AutoML TPOT with XAI analysis: optimization and interpretation of a machine learning model for the classification of epoxy composites*

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Abstract

The article presents an approach to predicting the type of filler in epoxy composites based on thermophysical parameters using AutoML TPOT and Explainable AI methods. The aim of the study was to create a highly accurate and transparent model of multi-class classification based on the following input features: thermal conductivity coefficient (CTC), mass fraction of filler (MFC), and test temperature (T). Based on the initial experimental data, 2,500 synthetic samples were interpolated and divided into training (70%) and test (30%) samples while maintaining class balance. AutoML TPOT performed an evolutionary search for the optimal pipeline, which included second-order polynomial feature expansion, a stack with DecisionTreeClassifier and GaussianNB as intermediate estimators, and a final RandomForestClassifier with 100 trees. The best pipeline showed an accuracy of over 95% on the Accuracy, Recall, Specificity, Precision, F-score, and G-Mean metrics and high AUC values (over 0.998) for all classes. The LIME method was used to interpret the model's decisions, which locally explains the influence of each parameter on the prediction. Analysis of sample #35 showed that MFC and CTC play the most important role in classification, ensuring clarity and confidence in the results. The combination of AutoML with XAI methods made it possible to automate the construction of highly efficient classification models and obtain transparent explanations of their predictions.

Keywords

epoxy compositions, machine learning, AutoML, TPOT, XAI

1. Introduction

The machine-building, energy, and aviation industries require materials with a complex set of properties: high strength, heat and wear resistance, processability, and durability. Traditional polymers do not always provide such a balance, so the creation of polymer composite materials and coatings based on them modified with fillers is becoming increasingly promising. The rheological behavior of polymer composites directly depends on their chemical nature. Technological properties are also significantly influenced by processing parameters such as temperature, pressure, strain rate, as well as the geometry and content of fillers. Thus, targeted control of the structure of the polymer matrix and the kinetics of its interaction with the surface of the filler particles makes it possible to predictably control the mechanism of composite formation and, accordingly, the properties of protective coatings [1,2].

Despite significant progress in the synthesis and processing technology of such materials, quantitative prediction of their properties remains a difficult task. The key reason for this is the nonlinear interaction between the matrix formulation and the forming modes. Machine learning

* *ITTAP'2025: 5h International Workshop on Information Technologies: Theoretical and Applied Problems, October 24-25, 2025, Ternopil, Ukraine, Opole, Poland*
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methods are radically changing this situation [3,4]. Research in the field of materials science confirms the feasibility of using machine learning methods to predict material properties [5-8]. Machine learning methods reveal hidden patterns even in small experimental data sets, build highly accurate predictive models, and assess the impact of individual technological factors on the final properties [9]. The use of machine learning algorithms in combination with Explainable AI (XAI) methods [10–12] significantly reduces the need for costly experiments, as it provides reliable prediction of material properties even with a limited amount of input data. This significantly speeds up the "design → prototype → evaluation" cycle and provides engineers with tools for targeted optimization of the strength and durability of composites. Article [13] summarizes current applications of artificial intelligence for predicting the mechanical properties of composites. It provides an overview of machine learning algorithms, model building stages, and validation methods. The theoretical foundations, advantages, and limitations of the methods are revealed, and the role of XAI in increasing predictions confidence is emphasized. In study [14], six machine learning algorithms were used to predict the tribological characteristics of epoxy coatings under variable loads and filler content. Study [15] is devoted to the erosion wear of ramie fiber-reinforced epoxy composites under various high-temperature conditions. SVM, Decision Tree, Random Forest, and Gradient Boosting were used to predict wear. Study [16] proposes a method for optimizing multicomponent epoxy systems that combines molecular dynamics simulations with machine learning. Study [17] shows the possibility of assessing damage to glass-epoxy fabric laminates using machine learning. In the study [18] there was emphasised the possibility of remote detection of fatigue damage in glass-epoxy composites using thermal images trained on synthetic data. In [19], there was proposed an approach that combines the finite element method and a convolutional neural network to predict the macroscopic elastic characteristics of composites with complex microstructures. The trained CNN directly estimates the effective Young's modulus and Poisson's ratio for any shapes and distributions of inclusions. In study [20], four ML algorithms, such as decision trees, SVR, Gaussian Regression, and ensemble methods, were compared for predicting the tensile strength of carbon-plastic and glass-plastic thermoplastic composites. The article [21] summarizes the application of machine learning algorithms for all stages of the life cycle of fiber-reinforced polymer composites: from raw material selection and optimization of technological parameters to material ranking and validation of final products. Optimization models, ranking methods, and databases that support the design of composites with specified properties are considered. It is shown how ML outperforms traditional tools, accelerates the development of new products, and shapes the direction of future research and industrial applications. The authors of papers [22,23] used neural networks to model the mechanical properties of epoxy composites that were treated by the electric spark hydroimpact method. In work [24], a machine learning-based approach to predicting the thermal conductivity of composites, alternative to classical models, was proposed. The work confirms that machine learning algorithms provide a fast and accurate determination of the thermal conductivity of composite materials. In study [25], a machine learning-based tool was proposed for rapid prediction of the thermal conductivity of composites with hollow glass microspheres. ML models Random Fores, k-Nearest Neighbors, Support Vector Regression, and Artificial Neural Network were used. The authors of article [26] studied the tribotechnical characteristics of epoxy composites using neural networks.

