without the need for laborious and computation-intensive FE simulations. It is, therefore, evident that, although the use of deep learning in composites design has now started to be realised, the difficult-to-follow processing principles applied, and the lack of materials data hinder the desired accuracy that the ML models need to achieve. In order to be able to identify, quantify and decide on fabrication-induced defects in composite materials and evaluate the evolution of damage under different loading conditions that a composite structure may undergo, more reliable algorithms and materials models are required to assist the effectiveness and accuracy of the deep learning processes.

In this paper, the performance of sustainable composite laminates manufactured using a variety of different fabrication parameters was investigated under tensile testing, flexural testing, and shore hardness testing. The composite laminates were fabricated using hand lay-up and compression moulding process, considering different fabrication parameters combinations. Gaussian Process Regression (GPR) and Bayesian Regularized Artificial Neural Network (BRANN) models were developed and implemented with categorical covariates to predict several different mechanical properties, including shore hardness, flexural modulus, flexural strength, tensile Young's modulus, tensile strength and tensile strain at break. The generalization performance of both models was evaluated using k-fold and leave-one-out cross-validation procedures.

2 MATERIALS AND MANUFACTURING

For this study, a series of sustainable composite laminates was manufactured using compression moulding process and hand lay-up with a combination of non-woven flax (F) fabric and 2x2 twill woven basalt (B) fibre fabric reinforcing an epoxy resin matrix (EL2, EasyComposites). The fabrication process was based on the Design-of-Experiment (DoE) constructed to incorporate different fabrication parameters. Four variable manufacturing parameters were studied: (i) the lay-up configuration of the plies, (ii) the curing temperature, (iii) the curing time and, (iv) the curing pressure during the curing cycle. Each parameter had two levels of variation and curing temperature had three levels of variation, as shown in Table 1. A total number of 24 laminates were manufactured for the current study.

Table 1: Manufacturing parameters used for composite laminates fabrication.

Variables	Unit	Level 1	Level 2	Level 3
Lay-up	-	F-B-F-B-F-B	B-F-F-F-B	-
Curing temperature	°C	50	70	90
Curing time	min	120	150	-
Curing pressure	MPa	80	110	-

Different testing coupons were cut from these panels using a laser cutting process, including 5 tensile testing coupons from each laminate, according to the ASTM D3039 standard and 5 3-point bending coupons from each laminate, according to the ASTM D7264 standard. Samples from each laminate are shown in Figure 1.

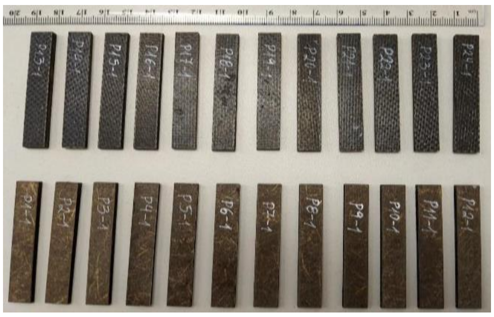


Figure 1: Samples cut from 24 composite laminate panels.

3 EXPERIMENTAL METHODS AND RESULTS

The experimental strategy followed in this work included three testing procedures in order to identify important mechanical performance and characteristics of the fabricated laminates, in order to be used for the statistical analysis. The experimental tests conducted are: (i) shore hardness testing, (ii) tensile testing and, (iii) flexural testing.

