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A MACHINE LEARNING APPROACH TO PREDICT MECHANICAL PROPERTIES OF CFRPS USING WCM PROCESSING PARAMETERS

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ABSTRACT

In the automotive industry, the final part quality is paramount to achieving the required mechanical properties. The part quality is determined during the manufacturing process and is dependent upon the manufacturing parameters used during production. One way to better define the set parameters that can deliver the highest part quality is by using Machine Learning (ML) models. For this study, flat plaques were produced by the Wet Compression Molding (WCM) process, and their respective manufacturing parameters such as thermal gradients, demolding characterization, and pressure profile were used as training data for the ML models. The ML models include Random Forest (RF), Gradient Boosting (GB), Multi-linear (MLR), and Support Vector Regression (SVR). Each model's predictive capabilities are validated by combining data obtained experimentally. Subsequently, the predictions are made to lessen resource-intensive experimental testing in future trials. This study aims to identify optimal processing parameters using the model to expedite the product development process, which currently employs a trial-and-error method.

1 INTRODUCTION AND STATE OF THE ART

WCM is a manufacturing process that can offer cycle times of less than five minutes, which is ideal for mass production in the automotive industry. In recent years, predictive ML models have become crucial, providing researchers with generalized models trained on experimental data, and ensuring high prediction accuracy. Once validated, coupling such a model with a new manufacturing process, material, or dataset is fast and reliable, eliminating the need for an inefficient trial-and-error approach to determine desired processing parameters.

When choosing a robust model, consideration of data types, desired outcomes, and computational time for training and testing must be at the forefront. In 2019, Golkarnarenji et al. [1] compared SVR with Artificial Neural Networks (ANNs) and determined that SVR outperformed ANNs for Young's modulus prediction with an average error of less than ±2.4%. In 2021, Chahboun et al. [2] compared MLR, SVR, and RF, for the hourly prediction of the power produced by photovoltaic solar panels. SVR demonstrated superior accuracy with a coefficient of determination (R^2) of 96% and a root mean squared error ($RMSE$) of 0.39 kW. In 2023, Omar et al. [3] evaluated ML models for crack propagation, with GB performing best compared to RF and SVR models. The objective of this study is to develop four ML models for the comparison and prediction of CFRP mechanical properties of WCM parts based on manufacturing parameters, and the flexural and interlaminar shear strength results supplied by the University of Windsor and the University of Waterloo.

2 MACHINE LEARNING MODELS

For this study, four models were trained and tested based on the following techniques: RF, GB, MLR, and SVR. These ML models were developed using input-output pairs composed of manufacturing parameters and experimental results obtained from mechanical testing. The model architecture and performance metrics are provided in Figure 1.