Thus, the use of advanced machine learning algorithms opens up new prospects for improving the accuracy of forecasts and optimizing the technological processes of composite materials production. The goal of our research is to create a highly accurate model for predicting the properties of composite materials, developed using AutoML TPOT and Explainable AI methods, which automates the selection and optimization of hyperparameters while transparently explaining the impact of input parameters on the prediction.

2. Materials and methods

The experimental basis for our study was formed on the basis of work [27], in which the author thoroughly investigated the thermophysical properties of epoxy composites reinforced with glass fiber.

Three physical parameters were used as input features to build the machine learning model: experimentally measured composite thermal conductivity coefficient (CTC), mass fraction of filler (MFC), and test temperature (T). The output variable was a categorical feature denoting the type of filler used in the epoxy matrix: aerosil, coded as class 1, γ-aminopropyl aerosil as class 2, aluminum oxide as class 3, and chromium oxide as class 4.

The experimental data contained a limited number of primary samples that reflected the thermophysical properties of composites only for certain combinations of CTC, MFC, and T. For full training of machine learning models, a denser and more homogeneous data set is needed to minimize the risk of overfitting and underfitting, improve the model's ability to generalize, and ensure correct cross-validation. To increase the sample size without additional expensive measurements, 2,500 synthetic samples were interpolated based on the initial experimental data. These were used to form the dataset. The dataset was randomly divided in a 70/30 ratio, i.e., 1,750 samples were included in the training sample, and the remaining 750 remained as a test set. The distribution was performed taking into account the filler class so that the proportions of classes in the subsets reproduced the initial data structure.

In this study, the AutoML concept was used to build a machine learning model, which automates the entire lifecycle of machine learning model creation, from initial data analysis to obtaining a ready-made pipeline with configured hyperparameters [28]. The idea of AutoML arose in response to the rapid growth in data volumes and algorithm complexity, as well as the limited time available to specialists who have to manually sift through hundreds of combinations of models, transformers, and settings to achieve acceptable accuracy. Within AutoML, this process is delegated to a meta-algorithm, which first generates an initial set of pipelines, then evaluates their performance according to a defined metric, and gradually improves them through search strategies, the most common of which are Bayesian optimization, genetic programming, stochastic local search methods, or gradient procedures. During each iteration, the system performs cross-validation to prevent overfitting and adjusts the balance between forecast quality and pipeline complexity, often using multi-criteria optimization to minimize time and computational resource costs. Based on the search results, AutoML returns a ready-made machine learning model and a configuration file that specifies the preprocessing steps, the selected estimator, the optimal hyperparameters, and the ensemble assembly rules, if this proved to be more advantageous. The practical value of AutoML lies in significantly reducing research time and objectively comparing a large number of models. The AutoML method was implemented using the Tree-based Pipeline Optimization Tool (TPOT) [29-31]. This is an open Python library that automates the selection and configuration of machine learning pipelines through genetic programming techniques. It works in the scikit-learn ecosystem and treats each machine pipeline as a “chromosome,” which is a sequence of processing steps, including data preparation, feature transformation, and the application of the final algorithm for prediction. First, TPOT randomly creates a population of such pipelines, then cyclically applies selection, crossover, and mutations to obtain increasingly perfect combinations in subsequent generations. The quality of each individual is evaluated using a selected metric through cross-checking, and the evolution process continues until the specified time limit or number of generations is exhausted, or improvements cease.

