IJRESM
International Journal of Research in Engineering, Science and Management
Volume 9, Issue 4, April 2026
www.ijresm.com | E-ISSN: 2581-5792 | RESAIM Publishing | www.resaim.com

Machine Learning-Based Analysis for Thermal Properties of MWCNTs/Polymer Composites

Satish Geeri[1*], Gantyada Amaladevi[1]
[1]Department of Computer Science and Engineering, Visakha Institute of Engineering & Technology (A), Visakhapatnam, India

***Abstract*: This article discusses thermal prediction and data-based prediction of E-glass fiber polymer composites reinforced with multi-walled carbon nanotube (MWCNT). The hand lay-up technique was used to make the laminates by the use of woven roving E-glass mats oriented at 0º/90º, 0º/45, and 0º/135º. The volume fractions of MWCNTs into the polymer matrix were 0%, 1%, 3%, 5% and 7%, which developed fifteen different composite configurations. The Thermogravimetric Analysis (TGA) was used to find out the thermal properties of the material including weight loss, degradation and decomposition behavior. These findings indicate that the orientation of fibers and MWCNT content are crucial determinants of thermal stability and that increased resistance exists at maximized filler loadings. A number of machine learning models were developed and trained using experimental data to increase predictive power. The performance of the models was measured using standard evaluation metrics and the importance of features analysis was conducted to identify important parameters on the thermal behavior. The integrated experimental and machine learning method offers a developed framework to predict thermal properties and optimize composite design, valuable information to be used in the advanced structural and thermal applications.**

***Keywords*: Machine Learning, Thermal Properties, MWCNTs, Polymer Composites, Data-driven Prediction.**

1. Introduction

Electromagnetic Interference (EMI) has become a major problem affecting the performance and reliability of devices with the development of electronic and communication systems. EMI shielding materials that are made of polymer composites are popular due to their light weight, resistance to corrosion, and flexibility in design. They are however prone to high temperatures in aerospace and automotive electronics and telecommunications [1], [2]. Thus, thermal properties, particularly stability, degradation behavior, and decomposition resistance, are crucial for consistent EMI shielding and durability. Low thermal conductivity may lead to degradation of the structure which degrades shielding and performance [3]. Polymer composites are appreciated because of their strength-to-weight ratio, processability and their multifunctional uses. Glass fiber reinforced polymer (GFRP) is popular due to its affordability and mechanical characteristics. Though these have such advantages, high temperature thermal stability is a persistent issue and incorporation of nanofillers improves the functional properties of the polymer composites [4]. Common nanofillers are nanoclays, graphene nanoplatelets, silica nanoparticles, carbon black, and carbon nanotubes (CNTs). Carbon nanotubes (MWCNTs) have a high aspect ratio, thermal conductivity and mechanical strength which make them especially promising in enhancing thermal resistance and slowing degradation [5]. Various fabrication methods, such as hand lay-up, compression molding, resin transfer molding (RTM), and vacuum-assisted resin infusion (VARI), are used for polymer composites [5], [6]. The simplicity, low cost, and effectiveness of the hand lay-up technique in large structures make it popular.

The problems such as homogenous dispersal of nanofillers and laminate uniformity have to be addressed to achieve maximum performance. Multi-walled carbon nanotubes (MWCNTs) are chosen as reinforcing nanofillers due to their improvement of thermal stability and creation of conductive networks in the polymer matrix [6]. Composite fabrication is done by hand lay-up because it is economical and flexible to different fibre orientations allowing hybrid composites to have better thermal properties. The orientation of fibers has a great impact on the performance of composites. The 0º/90º, 0º/45, and 0º/135º reinforced with E-glass woven roving mats provide different reinforcements that have an impact on thermal behavior [7]. The thermal degradation and stability depend on the reinforcement mechanism between fiber orientation and nanofiller content. Filler loading is crucial in order to maximize the properties of composite. The volume fraction of MWCNTs (0%, 1%, 3%, 5%, and 7%) is used to determine the optimum filler content and evaluate the agglomeration effect at higher concentrations [8]. Although advances have been made the joint influence of nanofiller content and fibre orientation on thermal properties is poorly studied [9], [10].