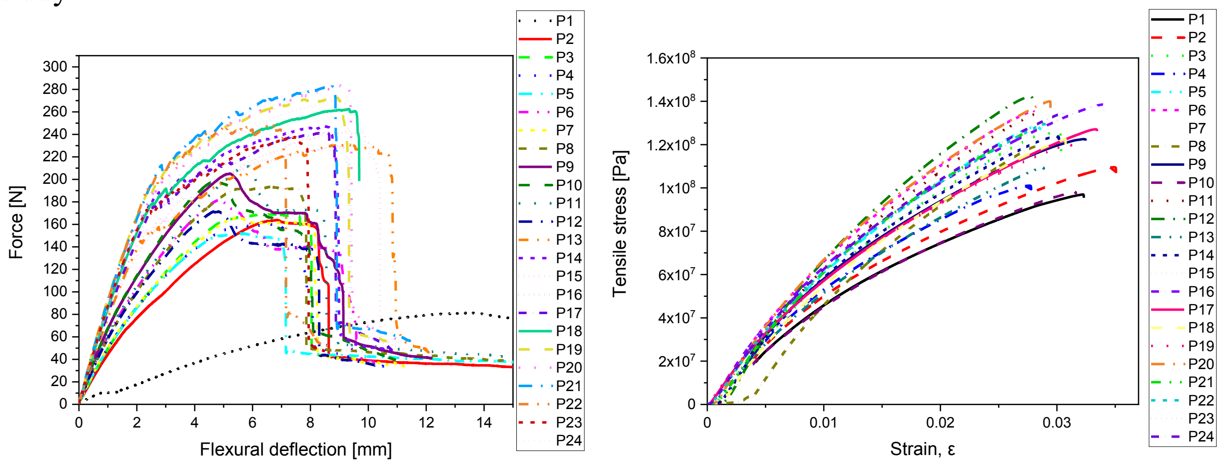
3.1 Shore hardness test

The hardness of the front and back faces of each panel was measured using a Zwick Roell

Shore D hardness tester. A total of ten measurements were taken at different locations on each face of the panel and their average was reported as the hardness value.

3.2 Flexural test

The flexural tests were performed on the 5 coupons from each laminate using a Universal Testing Zwick machine with a maximum load cell of 30 kN according to ASTM D7264 standard. The average flexural deflection-force curves that describe the flexural behaviour of each laminate are shown in Figure 2(a). The differentiation that is observed in the flexural response of the coupons from Panel 1 is due to the different span length that was used during the test. However, it can be assumed that the values of flexural strength are not significantly affected [17]. From each test, the flexural modulus and the flexural strength were calculated and considered as the output variables for the training of the predictive models used in this study.



(a) (b)

Figure 2: (a) Flexural deflection-force curves and (b) Tensile strain-stress curves for the 24 panels.

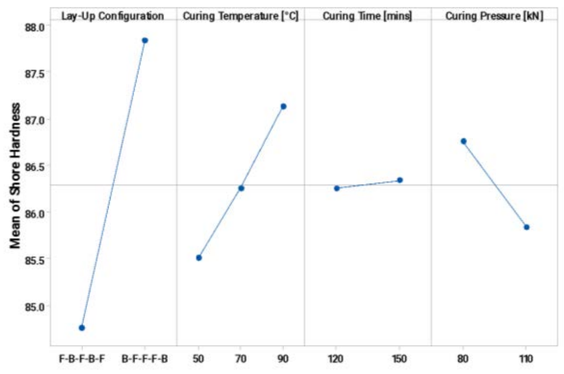
3.3 Tensile test

The tensile tests were performed on all 5 coupons from each laminate using a Universal Testing Zwick machine with a maximum load cell of 30 kN and in accordance with ASTM D3039 standard. The average strain-stress curves that describe the tensile behaviour of each laminate is shown in Figure 2(b) for the 24 composite laminates (P1-P24). From each test, the tensile Young's modulus, the tensile strain at break and the tensile strength were calculated and considered as the output variables for the training of the predictive models used in this study.

