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Original Research Article

Data-Augmented Deep Learning Models for Assessing Thermal Performance in Sustainable Building Materials

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ABSTRACT

Energy efficiency in buildings drives the development of sustainable materials, with Phase Change Materials standing out for their contribution to the construction sector. Phase Change Materials, integrated into materials like cement or concrete, regulate indoor temperatures by absorbing heat during the day and releasing it at night. Accurate thermal property assessment is crucial for optimizing these materials, yet conventional experimental methods are time-consuming, costly, and require specialized labor. While automation and machine learning streamline the process, they do not eliminate the need for expertise but rather shift the focus toward data-driven material innovation, complementing rather than replacing traditional roles. To enhance efficiency, our study integrates deep neural networks. A Generative Adversarial Network first augments the dataset, and a Multilayer Perceptron then predicts the properties of cementitious composites enriched with Phase Change Material and nano-silica aerogel. Using inputs such as mass composition and density, the model outputs compressive strength and thermal conductivity. Training with synthetic data yields high predictive accuracy, highlighting the potential of data augmentation in domains with limited datasets. This approach enhances the precision and efficiency of assessing thermal performance in innovative construction materials while supporting the evolving role of experts in the field.

KEYWORDS

Energy Efficiency, Phase Change Materials, Deep Neural Networks, Multilayer Perceptron, Data Augmentation, Thermal conductivity.

INTRODUCTION

Energy efficiency in buildings is essential for reducing energy consumption while maintaining thermal comfort and minimizing environmental impact. A key strategy to achieve this lower energy consumption involves integrating materials with enhanced thermal performance, reducing reliance on active heating and cooling systems [1]. Among these materials, phase change materials (PCMs) have gained prominence due to their ability to absorb and release thermal energy as they transition between phases, improving indoor temperature regulation and overall energy efficiency [2].

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Concrete, widely used in construction for its high compressive strength, durability, and affordability, presents opportunities for improved sustainability when combined with PCMs and other thermal-enhancing materials. By precisely tailoring the concrete composition, its thermal performance can be optimized without compromising structural integrity. Several studies have demonstrated the benefits of PCM integration in building envelopes [3]. For instance, Rajesh et al. [4] reported a 20% reduction in energy consumption when using PCM-modified mortar, while Qu et al. [5] employed EnergyPlus simulations to assess thermal comfort improvements. Other experimental and numerical studies [6,7] have reinforced the potential of PCM-enhanced materials in mitigating temperature fluctuations and reducing heat transfer into buildings.

Given the growing emphasis on sustainable construction, accurately assessing the thermal and mathematical properties of these advanced materials is critical. Traditional experimental methods, while reliable, are often time-consuming, costly, and require specialized labor. Predictive modeling offers an efficient alternative, enabling material performance evaluation without extensive physical testing. Beyond thermal conductivity, compressive strength remains a fundamental property for ensuring structural integrity. Therefore, an effective approach must balance both thermal and mechanical performance for practical implementation [8].

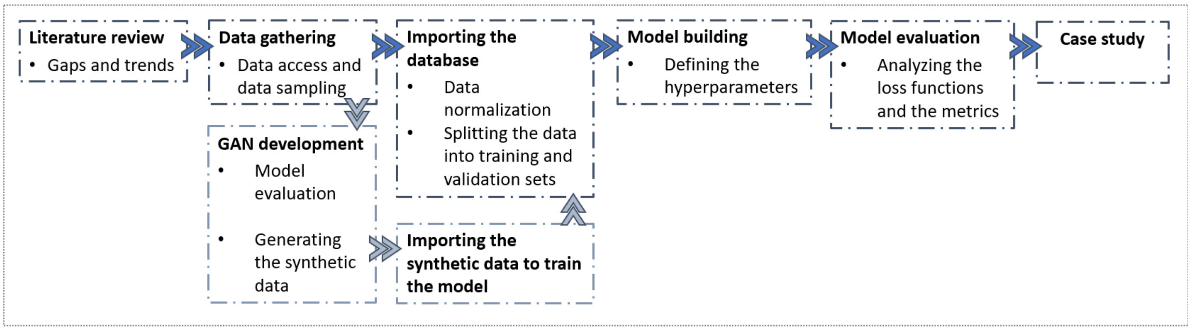
Machine learning (ML) and deep learning (DL) have emerged as powerful tools for predicting material properties, leveraging large datasets to identify patterns and improve accuracy [9]. ML models have been successfully applied to predict the properties of concrete. Mehta [10] compared some models to predict the strength of concrete with waste foundry sand, finding ANN to be the most accurate. Ji et al. [11] introduced five key mix parameters and used ANN-based models to optimize concrete mix design, improving efficiency, durability, and sustainability tensile strength. Song and Kwon [12] proposed a neural network-based technique to predict chloride diffusion in high-performance concrete, improving evaluation accuracy and efficiency. However, studies focusing on ML-based predictions of thermal properties remain limited. Among ML models, artificial neural networks (ANNs) are particularly effective for capturing complex relationships between material composition and performance [13,14].