New studies of polymer composites enhance materials with small fillers and data methods. Modelling and improving properties become applicable with the help of machine learning (ML) and artificial intelligence (AI). According to Mahadeva R et al. [11], ML and AI forecast material behavior, save costs and design faster. Hamidi YK et al. [12] demonstrated the effectiveness of ML in forecasting mechanical and thermal characteristics, which can help with the assessment. The reviews of the ML use by Maniraj J et al. [13] and Karuppusamy M et al. [14] show that it has made progress in

*Corresponding author: geerisatish@gmail.com

Table 1
Literature review and gaps from previous works

S. No.	Filler Materials	Fabrication Process	Remarks	Research Gap	Ref.
1	Carbon-based fillers (CNTs, graphene)	Various methods	Sebastian A et al. used ML to improve EMI shielding.	Research efforts have been sparse in merging thermal analysis with machine learning across different fiber orientations.	19
2	Biofibre + Glass fiber (hybrid)	Hand lay-up	Razzaq MEA et al. showed improved mechanical properties.	The emphasis has predominantly been on mechanical properties, leaving a gap in comprehensive thermal behaviour studies.	20
3	Polymer composites (general)	Machine learning model	Li Z et al. developed ML models for interface behaviour.	Experimental validation, particularly with nanofillers like MWCNTs, is missing.	21
4	Polymer composites (interface study)	Data-driven approach	Li Z et al. provided ML datasets for composite analysis.	Furthermore, there is a disconnect between these studies and practical fabrication methods, as well as real-world thermal testing.	22
5	Glass fiber composites	Hand lay-up	Anwar AM et al. studied composites for space use.	The exploration of nanofiller incorporation (MWCNTs) and predictions based on machine learning remains unexplored.	23

modelling, optimization, and feature analysis, but with such problems as a limited amount of data and the necessity of powerful experimental checks. Sharma A and Kushvaha V [15] wrote about the broad application of ML to design, and Kharb SS et al. [16] applied the data-driven method to predict erosion in reinforced polymers, proving the versatility of data-driven methods. Composites are improved by the use of carbon-based fillers, particularly, the MWCNTs. Wang MW et al. [13] investigated MWCNT alignment, which yielded better properties and interactions. Recently, Laad M et al. [17] discovered that MWCNT- and graphite-reinforced composites are more thermal stable and structure because of better filler dispersion and network formation.

Not much research attention has been given to the use of ML to forecast thermal properties in composites, as presented in Table 1 and literature review. The research will be used to fabricate MWCNT reinforced E-glass fiber polymer composite with various fiber orientations using hand lay-up process, to ascertain thermal properties of MWCNT loading, fiber orientation interaction during thermal stability, to produce and analyze ML models to predict thermal properties, and to establish significant parameters that are used to control thermal behavior.

2. Methodology

A. Materials, Fabrication Process and Characterization

A basic hand lay-up technique was utilized to make the composites. To prepare the polymer resin (Epoxy HY951), the appropriate quantity of MWCNTs was incorporated (0%, 1%, 3%, 5%, and 7%) into the polymer. This was achieved through stirring and occasionally sound waves were used to evenly distribute them and avoid clumping. Then a hardener (LY556) was put in in the correct quantity. Mats of E-glass fibres were cut to the required sizes and put in the mold for different orientations (0º/90º, 0º/45, and 0º/135º). MWCNTs resin was applied uniformly on each layer using brushes or rollers to ensure that it soaked. Air bubbles were eliminated with the help of rollers and enhanced the quality of the laminate.

The laminates were allowed to dry at room temperature in 24 hours. In some cases, additional curing was implemented in order to reinforce the bonds. The composites were cured in the mold and removed after curing and then cut into pieces to be subjected to thermal testing. The thermal properties were checked using thermogravimetric analysis (TGA). Samples were warmed up at a constant rate at room temperature up to a high temperature (such as 600-800ºC) in a controlled atmosphere. The test measured weight loss (%), the temperature when degradation starts, the highest degradation temperature, and the leftover weight. The work flow of the methodology is represented in the Fig. 1.

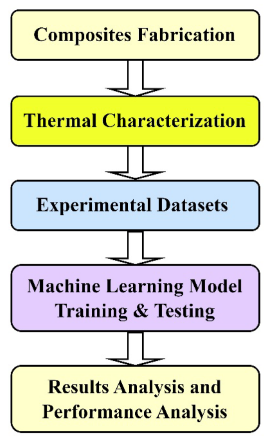

Fig. 1. Flow diagram of work

B. Machine Learning Models

After thermal characterization, for experimental datasets of 37564 was split in the ratio of 70:30 in the view of training the models and testing. A total of six different regression-based machine learning models were selected, in order to capture the linear and nonlinear trend of datasets. The machine learning models like Linear Regression, Ridge Regression, Lasso Regression, K-Nearest Neighbors, Gradient Boosting and Random Forest were simulated. The performance was evaluated based on parameters like R^2, MAE, MSE, and RMSE.