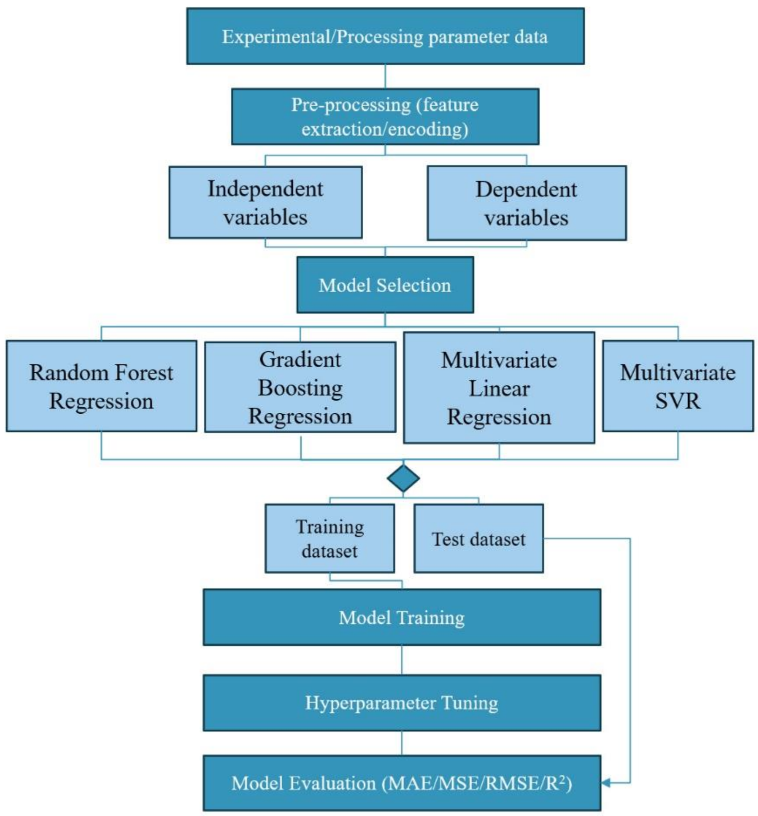

Figure 1: ML model architecture

Following pre-processing, the independent features with the highest correlation to part quality were chosen for model training. For each model development, 70% of the data was used for training, and 30% for testing the model. RF employs ensemble learning by averaging predictions from multiple decision trees trained on k samples from the dataset, where k is a hyperparameter chosen by the developer to reduce overfitting and enhance robustness. RF performs effectively on both large and small datasets but can be computationally expensive. GB sequentially builds trees to correct errors made by previous ones, refining predictions iteratively by training on residuals. While GB handles complex relationships, GB is prone to overfitting and requires careful tuning. MLR predicts a dependent variable based on multiple independent variables by fitting a linear equation, offering simplicity but assuming a linear relationship, which may not always hold true. SVR finds a hyperplane in N-dimensional space, where N is defined by the number of features in the dataset. SVR represents the relationship between variables, aiming to minimize error and maximize margin but may be sensitive to kernel choice and be computationally expensive. Subsequently, each model undergoes fine-tuning through hyperparameters, intricately steering the algorithm's learning trajectory and wielding considerable influence over the model's behavior. The models were then assessed based on prediction accuracy before being integrated into the system.

3 MATERIALS AND METHODOLOGY

3.1 Materials

For this study, sixty-seven panels were manufactured with bindered, unidirectional non-crimp fabric (UD-NCF), PX35-UD300 from Zoltek Corporation [4], and the resin EPIKOTE TRAC 6150 by Westlake Epoxy [5]. These panels were produced by using a 100 ton Wabash or a 25 000 kN hydraulic Dieffenbacher press with parallelism control, reaching a maximum closing speed of 800 mm/s. Additionally, the flat plaques analyzed presented two stacking sequences of $[0/90]_s$ and $[0]_8$ and dimensions of 550 x 900 mm^2 and 300 x 300 mm^2 , respectively, as shown in **Error! Reference source not found.**. Note the initial and secondary resin dispersion regions and i nstitutions. 710 samples received a pre-activated binder the remaining 35 samples were not activated or were unbindered.

3.2 Methodology

To better analyze the influence of the resin area on the mechanical properties, the plaques were sectioned into initial resin dispersion regions (regions A and C), and secondary resin dispersion regions (regions B, D, E, and F through J).