A major challenge in developing accurate ML models is the need for large, high-quality datasets. Insufficient data can hinder model generalization and lead to suboptimal predictions. To overcome this limitation, data augmentation techniques, such as Generative Adversarial Networks (GANs), have been increasingly utilized. Originally introduced by Goodfellow et al. [15] for image generation, GANs have since been adapted to generate synthetic tabular data, addressing data scarcity issues in various fields. Techniques such as Conditional Tabular GAN (CTGAN) [16] and CopulaGAN [17] have demonstrated success in augmenting real datasets to improve model performance. Despite extensive research on ML applications in concrete property prediction, the integration of advanced generative models like GANs for predicting both thermal and mechanical properties remains relatively unexplored.

This study builds upon prior research [18] that developed a generalist model for predicting the thermal conductivity of concrete. Expanding on that approach, this work addresses the challenge of predicting both thermal conductivity and compressive strength using a limited dataset. A multilayer perceptron (MLP) model is employed for property prediction, while a CopulaGAN model is used to generate synthetic tabular data based on published studies. This combination enhances predictive accuracy and demonstrates the feasibility of integrating real and synthetic data. By improving the precision of material property assessment, this study contributes to the development of energy-efficient construction materials while maintaining structural integrity, supporting the broader goal of sustainable building practices.

METHODS

The proposed methodology builds upon the foundation of a previously developed approach, refining and extending it through the incorporation of two key components: (1) the development of a Multilayer Perceptron (MLP) model designed to predict material properties based on their unique features, and (2) the implementation of a Generative Adversarial Network (GAN) for data augmentation. This dual-step process tackles the challenge of limited datasets by generating synthetic data to complement real data, ultimately improving the predictive accuracy and overall performance of the MLP model. The workflow followed in this study is outlined in Figure 1, which outlines each stage, from data gathering to model evaluation. This workflow was designed based on prior research and refined to address the specific challenges of predicting material properties using machine learning.



Data processing

To ensure consistency and reliability, data normalization was performed before training. The dataset underwent min-max scaling, transforming all input features to a range of [0,1] to prevent scale dominance and facilitate stable training. This normalization step was applied to both the real and synthetic datasets to maintain uniformity.

Generative Adversarial Network

Given the limited availability of real-world data, a CopulaGAN model was used to generate synthetic data while maintaining the statistical patterns of the original dataset. The GAN was trained with an adaptive learning rate and optimized to reduce differences between real and synthetic data. Once trained, it generated 1,000 synthetic data points, which were combined with the original dataset for model training. The quality of the synthetic data was evaluated by comparing its statistical properties to the real data using Kolmogorov-Smirnov (KS) tests and correlation matrix comparisons.

Model building

The Multilayer Perceptron (MLP) model was developed to predict material properties based on key input features. Its architecture included an input layer for processing normalized data, multiple hidden layers with activation functions to capture complex patterns, and an output layer tailored to the prediction task. The model was trained using an optimization algorithm with a predefined learning rate, while a loss function was employed to minimize prediction errors. The dataset was divided into training and validation sets to ensure balanced learning and hyperparameter tuning was conducted to enhance model accuracy and generalization.

Validation and case study

To assess the model's reliability, a validation process was conducted by training and testing it under three different scenarios: one using only real data, another relying solely on synthetic data, and a third combining both datasets. This comparison allowed for a detailed evaluation of how data augmentation influences predictive accuracy and generalization. Model performance was analyzed by tracking the loss function's behavior and comparing predicted values against actual measurements.

To further validate the approach, a case study was carried out to test the model's effectiveness in predicting thermal and mechanical properties on unseen data. This practical assessment provided insights into the model's adaptability and robustness in real-world applications. The results demonstrated that incorporating synthetic data significantly enhanced prediction accuracy, reinforcing the effectiveness of GAN-based data augmentation in overcoming dataset limitations.