To interpret the machine learning model, there was employed the Local Interpretable Model-agnostic Explanations (LIME) method from the Explainable AI arsenal, which provides explanations by constructing simple local approximations [32-33]. Its key idea is that even if the global behavior of a complex algorithm is incomprehensible, in the immediate vicinity of a single prediction object, it can be well enough described by an elementary, intuitively understandable

model. To obtain such a local picture, LIME first creates artificial "neighboring" observations: it randomly disturbs the initial features. For each disturbed sample, the base model generates a prediction, after which the algorithm assigns weights to the samples that decrease with distance from the point of interest. Based on the weighted set of "pseudo-observations" obtained, LIME trains a simple linear model or a small decision tree that minimizes prediction error in this local context. The coefficients of such a model serve as understandable explanations. They indicate how much each feature pushes the prediction up or down for the selected object. The advantage of LIME is that it is independent of the type of base model and the nature of the data. It works with any estimator that returns probability predictions or estimates, and the procedure itself generates understandable numerical weights. This approach makes it possible to verify the plausibility of a decision, identify potential biases, and adjust the model or data. The limitations of the method stem from its local nature. The explanations apply only to a single sample.

The values of Accuracy, Recall, Specificity, Precision, F1-score, and G-Mean metrics were calculated using classical formulas (Table 1) and four basic classification error values: true positives (TP), true negatives (TN), false positives (FP), and false negatives [34].

Table 1
Performance Metric Calculation Formulas

Formula	Description
$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$	It shows the proportion of all correctly classified samples out of the total number of samples.
$Recall = \frac{TP}{TP + FN}$	It reflects the model's ability to identify all samples belonging to a specific class.
$Specificity = \frac{TN}{TN + FP}$	It reflects the model's ability to avoid false positive classifications.
$Precision = \frac{TP}{TP + FP}$	It shows the proportion of samples predicted as positive by the model that actually belong to the positive class.
$F1 - Score = 2 \times \frac{Precision \times Recall}{Precision + Recall}$	The harmonic mean of Precision and Recall, reflecting the balance between them.
$G - Mean = \sqrt{Recall \times Specificity}$	The geometric mean of Recall and Specificity, which allows evaluating the model's balance across both positive and negative classes.

Calculating a set of metrics provides a comprehensive picture of how the model classifies samples. Accuracy shows the overall percentage of correct decisions and is useful when classes are balanced. Recall answers the question of how many samples of the positive class were detected, while Specificity reflects the model's ability to avoid mistakes regarding negative samples. Precision shows what proportion of the predicted positive samples the model actually classified correctly. F1-score combines Precision and Recall into a single value, thus showing how successfully the model finds a compromise between these two indicators. G-mean is the geometric mean of Recall and Specificity, so it characterizes the uniformity of the model's performance on

both classes and is especially valuable when the data is imbalanced. Together, these metrics help to assess overall accuracy.

3. Results and discussion

3.1. Structure and performance evaluation of the AutoML TPOT pipeline

During the evolutionary search, the AutoML TPOT algorithm formed a composite pipeline that begins with the expansion of the initial features using second-order PolynomialFeatures without adding a constant column. This way, all squares and pairwise intersections of the initial variables are included in the dataset, allowing the model to capture nonlinear relationships between thermal conductivity, filler concentration, and temperature (Figure 1).

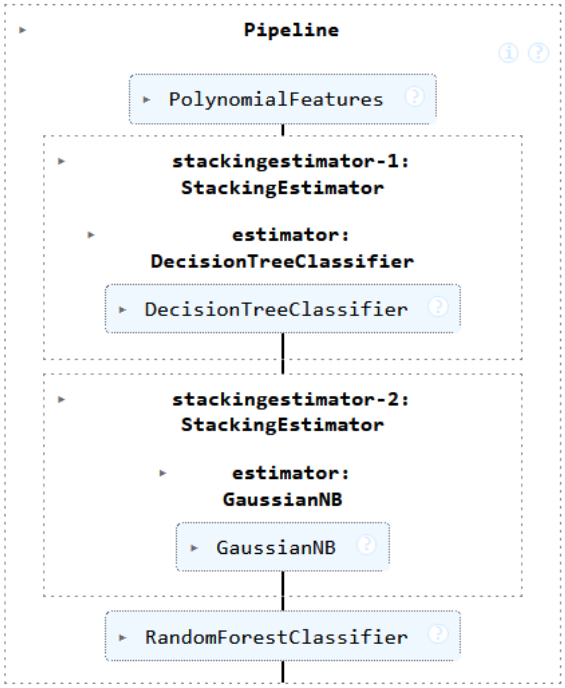

Figure 1: Optimized AutoML TPOT Pipeline Diagram.