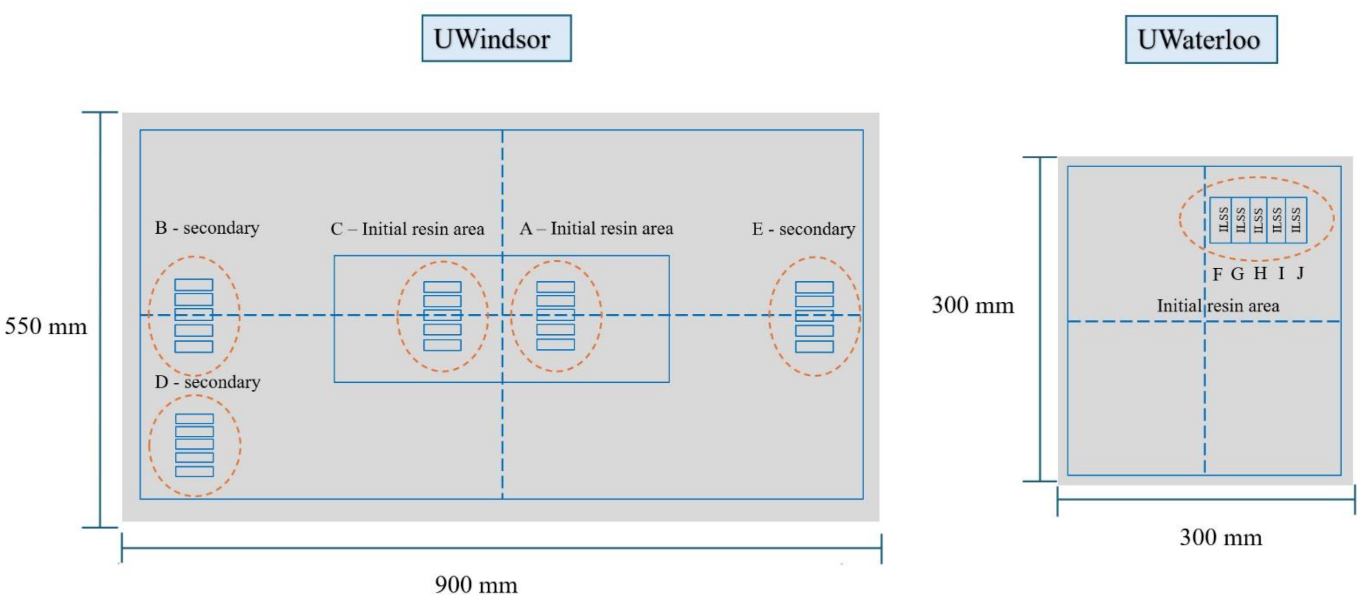

Figure 2: CFRP flat plaque dimensions and test sample locations

745 samples were tested for flexural modulus, maximum flexural strength, and strain at break or interlaminar shear stress. An MTS Criterion Model 43 and Quasi-static testing frame followed ASTMs D7264 and D2344, respectively. The features were evaluated using the SHAP (SHapley Additive exPlanations) method to provide insights into the contribution of each feature to the model's prediction. Positive SHAP values indicate a feature's positive contribution to the prediction, increasing the output value, and the opposite for negative values. Zero values signify minimal influence on the prediction. SHAP provided insights into the overall behaviour of the model and was applied to the model with the highest R^2 test value. Concurrently, the nominal, ordinal, and continuous data were pre-processed in Python© v. 3.10, normalized, and encoded to ensure proper weighting and outlier management. Libraries such as SHAP, Seaborn, Sklearn, Numpy, Pandas, Statistics, and Matplotlib provided correlation and analysis tools, and evaluation metrics to visualize the model comparisons.

4 RESULTS

Table 1 presents the outcomes forecasting the maximum ILSS or the utilization of the binder in relation to the independent variables. Following training on 70% of the data, the model undergoes validation using undisclosed test data. In both scenarios, the RF model demonstrated superior performance, achieving a 98.28% accuracy rate in predicting maximum ILSS based on the test data. In Case #2, the RF model exhibited a 99.97% accuracy rate in predicting binder usage on the test data. It is noteworthy that predictions for maximum flexural strength, as well as resin dispersion regions, also attained RF accuracies of 97% or higher. A model demonstrating training and testing accuracies of 90% or higher is deemed competent, while a model with an accuracy of 95% or greater is regarded as high fidelity.

Table 1: Training and testing results by ML model

Features
Plaque location
Institution
Mold type
Mold Temp. (°C)
Resin Set Time (sec)
Mold Curing Time (sec)
Binder/Inact/Non-binder
Initial/secondary

Responses
Maximum Flexural Strength (MPa)
Max shear stress (MPa)
Binder/Inact/Non-binder
Initial/secondary

Outcome

Case # 1 (Response: Max shear stress (UWaterloo & UWindsor))

Metric	**RF**	**GB**	**MLR**	**SVR**
MAE_train	0.4139	0.7535	0.7213	3.7086
MSE_train	1.1732	3.7077	3.7287	67.1235
R2_train	**99.67%**	**99.11%**	**99.10%**	**83.84%**
MAE_test	1.0156	1.1475	1.5882	3.6115
MSE_test	2.6195	8.6607	14.6343	7.8172
R2_test	**98.28%**	**97.83%**	**96.33%**	**84.69%**

Case # 2: (Response: Binder (UWaterloo & UWindsor))

Metric	**RF**	**GB**	**SVR**
MAE_train	0.00	0.00	0.14
MSE_train	0.01	0.00	0.05
R2_train	**99.95%**	**99.97%**	**67.75%**
MAE_test	0.00	0.00	0.13
MSE_test	0.01	0.00	0.18
R2_test	**99.97%**	**99.98%**	**79.47%**

The evaluation metrics utilized to assess the disparity between observed and predicted values consist of the mean absolute error (MAE), mean squared error (MSE), and coefficient of determination (R^2). They were determined by the following equations:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|, \qquad MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2, \qquad R^2 = 1 - \frac{\sum(y_i - \hat{y})^2}{\sum(y_i - \bar{y})^2} \tag{1}$$

where $\hat{y}$ was the predicted value of y and $\bar{y}$ was the mean value of y. Once optimized, the RF model predicted feature contribution for unseen inputs. Table 2 illustrates the maximum strength case where T_{before}, resin temperature, and resin set time are 79.11% of the contribution to the predicted strength.

Table 2: Input parameter feature importance (%)

	Location	Resin temp.	Mold temp.	Resin Set Time	Mold Curing Time	Tbefore	Degree	Predicted Max. Strength
Input (feature)	E	60	110	0	300	114.45	1	356.63 MPa
Contribution (%)	5.89%	14.95%	6.48%	20.20%	2.37%	43.96%	6.09%	

Additionally, a SHAP evaluation was conducted to ascertain significance. Figure 3 visualizes the distribution and density of SHAP values corresponding to features as they relate to the maximum ILSS.