This approach demonstrates how combining GAN-based data augmentation with MLP predictive modeling can enhance property assessment, providing a scalable and efficient solution for sustainable construction research.

CASE STUDY

The proposed model is applied to a case study focused on concrete mixtures enhanced with Phase Change Materials (PCM) and nano-silica aerogel. As emphasized in the introduction, thermal conductivity (TC) and compressive strength (CS) are critical properties that significantly influence a building's thermal performance and structural resistance. These properties are highly dependent on the type and proportion of the constituents within the concrete mixture. Therefore, this study aims to predict TC and CS based on the mass composition of the mixture's components.

To address the challenges associated with limited datasets, this study utilizes 33 experimental samples, each representing unique compositions of Phase Change Material (PCM) and nano-silica aerogel. These samples were sourced from relevant literature, ensuring a diverse dataset to support model development [19]. Seven critical input parameters that influence thermal conductivity (TC) and compressive strength (CS) were identified for this analysis: density (D), cement content (C), sand content (S), aerogel aggregate content (AAg), PCM aggregate content (PCMAg), water content (W), and superplasticizer content (Sp). Figure 2 provides a schematic illustration of the neural network architecture used in this case study, highlighting the relationship between the input parameters, the processing layers, and the predicted outputs.

Table 1 offers a comprehensive summary of the range of values for each input parameter, along with the corresponding TC and CS outputs, illustrating the variability within the dataset. The measured TC values range from 0.19 to 1.80 W/m·K, with a standard deviation of 0.4 W/m·K, while CS values span from 1.4 to 42.0 MPa, with a standard deviation of 11.5 MPa. This variability underscores the significant role that compositional differences play in determining the thermal and mechanical properties of the mixtures, emphasizing the importance of developing a robust predictive model capable of accurately capturing these complex relationships.