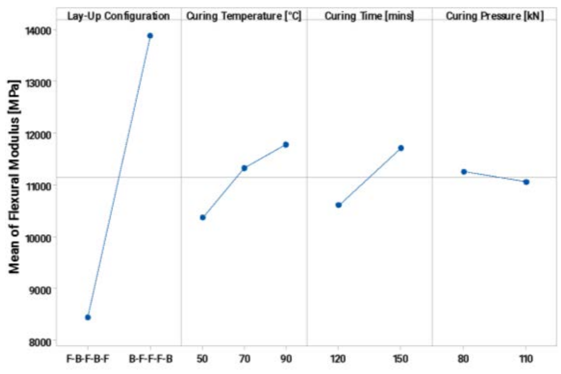
4 ANOVA AND PREDICTIVE MODELLING

4.1 Main effects plots

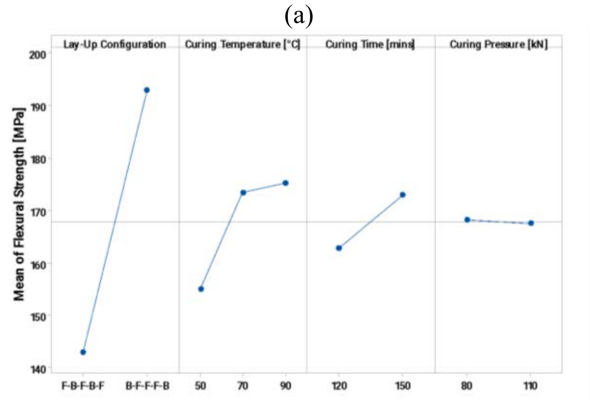
A general full factorial design was adopted with four experimental factors, as shown in Table 1, (i) lay-up configuration (two levels), (ii) curing temperature (three levels), (iii) curing time (two levels) and, (iv) curing pressure (two levels). Figure 3 shows the main effect plots that were created using Minitab for all the output variables studied, namely shore hardness, longitudinal Young's modulus, tensile strain at break, tensile strength, flexural modulus and flexural strength. As can be seen, the lay-up configuration greatly affects all the output variables, demonstrating the highest contribution on the outputs, apart from the tensile strength (Figure 3(f)), that the effect of the lay-up is less than the other outputs. The results indicate that the basalt (B) layer on the top and bottom surfaces of the composite laminate (B-F-F-F-B laminate) increases all the mechanical properties studied, providing a better longitudinal and flexural performance overall. A similar behaviour is observed for the curing temperature across all the studied outputs, which demonstrates an increase with increasing temperature. The only output that the curing temperature does not have a great influence is the tensile strain at break, as shown in Figure 3(e), where the line is almost horizontal, showing a minor effect. The change in curing time from 120 min to 150 min also increases the value of all the outputs, with the greatest influence being on the tensile Young's modulus (Figure 3(d)) and the lower effect being observed for the shore hardness (Figure 3(a)), where the line appears almost horizontal. Finally, the curing pressure seems to affect the least all the selected output variables, apart from the shore hardness (Figure 3(a)), which demonstrates the most influence due to the increase of the curing pressure.



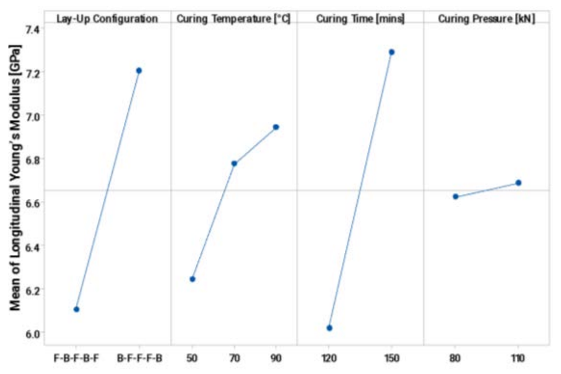
(a)



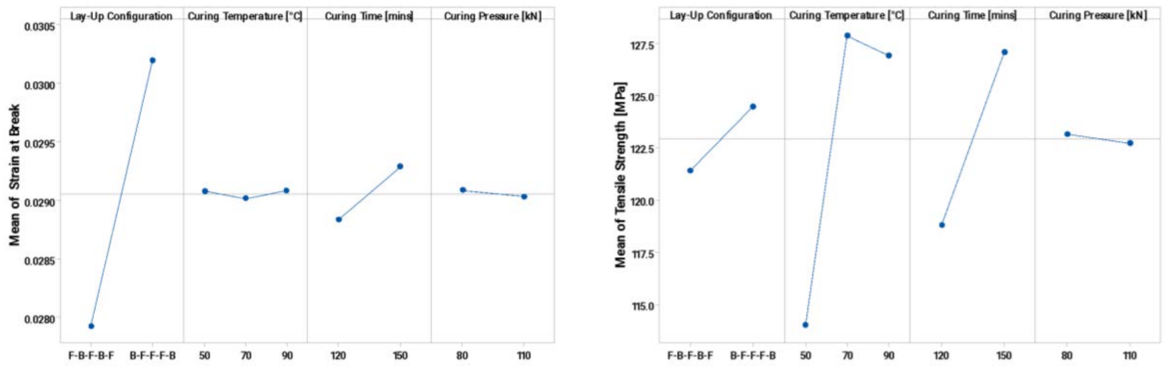
(b)



(c)



(d)



(e) (f)

Figure 3: Plots of main effects for (a) shore hardness, (b) flexural modulus, (c) flexural strength, (d) longitudinal Young's modulus, (e) tensile strain at break and, (f) tensile strength.