Next, a stack of two basic estimators was built. The first is a small DecisionTreeClassifier, limited to a depth of two levels and strict thresholds for minimum samples in nodes (17 samples in leaves, 10 to split), which reduces the risk of overfitting and at the same time generates simple, interpretable rules as new synthesized features. The second layer adds the result of GaussianNB to these features, which takes into account the conditional independence of polynomial components and works as a fast, linear classifier. Finally, all primary and intermediate representations are fed into a RandomForestClassifier, configured for 100 trees with no depth limit, but with an aggressive threshold of max_features = 0.3 so that each tree sees only a third of the features, and with moderate regularization via min_samples_leaf = 2 and min_samples_split = 4. Evolution parameters such as twenty generations of twenty individuals with five-fold cross-validation and accuracy metrics allowed TPOT to explore four hundred unique pipelines, each with its own hyperparameters, while parallel execution (n_jobs = -1) ensured acceptable optimization time. Random initialization with random_state = 42 guarantees reproducibility (by running the search with the same seed, you can get the same pipeline composition). A high verbosity level = 3 during the process allowed us to track the progress of each generation in detail. As a result, the resulting stack shows the best balanced accuracy among the tested combinations, combining the ability to

capture complex cross-effects with control over generalization ability thanks to conservative tree and forest settings.

Figure 2 shows a confusion matrix demonstrating the classification results, where each class corresponds to a specific type of epoxy composite with different fillers.

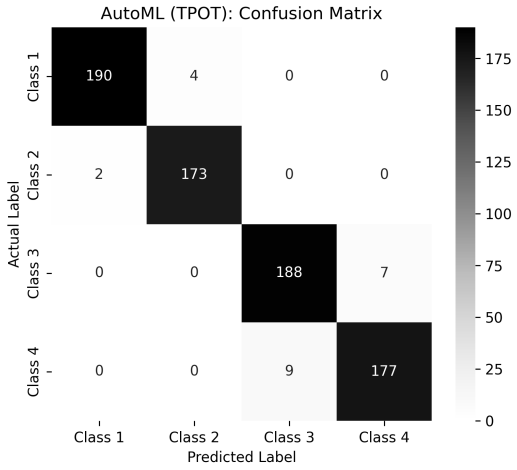

Figure 2: Confusion matrix.

The confusion matrix confirms the effectiveness of the constructed machine learning model for composite type recognition tasks based on thermophysical parameters.

Figure 3 shows the Precision–Recall and ROC curves with AUC indicators for multi-class classification.

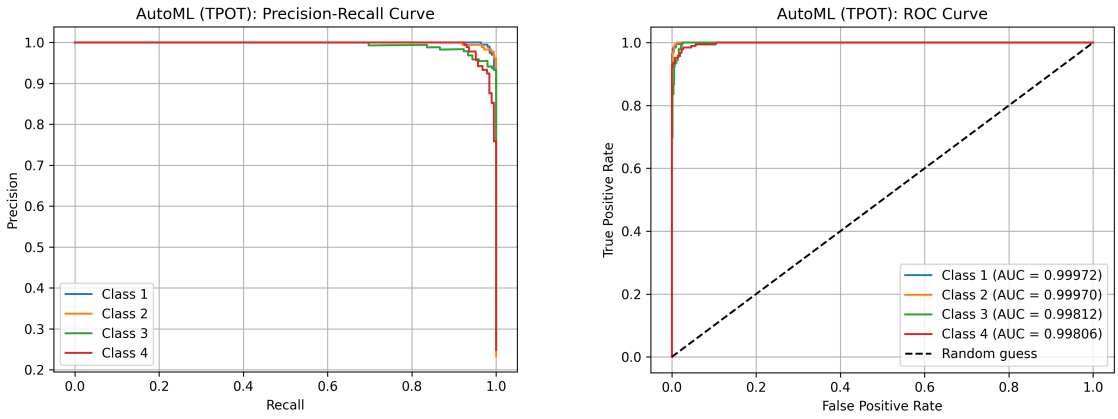

Figure 3: Precision–Recall and ROC curves with AUC metrics for multi-class classification.