3. Results and Discussions

The main aim of the present work was to perform analysis for the machine learning model outputs parameters. To identify the best suitable model for the experimental dataset and to identify the most influential feature parameter on the output thermal behavior properties.

The performance of the Linear Regression (LR) model is shown in Fig. 2, through the Actual vs. Predicted plot. Ideally, everything ought to be in line with the 45º diagonal and this means that there is complete agreement between the experimental and predicted values. The visualized scatter, however, shows that there is a significant deviation, which highlights the limitations of the linear model. The plotted data depict a clustered and curved distribution especially in the mid-range (30-70) and higher values (>90). This implies that there is a nonlinear dependence between the input parameters (MWCNT filler content, fiber orientation, and temperature) and the thermal properties.

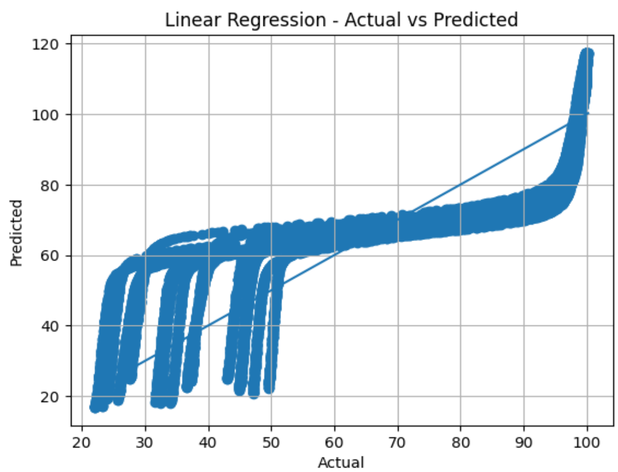

Fig. 2. Linear regression - Actual and Predicted data

As a result, the Linear Regression model cannot capture these complicated interactions as shown in Table 2 & Fig. 2. The R^2 value of about 0.82 indicates the model accounts for only 82% of the variance in the experimental data, relatively low compared to advanced models. The high values of MAE and RMSE are another indication of important prediction errors. These results suggest a false high weight to filler content and low weight to the effect of temperature in the Linear Regression model. This is contrary to the physical expectations whereby temperature is generally the most important determinant of thermal degradation. On the whole, the Linear Regression model is not suitable to model the thermal behaviour of developed composites. The nonlinear data requires a higher level of machine learning models like KNN, Random Forest or Gradient Boosting to predict it with accuracy as presented in Table 3.

The Actual vs Predicted plot of the Ridge Regression model indicates a similar trend with Linear Regression as shown in Fig. 3. Although Ridge has been regularized to minimize overfitting, the scatter plot does not follow the desired diagonal line. The predicted values do not have a linear alignment, but rather a band shape that is curved, particularly in the mid-range (3070) and the high-value (>90) ranges. This implies that Ridge Regression too does not help to capture the nonlinear relationships in the dataset. The clustering of points to systematic prediction errors, which show the limitations of the model as shown in Table 2. These values are almost the same as Linear Regression, which shows that regularization does not make much of an improvement. The Ridge Regression is inappropriate in predicting the thermal properties in the study due to low R2 and high error values. In contrast to Linear Regression, Ridge gives temperature a prevailing weight, which is more consistent with predicted behavior of thermal degradation as shown in Table 3. Nevertheless, even with the enhanced interpretation of features, predictive capability is not satisfactory. To conclude, although Ridge Regression can provide better feature interpretation than Linear Regression, it does not enhance prediction performance. This application cannot be performed with the model because it cannot model nonlinear relationships, which highlights the importance of advanced machine learning models such as KNN and Random Forest to predict thermal properties.