4.2 Gaussian Process Regression and Bayesian Regularized Artificial Neural Networks

In this work, supervised learning models for regression with categorical covariates were developed and implemented in MATLAB. Therefore, dummy variables have been created from the design matrix. ML models including GPR and BRANNs were trained to predict the mechanical behaviour of composite laminates. GPR models are non-parametric kernel-based probabilistic models that are widely used to learn input-output mappings from data [18]. In particular, a Gaussian process is fully specified by its mean, $m(\mathbf{x})$, and covariance (kernel), $k(\mathbf{x}, \mathbf{x}')$, functions, where $\mathbf{x}$ and $\mathbf{x}'$ are input variables of dimension d. The mean function and the covariance function of a real process, $f(\mathbf{x})$, are defined as

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})] \tag{1}$$

and

$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))], \tag{2}$$

respectively. The Gaussian process can be written as

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')). \tag{3}$$

Given an input-output training dataset of n observations, $\mathcal{D} = \{(\mathbf{x}_i, \mathscr{y}_i) | i = 1, \ldots, n\}$, where $\mathscr{y}$ denotes a (scalar) dependent variable, it is typical to assume that the true response $\mathscr{y}$ differs from $f(\mathbf{x})$ by additive noise that follows an independent, identically distributed Gaussian distribution with zero mean and variance σ_n^2, thus $\mathscr{y} = f(\mathbf{x}) + \epsilon$, with $\epsilon \sim \mathrm{N}(0, \sigma_n^2)$. The variance σ_n^2 is estimated from the data. It is common to consider Gaussian processes with a zero mean function. Therefore, the joint distribution of the true responses, $\boldsymbol{\mathscr{y}}$, and the test responses, $\boldsymbol{f}_*$, under the prior $\mathrm{cov}(\boldsymbol{\mathscr{y}}) = K(X, X) + \sigma_n^2 I$, can be written as

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathrm{N}\left(\mathbf{0}, \begin{bmatrix} K(X,X) + \sigma_n^2 I & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}\right), \tag{4}$$

where I is the $n \times n$ identity matrix, X is the $n \times d$ matrix of the training inputs, X_* is the $n_* \times d$ matrix of test inputs, $K(X,X)$ is the $n \times n$ covariance matrix, and $K(X,X_*)$ $K(X_*,X)$ and $K(X_*,X_*)$ denote the matrices of the covariances evaluated at all pairs of training and test points, test and training points, and test points solely, respectively. GPR with linear kernel is equivalent to Bayesian linear regression. When there is no or limited prior knowledge about the input-output mapping function, a zero mean function and a squared exponential kernel function are generally used. In this work, GPR models using a linear basis function and a squared exponential kernel function were developed to predict the mechanical properties of composite laminates.

BRANNs represent a robust class of ANNs that can reduce or even eliminate the need for cross-validation [19]. The developed BRANNs are feedforward neural networks with a single hidden layer of 5 tan-sigmoid neurons followed by a linear output layer. The BRANN models were trained for a different number of epochs up to 1000. Figure 4 shows a schematic representation of a neural network with a single hidden layer.