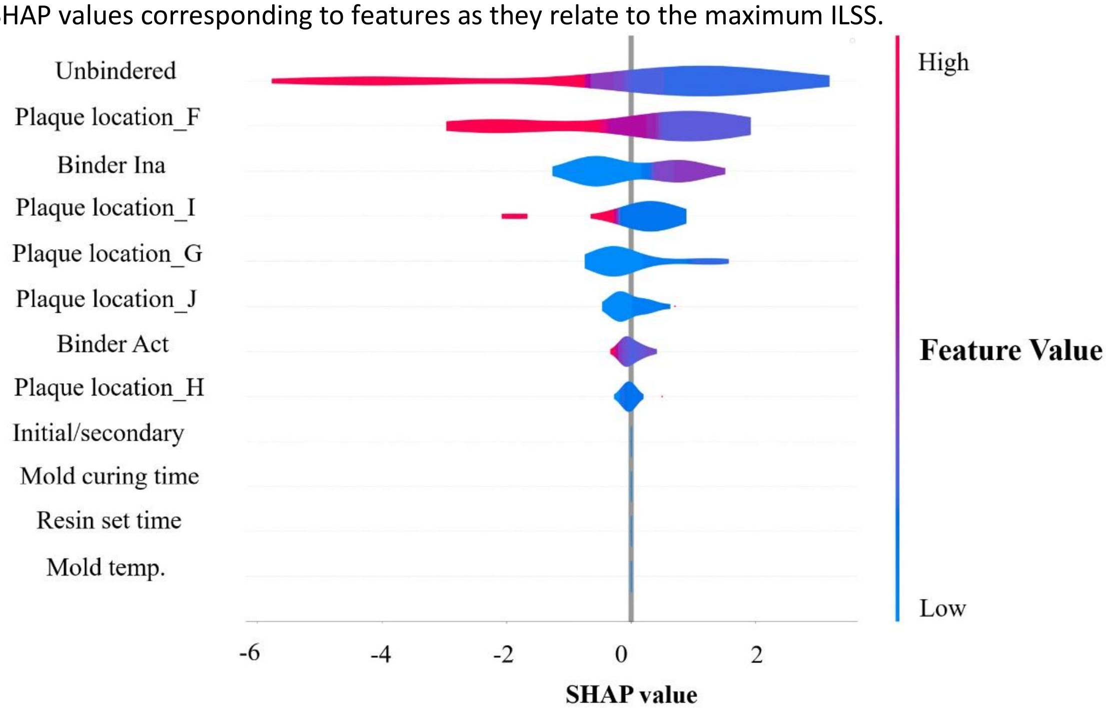

Figure 3: SHAP values for feature contribution to maximum ILSS

The SHAP values were calculated from the following equation:

$$\phi_i(v) = \sum S \subseteq N\{i\} \frac{|S|!\,(|N| - |S| - 1)!}{|N|!}[v(\,S \cup \{i\}) - v(S)] \tag{2}$$

where $\phi_i(v)$ is the SHAP value of feature i, $v(S)$ is the model's prediction when considering the feature subset S, and N is the set of all features. For the maximum ILSS prediction, the inputs with the highest impact were the unbindered plaques, plaque location F, and binder inactivated plaques. For the maximum flexural strength prediction, the inputs with the highest impact were mold temperature, resin set time, and resin temperature. When predicting the use of binder, the inputs with the highest impact were the mold temperature and mold curing time.

5 DISCUSSION AND FUTURE WORK

Based on the preceding analysis, the RF model emerges as the most effective predictor due to its ability to mitigate overfitting and tune the hyperparameters using a randomized grid search technique instead of a trial-and-error method. The RF model is recommended for cases involving continuous or ordinal input parameters, continuous outputs, and regression analysis needs. It is recommended that at least two data sources be considered for studies of this type due to the increase in testing accuracy from 22.61% to 98.28%. The feature importance and SHAP significance played a role in determining the optimal parameters and their respective contributions. The optimal parameters for maximizing ILSS were a mold temperature of 122.5°C, zero resin set time, the secondary resin dispersion region, unbindered, or binder-activated plaques. For maximizing flexural strength, optimal parameters were a resin temperature of 50°C, mold temperature of 110°C, zero resin set time, the initial resin dispersion regions, and the binder-activated plaques. When predicting binder, the outcome relied heavily on mold temperature and curing time. These results can be validated with a sensitivity analysis in the future.

In conclusion, researchers can readily deploy this model to forecast the chosen response variables for a set of features not included in the training set. As additional mechanical testing, such as tensile or flexural, becomes available, the model can be adapted to evolving industry requirements. With an expanded training set, the reliance on resource-intensive experimental testing for composites manufactured using WCM will diminish.

6 REFERENCES

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