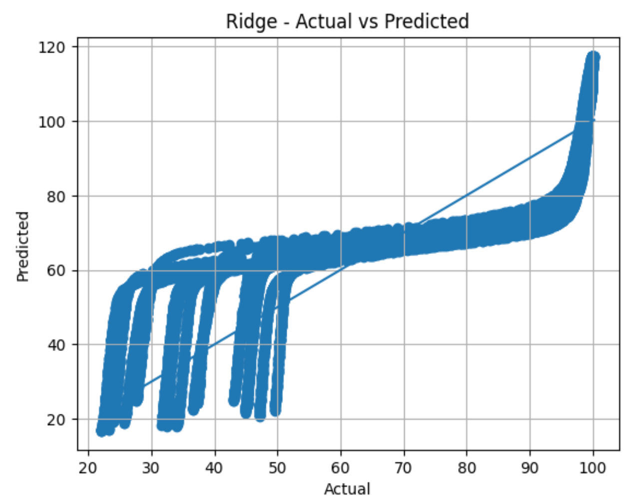

Fig. 3. Redge regression - Actual and Predicted data

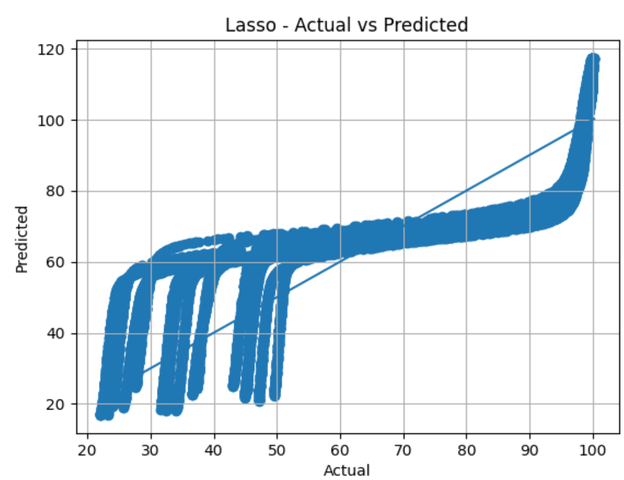

Fig. 4. Lasso regression - Actual and Predicted data

Based on the Fig. 4 of the Lasso Regression model is similar to that of the Linear and Ridge models. The data points are highly spread and do not follow the 45-diagonal line, which means that they are not optimally predicted. The distribution in the mid-range (3070) and higher (>90) values shows a curved and clustered distribution. This supports the hypothesis that Lasso Regression, even with L1 regularization, is unable to capture the nonlinear correlation between the input parameters and the thermal properties indicating systematic underfitting.

These values are almost the same as Linear and Ridge models, which means that Lasso does not improve the predictive performance significantly. Low values of R2 and high values of error also support the fact that the model failed to model the thermal behavior of composites as shown in Table 2. Lasso is right by putting temperature as the leading factor with a contribution of more than 90% and filler content has secondary contribution and fiber orientation shows minimal contribution as presented in Table 3. This is in agreement with the physical interpretation of the mechanism of thermal degradation. In general, Lasso boosts feature interpretability but does not make predictions more accurate. The model is not applicable to this study since it cannot take into consideration nonlinear relationship.

In the Actual vs Predicted plot of the K-Nearest Neighbors (KNN) model, the curve is nearly parallel to the straight line fit and this indicates a high concordance between experimental and predicted values presented in Fig. 5. Compared to linear models, there is no apparent dispersion or variation throughout the range (20-100). The predictions closely follow the real data, demonstrating how the KNN model can be effective in the complex relationship between the input variables and the thermal properties. Findings indicate close to perfect prediction accuracy, as indicated by a high R^2 value, which means that the model explains almost all the variance as shown in Table 2. Very low Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) mean that there is a low prediction error. This distribution indicates that temperature is the most key factor affecting the thermal behavior, Multi-Walled Carbon Nanotube (MWCNT) filler content has a moderate impact, and fiber orientation has a minor impact as shown in Table 3. The high performance of KNN model is attributed to the fact that it does not assume predetermined relationships between variables. Rather, it forecasts values using their similarity to neighboring data points so it is very useful with nonlinear data. The model elucidates the local variations, which are important in modelling of complex interactions among temperature, filler content, and fiber orientation. KNN works well where the experimental data are limited hence it is applicable in materials science.