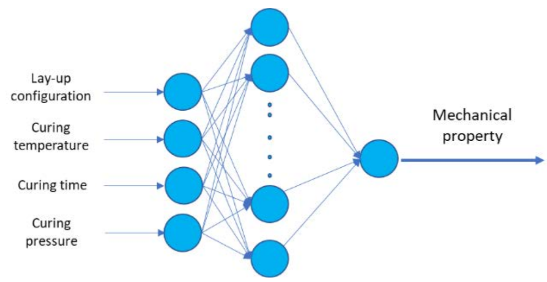


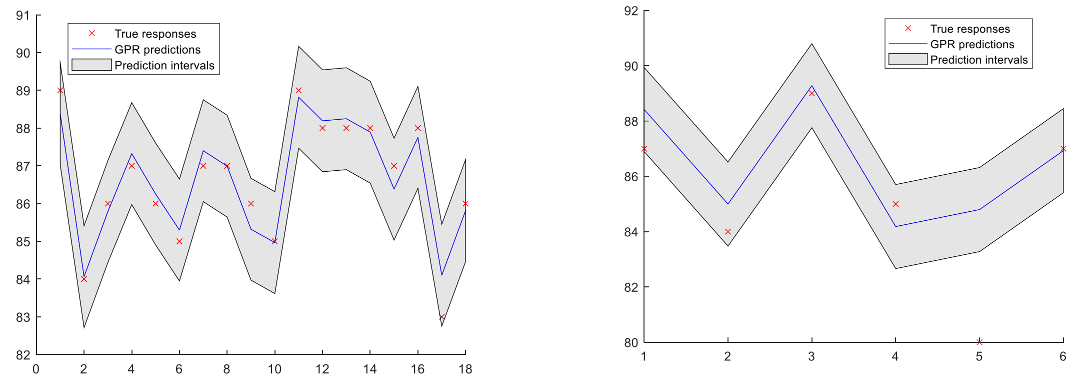
Figure 4: Schematic illustration of the ANN architecture.

To avoid overfitting, cross-validation procedures were used to assess the effectiveness of the models. Cross-validation is a statistical method of evaluating the generalization performance of a ML model. This method is commonly used to compare different ML models because it is more stable and thorough than using a simple train/test split approach [20]. There are various cross-validation techniques, such as *k*-fold cross-validation and leave-one-out cross validation. When performing *k*-fold cross-validation, the dataset is first randomly partitioned into *k* number of parts (of approximately equal size), called folds, where *k* is typically a user-specified number. Then, a sequence of models is trained using the *k-1* folds as the training set and tested using the remaining k^{th} fold. This process is repeated *k* number of times such that each fold is used as the test set once. In the end, an average value of the training and testing errors across all folds is calculated.

The dataset was split randomly into 4 folds of equal size to evaluate the ML models for each response variable (mechanical property) using *4*-fold cross-validation. In addition, the leave-one-out cross-validation was used to cross-validate the models due to the small size of the dataset. The leave-one-out cross-validation is a particular case of *k*-fold cross-validation, where

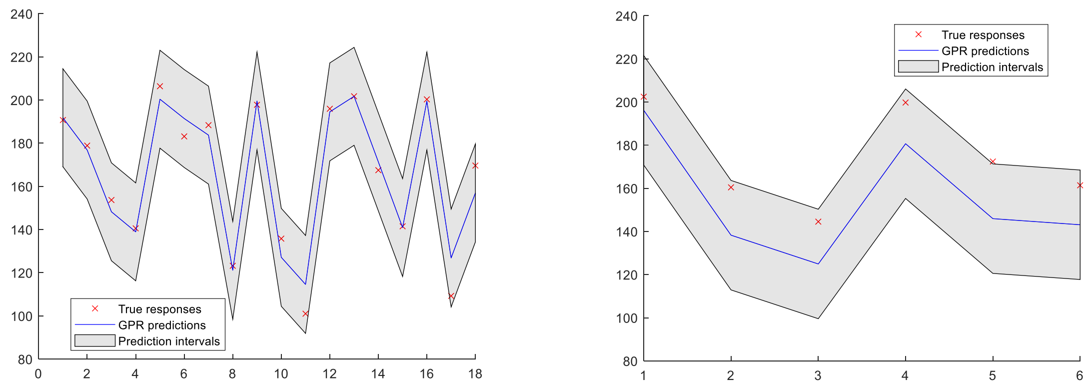
k is set to the total number of observations in the dataset. The leave-one-out cross-validation is particularly useful when dealing with small datasets since the model will use more training data points for learning in each iteration. The Root-Mean-Square-Error (RMSE) was utilized to evaluate the training and testing performance of the models.

As an example, Figures 5-7 show the observed data points, the GPR predictions and the 95% prediction intervals for different folds of the GPR *4*-fold cross-validation for some of the mechanical properties. The width of the prediction intervals represents the uncertainty in the predictions. The results show that the predicted responses cross or are close to the true responses, with almost all predicted responses being inside the prediction intervals. Tables 2 and 3 show the *4*-fold and leave-one-out cross-validation results, respectively, of both models for each mechanical property. A large difference between the training RMSE and the testing RMSE may be a sign of overfitting of the ML model. As can be seen from the results, both models are able to provide predictions of acceptable accuracy, especially by using the leave-one-out cross-validation approach due to the small size of the dataset. GPR models provide uncertainty estimates for their predictions, but the BRANNs were able to provide a greater balance between the accuracy of training and testing results compared to the GPR models in this case.