The Precision–Recall curve shows the reliability of the model for multi-class classification tasks, where it is important to maintain a balance between Precision and Recall for each individual class. On the ROC graph, the area under the curve (AUC) exceeds 0.998 for each class. From the perspective of ROC analysis, the classifier provides extremely high discriminatory power for all four types of fillers.

Figure 4 shows the performance indicators of the machine learning model.

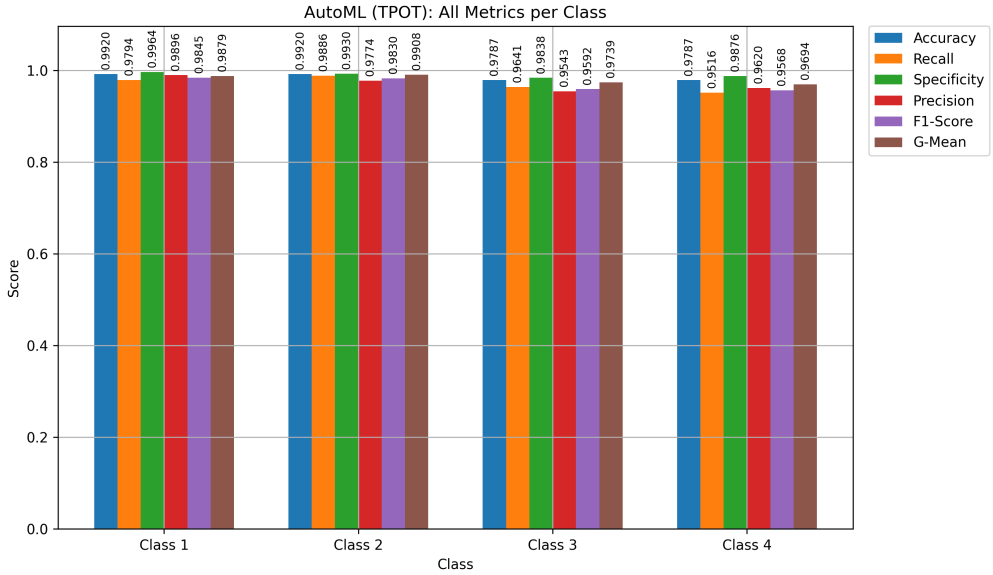

Figure 4: Machine learning model performance metrics.

The histograms clearly confirm that the model works in a balanced and stable manner, as all metrics, including the lowest ones, have values above 95%, which indicates high classification reliability for each of the four classes. The F1-Score metric responds to any imbalance between correctly found positive samples and false predictions. For classes 1 and 2, the F1-Score values are 98.45% and 98.30%, respectively, indicating an almost perfect combination of Precision and Recall for these types of fillers. For classes 3 and 4, the F1-Score drops to 95.92% and 95.68%, respectively. G-Mean reflects the balance between Recall and Specificity. For classes 1 and 2, G-Mean reaches 98.79% and 99.08%, which shows the high ability of the ML model to minimize false positive and false negative decisions. G-Mean values of 97.39% and 96.94% for classes 3 and 4 reflect a slight decrease in the model's ability to simultaneously detect positive samples and minimize false positives for these two classes. Thus, the simultaneously high F1-Score and G-Mean values confirm that the AutoML TPOT pipeline not only provides high overall efficiency but also balanced classification across all four classes.

3.2. Interpretation of the machine learning model

The LIME explanation for sample #35 demonstrates how the machine learning model formed a prediction in favor of class 3 by analyzing the influence of MFC, CTC, and T (Figure 5).