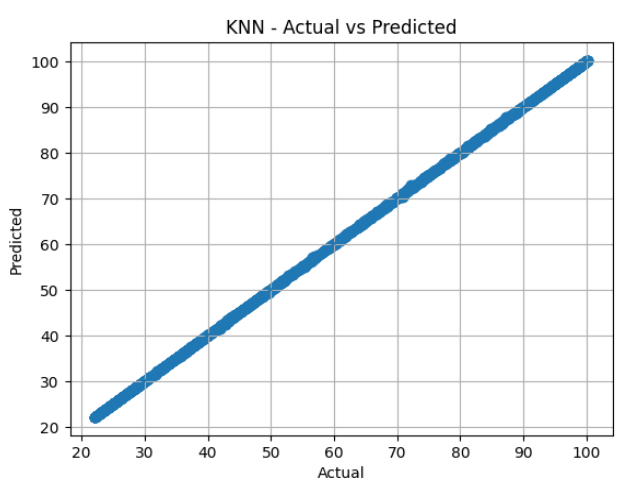

Fig. 5. KNN - Actual and Predicted data

The actual vs. predicted plot of the Random Forest (RF) model shows that the data points almost perfectly align with straight line, meaning that there is a high level of concordance between the predicted and experimental values as shown in Table 2 & Fig. 6. The RF model shows very little deviation and the model shows negligible scatter over the whole range of values as compared to linear models. The data values are tightly clustered around the ideal line, which confirms the ability of the model to effectively describe the underlying relationships in the data. The value of the R^2 is close to 1 which shows that the model explains almost all the variability of the data as in Table 2. The error values are very low which supports the high prediction accuracy of the model. The most powerful parameter that appears is temperature which mostly impacts on thermal behavior. MWCNT filler content has a moderate influence on thermal stability, whilst fiber orientation has a relatively small impact on thermal degradation as noticed in Table 3. Random Forest model is one of the most credible models in this study as it offers very accurate and consistent predictions of thermal properties. Despite being marginally less accurate than KNN, it has better robustness and generalization potential, making it very appropriate to be used in practical tasks in composite material prediction.

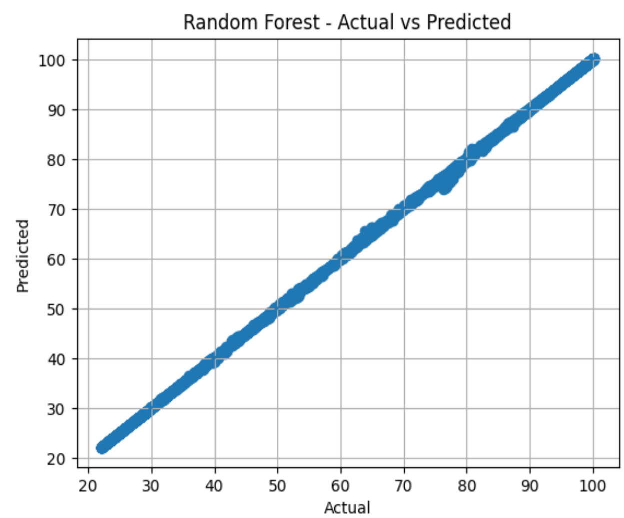

Fig. 6. Random Forest - Actual and Predicted data

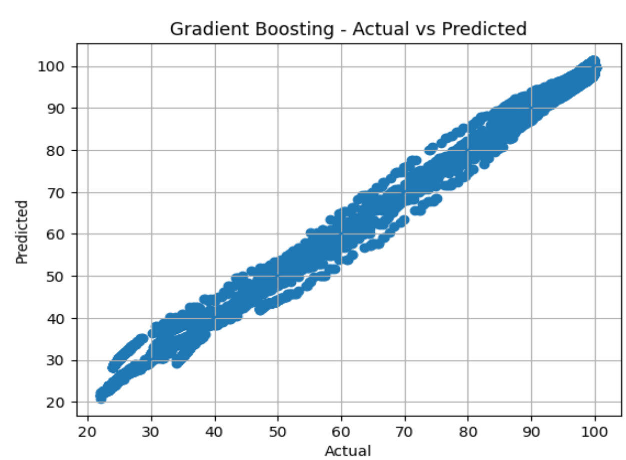

Fig. 7. Gradient Boosting - Actual and Predicted data

Table 2
Performance evaluation parameters

S.No.	Model	R^2	MAE	MSE	RMSE
1	Linear Regression	0.819819	10.593617	160.186193	12.656468
2	Ridge	0.819819	10.593551	160.185901	12.656457
3	Lasso	0.819824	10.592942	160.182278	12.656314
4	KNN	0.999996	0.020353	0.003182	0.056413
5	Random Forest	0.999985	0.031159	0.01293	0.113709
6	Gradient Boosting	0.995628	1.274107	3.886717	1.971476