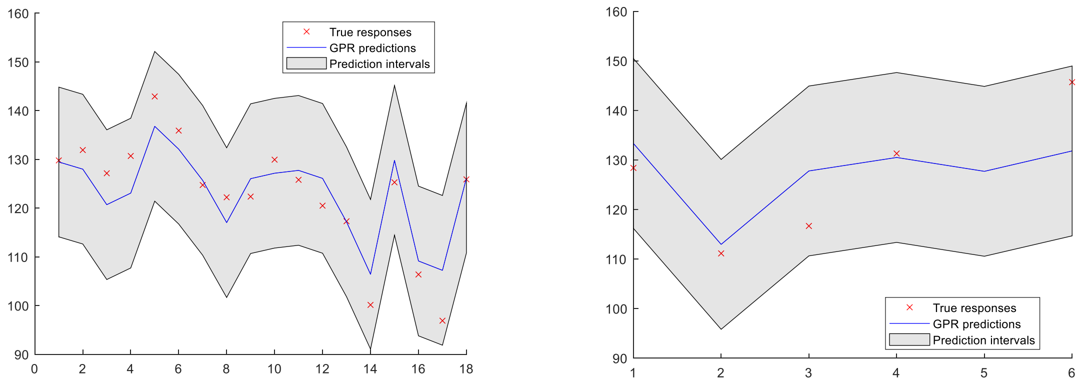
(a) (b)

Figure 5: GPR for shore hardness (Fold 3) (a) Train and (b) Test.



(a) (b)

Figure 6: GPR for flexural strength [MPa] (Fold 1) (a) Train and (b) Test.



(a) (b)

Figure 7: GPR for tensile strength [MPa] (Fold 4) (a) Train and (b) Test.

Table 2: *4*-fold cross-validation results.

Mechanical property	GPR		BRANN	
	Training RMSE	**Testing RMSE**	**Training RMSE**	**Testing RMSE**
Shore hardness	0.5719	1.4178	1.0302	1.5755
Flexural modulus [MPa]	498.9573	1238.4245	1766.6855	1484.9250
Flexural strength [MPa]	7.0574	19.1712	11.3632	19.5431
Young’s modulus [GPa]	0.4811	1.4386	0.8093	1.4365
Strain at break	0.0015	0.0030	0.0022	0.0026
Tensile strength [MPa]	4.7696	14.4552	9.9279	13.9368

Table 3: Leave-one-out cross-validation results.

Mechanical property	GPR		BRANN	
	Training RMSE	**Testing RMSE**	**Training RMSE**	**Testing RMSE**
Shore hardness	0.5987	1.0509	1.1279	1.1778
Flexural modulus [MPa]	517.5820	996.6772	801.8487	1240.6323
Flexural strength [MPa]	7.4580	13.6216	11.3592	15.4089
Young’s modulus [GPa]	0.4850	1.0416	0.9149	1.1828
Strain at break	0.0015	0.0022	0.0024	0.0019
Tensile strength [MPa]	5.1384	10.3356	9.9047	10.5260

5 CONCLUSIONS

In this preliminary study, a machine learning modelling approach has been employed to predict the mechanical properties (shore hardness, flexural modulus, flexural strength, Young’s modulus, strain at break and tensile strength) of flax/basalt composite material. Gaussian

Process Regression (GPR) and Bayesian Regularized Artificial Neural Network (BRANN) models were developed and implemented with categorical covariates and trained using experimental data to determine the effects of four manufacturing parameters namely (lay-up configuration, curing temperature, curing time, and curing pressure) on the aforementioned mechanical properties. The generalization performance of both models was evaluated using *k*-fold and leave-one-out cross-validation procedures. The performance metric utilised for evaluating the models was the Root-Mean-Square-Error (RMSE). The leave-one-out cross-validation of both models provided an improvement on the modelling accuracy as compared to the *4*-fold cross-validation due to the limited size of the dataset. The testing performance of the GPR model was slightly better compared to the BRANN for most mechanical properties, but the BRANN was able to provide a better balance between the accuracy of training and testing results. Although the proposed methodology can be used to determine effectively the optimum manufacturing parameters required to obtain the desired mechanical properties of the fabricated laminate, the developed models will benefit from additional data. Therefore, additional experiments will be carried out in future work.

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