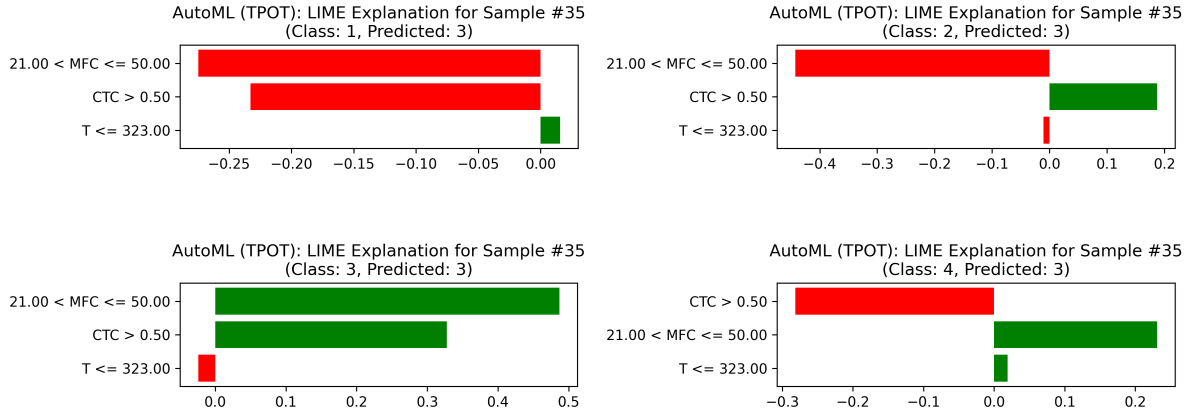

Figure 5: LIME explanations for sample #35 across all four classes.

Histograms illustrate the local contributions of features to the predicted probability for each class. Green (positive) and red (negative) bars reflect the direction of the influence of features. For class 1, the LIME explanation shows the overall negative impact of the main parameters on the probability of assigning sample #35 to this class. MFC has the greatest significance, reducing the probability of belonging to class 1 by 0.2748. This indicates that such a concentration is not characteristic of composites of this type. Thermal conductivity further reduces classification confidence, subtracting another 0.2329 from the weight contribution. Temperature has a minimal positive effect (0.0156), but it is not enough to compensate for the negative contribution of other features. As a result, the overall effect is negative, which explains why the model did not classify this sample as belonging to class 1. For class 2, the main negative impact on the probability of classifying the sample into this class is MFC, which reduces the corresponding weight contribution by 0.4428. This indicates that the model considers such a concentration to be atypical for composites of this class. At the same time, the thermal conductivity value has a moderately positive effect, increasing the probability of classification into class 2 by 0.1871, which indicates partial compliance with this CTC value for this type of composite. Temperature has an almost neutral effect, with a slight negative contribution of 0.0105. Together, these values form an overall negative effect, which explains why the model did not assign the sample to class 2, despite the partially favorable thermal conductivity parameters. For class 4, CTC has the greatest negative impact on the probability of assigning sample No. 35 to this class, reducing the class 4 rating by 0.2817. This indicates that this level of thermal conductivity is atypical for composites of this type. At the same time, MFC makes a positive contribution, increasing the probability of class 4 by 0.2306, which means partial compliance with this concentration for this type of material. Temperature has a negligible positive effect (0.019), which indicates its weak role in determining this class for the current sample. As a result, the negative contribution of the CTC feature outweighs the positive effect of MFC and T, which is why the model does not favor class 4 when classifying this sample. For class 3, the LIME explanation indicates a clear positive total contribution of parameters to the model decision in favor of this class. MFC has the greatest influence, with a weight contribution of +0.487. This indicates that such a concentration is a typical feature of composites with the third type of filler. CTC is also a significant positive factor, adding another 0.328, confirming that this parameter is well aligned with the properties of class 3 composites. Temperature has a weak negative impact of 0.024, meaning that its value is not decisive. As a result, the combined effect of MFC and CTC significantly prevails, which determined the choice of the model — sample #35 was classified as a representative of class 3.

The overall picture shows that the model makes decisions based on a combination of features, and it is MFC and CTC that are decisive for classifying this sample as a representative of class 3. Thus, the LIME explanation allows us to understand which parameters in the machine learning model had the greatest influence on the choice of filler class.

4. Conclusions

The study confirms the high efficiency of AutoML TPOT in the task of multi-class classification of epoxy composite filler types based on thermophysical parameters. Thanks to evolutionary search, an optimized pipeline was formed, combining polynomial feature expansion, a stack with DecisionTreeClassifier and GaussianNB, and the final RandomForestClassifier. This architecture provided balanced accuracy of over 95% across all key metrics. Of particular note is the high discriminatory power of the model (AUC greater than 0.998), as confirmed by the ROC and Precision–Recall curves. The use of the LIME method provided a transparent explanation of the model decision-making process. Local explanations for the selected sample showed that it is the filler concentration and thermal conductivity that are the determining factors that direct the prediction towards the correct class. This increased confidence in the model results.

Declaration on Generative AI

During the preparation of this work, the authors used Grammarly in order to grammar and spell check, and improve the text readability. After using the tool, the authors reviewed and edited the content as needed to take full responsibility for the publication's content.

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