Table 3
Influential feature parameter on the thermal properties

S.No.	Model	Filler % (%)	Fiber Orientation (%)	Temperature (%)
1	Linear Regression	89.2	0.29	10.51
2	Ridge	8.83	0.41	90.76
3	Lasso	8.81	0.38	90.81
4	KNN	3.58	1.38	95.04
5	Random Forest	3.18	0.94	95.88
6	Gradient Boosting	3.05	0.69	96.26

The Actual versus Predicted plot in the case of the Gradient Boosting (GB) model illustrates that the data points are closer to the line implying that there is a high level of concordance between the predicted and experimental values as noticed in Fig. 7. Nevertheless, as opposed to the K-Nearest Neighbors (KNN) and Random Forest models, a slight deviation of points can be observed, especially in the central range (4080). This small dispersion indicates that although the model does a good job in capturing the overall trend, small prediction errors remain. The errors are also not that big and constant meaning that the model has a high degree of accuracy although it does not predict perfectly. These values indicate very high predictive performance, albeit a bit less than KNN and Random Forest. The R2 (>0.99) indicates an excellent fit of the model and the RMSE (~1.97) is also low but greater than that of KNN and Random Forest as shown in Table 2. The above findings strongly show that temperature is the most significant factor in determining thermal behavior, and MWCNT content moderately affects thermal stability, and fiber orientation has little impact as represented in Table 3. Gradient Boosting model is very accurate in its predictions and it is much better compared to the linear models. Though a little less precise than KNN and Random Forest, it is a strong and stable model to predict the thermal characteristics of polymer composites.

The comparative study of six machine learning models demonstrates that they have significant variations in their predictive power in terms of thermal properties of MWCNT-reinforced polymer composites. Among the models, KNN model was the most accurate (R2=0.999996) and least erroneous (RMSE = 0.056) with the second place going to the Random Forest model (R2=0.999985). Gradient Boosting also had high predictive power (R2=0.9956) but with a little more error than KNN and Random Forest. However, the performance of linear models like Linear Regression, Ridge, and Lasso was poor (R2= ~0.82) and had much higher error values, which highlights their inefficiency in the nonlinear relationships that exist in the data. The analysis of feature importance in all the models indicated that temperature was the most common variable when it comes to thermal behaviour (~90-96 percent), followed by filler content (MWCNT), and insignificant fibres orientation. In general, the results indicate that complex machine learning models, especially KNN and Random Forest are very effective in the accurate prediction of thermal properties, and simple linear models cannot be applied to such complex material systems.

4. Conclusion

MWCNT based polymer composites of E-glass fibre were successfully prepared in this study through the hand lay-up method with different fiber orientations (0º/90º, 0º/45, & 0º/135º) as well as filler loadings of 0%, 1%, 3%, 5% and 7 vol.% MWCNTs. The thermal properties of the composites developed were measured, and machine learning algorithms were used to estimate the thermal characteristics of the experiments. These findings showed that the presence of MWCNTs has a significant positive effect on the thermal stability of polymer composites in terms of weight loss and degradation delay. The input parameters that were found to have the greatest effect on the thermal behavior were temperature with a contribution of around 90-96%, then filler content and fibre orientation had the least contribution towards thermal degradation. A comparative study of six machine learning models indicated that sophisticated models perform much better than the traditional linear methods. K-Nearest Neighbors (KNN) model was found to have the best prediction accuracy ($R^2 \approx 0.99$) and minimum error followed by the Random Forest model. Gradient Boosting was also able to give good predictions, but Linear Regression, Ridge and Lasso models performed poorly because they failed to figure nonlinear relationships in data. Altogether, experimental analysis and machine learning modeling provide an effective structure to predict thermal properties and optimize the design of composite. The results highlight the possibilities of data-driven methods in the development of advanced materials and indicate that KNN and Random Forest algorithms are very well adapted to predicting the thermal behavior of polymer nanocomposites with high accuracy.

References

[1] Y. Zhang and J. Gu, "A perspective for developing polymer-based electromagnetic interference shielding composites," *Nano-Micro Letters*, vol. 14, no. 1, p. 89, 2022.

[2] R. K. Bheema *et al.*, "A review on recent progress in polymer composites for effective electromagnetic interference shielding properties—

structures, processes, and sustainability approaches," *Nanoscale Advances*, vol. 6, no. 23, pp. 5773–5802, 2024.
[3] J. Liu and V. Nicolosi, "Electrically insulating electromagnetic interference shielding materials: A perspective," *Advanced Functional Materials*, vol. 35, no. 18, 2024.
[4] R. A. Khan, "Thermo-mechanical properties and applications of glass fiber reinforced polymer composites," *MCMS*, vol. 5, no. 3, 2023.
[5] N. Das *et al.*, "Polymer nanocomposites and nanostructured polymers," in *IGI Global*, pp. 213–240, 2024.
[6] V. K. Vineet and X. T. Xiaowu, *New Horizons in Nanofillers Based Polymer Composites II*. Multidisciplinary Digital Institute, 2024.
[7] W. Zhao *et al.*, "Carbon-nanotube-templated carbon nanofibers with improved mechanical performance," *Journal of Applied Physics*, vol. 129, no. 4, Art. no. 044303, 2021.
[8] S. Kumar, A. Singh, and M. Tiwari, "Numerical and analytical modelling of effective thermal conductivity of multi-walled carbon nanotube polymer nanocomposites," *Nanocomposites*, vol. 9, no. 1, pp. 30–42, 2023.
[9] M. Karuppusamy *et al.*, "A review of machine learning applications in polymer composites: Advancements, challenges, and future prospects," *Journal of Materials Chemistry A*, vol. 13, no. 22, pp. 16290–16308, 2025.
[10] J. Han *et al.*, "Toward accurate machine learning-driven prediction of polymeric composites properties based on experimental data," *Materials Genome Engineering Advances*, vol. 3, no. 3, 2025.
[11] R. Mahadeva *et al.*, "Machine learning and artificial intelligence in polymer composites," in *CRC Press*, pp. 73–89, 2025.
[12] Y. K. Hamidi, A. Berrado, and M. C. Altan, "Machine learning applications in polymer composites," in *Proc. AIP Conference Proceedings*, vol. 2205, 2020.
[13] M. W. Wang, T. C. Hsu, and C. H. Weng, "Alignment of MWCNTs in polymer composites by dielectrophoresis," *European Physical Journal Applied Physics*, vol. 42, no. 3, pp. 241–246, 2008.
[14] J. Maniraj *et al.*, "Machine learning techniques for the design and optimization of polymer composites: A review," *E3S Web of Conferences*, vol. 428, Art. no. 02013, 2023.
[15] S. S. Kharb *et al.*, "Machine learning-based erosion behavior of silicon carbide reinforced polymer composites," *Silicon*, vol. 13, no. 4, pp. 1113–1119, 2020.
[16] A. Sharma and V. Kushvaha, "Applications of machine learning in polymer composites," in *Springer Nature Singapore*, pp. 1–17, 2022.
[17] M. Laad *et al.*, "Synthesis and characterization of carbon-based polymer composites reinforced with MWCNTs and graphite in PVDF matrix," *Scientific Reports*, vol. 15, no. 1, Art. no. 28928, 2025.
[18] A. Sebastian and D. Raghavan, "Machine learning techniques for the optimization of polymer composites used in EMI shielding," *International Research Journal of Advanced Science Hub*, vol. 7, no. 5, pp. 462–471, 2025.
[19] M. E. A. Razzaq *et al.*, "Mechanical properties of biofiber/glass reinforced hybrid composites produced by hand lay-up method: A review," *Materials Engineering Research*, vol. 3, no. 1, pp. 144–155, 2021.
[20] Z. Li *et al.*, "Machine learning framework for evaluating microscale interface cohesive zone models of polymer composites," *ACS Applied Materials & Interfaces*, vol. 17, no. 45, pp. 62590–62605, 2025.
[21] Z. Li *et al.*, "Machine learning framework for evaluating microscale interface cohesive zone models of polymer composites," *Figshare*, Nov. 2025.
[22] A. M. Anwar *et al.*, "Performance evaluation of irradiated space structure composites manufactured by the hand lay-up method," *IREASE*, vol. 11, no. 4, p. 155, 2018.