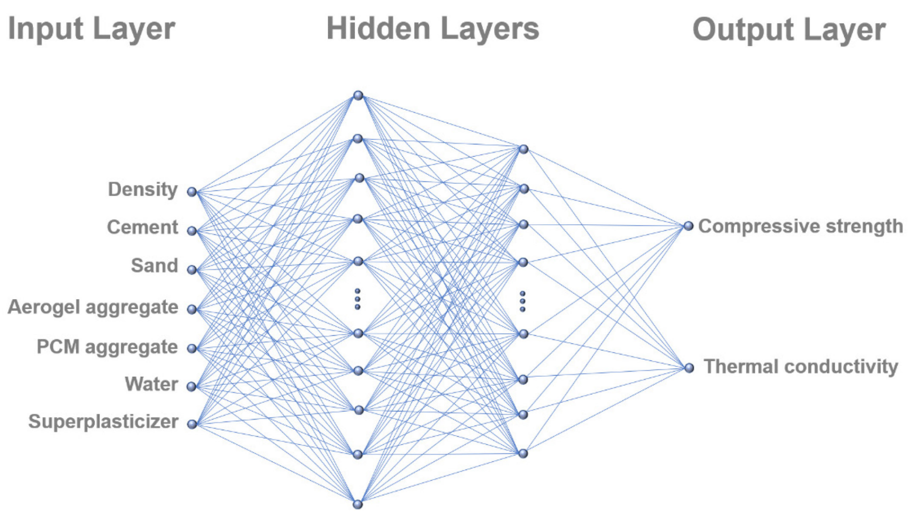


Figure 2. The multilayer perceptron model

Table 1. Summary of Input Parameters and Corresponding Outputs

D	C	S	AAg	PCMAg	W	Sp	CS	TC
2384.31	650	1741.00	0	0	247	9,75	42	1.8000
2378.27	650	1566.59	0	174.10	247	9.75	38	1.4046
2366.20	650	1479.85	0	261.15	247	9.75	35	1.3057
235412	650	1305.75	0	435.25	247	9.75	31	0.9556
2323.94	650	1218.70	0	522.3	247	9.75	28	0.9021
2251.51	650	1131.65	0	609.35	247	9.75	23	0.8815
2179.07	650	1044.60	0	696.40	247	9.75	20	0.8526
2046.28	650	957.55	0	783.45	247	9.75	19	0.7991
1949.70	650	783.45	0	957.55	247	9.75	16	0.7002
1883.30	650	696.40	0	1044.60	247	9.75	16	0.6879
1798.79	650	609.35	0	1131.65	247	9.75	14	0.6714
1720.32	650	522.30	0	1218.70	247	9.75	14	0.6508
1611.67	650	435.25	0	1305.75	247	9.75	10	0.6302
1490.95	650	261.15	0	1479.85	247	9.75	7.2	0.6014
1430.58	650	174.10	0	1566.90	247	9.75	6.9	0.5519
1376.26	650	87.05	0	1653.95	247	9.75	5.5	0.4902
1352.11	650	0	0	1741.00	247	9.75	5.2	0.4201
2354.12	650	1653.95	87.05	0	247	9.75	32	1.5034
2082.49	650	1479.85	261.15	0	247	9.75	23	1.1080
1991.95	650	1392.80	348.2	0	247	9.75	22	0.9021
1913.48	650	1305.75	435.25	0	247	9.75	20	0.8609
1859.15	650	1218.70	522.3	0	247	9.75	19	0.8197
1714.29	650	1044.60	696.4	0	247	9.75	14	0.7826
1635.81	650	957.55	783.45	0	247	9.75	12	0.6796
1515.09	650	870.50	870.5	0	247	9.75	7.6	0.5519
1442.66	650	783.45	957.55	0	247	9.75	6.3	0.4819
1219.32	650	609.35	1131.65	0	247	9.75	4.5	0.4325
1152.92	650	522.30	1218.7	0	247	9.75	3.3	0.3913
1038.23	650	435.25	1305.75	0	247	9.75	3	0.3501

820.93	650	261.15	1479.85	0	247	9.75	2.1	0.2636
754.53	650	174.10	1566.9	0	247	9.75	1.8	0.2018
712.27	650	87.05	1653.95	0	247	9.75	1.5	0.2018
688.13	650	0	1741.00	0	247	9.75	1.4	0.1854

The dataset is randomly divided into two subsets: 80% for training and 20% for validation. To evaluate the model's robustness and generalization capability, its performance is tested on an independent dataset. The reliability and reproducibility of the Artificial Neural Network (ANN) model are examined using established metrics such as Root Mean Square Error (RMSE) and the coefficient of determination (R^2). These metrics provide a comprehensive evaluation of the model's accuracy in capturing the complex relationships between input parameters and the target properties.

By combining experimental data collected from the literature with predictive modeling, this case study demonstrates the potential of ANN models to address data scarcity challenges while offering precise predictions for optimizing concrete mixtures. This approach not only ensures efficient material design but also contributes to advancing the integration of machine learning in material science applications.

RESULTS AND DISCUSSION

The initial step of this study focuses on developing a Multilayer Perceptron (MLP) model designed to predict two critical properties of concrete: compressive strength and thermal conductivity. These predictions are based on the mass composition of the concrete's constituents and its density, capturing the intricate relationships between material composition and performance. The configuration and design of the MLP model are detailed in Table 2, which provides a comprehensive summary of its essential components, including the selected hyperparameters, evaluation metrics, activation functions, optimization techniques, and loss functions.

Table 2. The main features of the model

Hyperparameters	
	Hidden layers = 2
	Neurons = [200,100]
	Batch size = 64
	Learning rate = 0.001
	Epochs = 100
Metrics	
	RMSE
	R^2
Activation function	
	ReLU
Optimization function	
	Stochastic Gradient Descent (SGD)
Loss function	
	MSE

The second step of this study focuses on evaluating the impact of synthetic data on the training of the MLP model. This analysis is conducted to determine whether a model trained with augmented data can produce results comparable to the performance achieved through training with real data and possibly enhance it. This study investigates two distinct scenarios: (a) training the MLP model exclusively with the real dataset containing 33 entries, and (b) training the model with the synthetic data consisting of 1000 entries first and then the real dataset.

Both scenarios utilize the same model architecture and hyperparameters to ensure consistency, with the key difference being the composition of the datasets used during the training and validation phases. Our approach in scenario (b) involves training the model first with synthetic data. Subsequently, the same model architecture uses the real dataset to enhance the model's performance. The results of the training phase reveal that scenario (b) outperforms scenario (a) in terms of overall metrics. For scenario (a), the model achieved a Root Mean Square Error (RMSE) of 0.0700 and a coefficient of determination (R^2) of 0.9940. In contrast, scenario (b) demonstrated improved performance with an RMSE of 0.0530 and an R^2 of 0.9971. Table 3 provides a detailed comparison of the validation and test results for both scenarios, highlighting the enhanced predictive accuracy achieved through synthetic data augmentation.

Table 3. Comparison between the performance metrics of the MLP model trained with both datasets

Scenario	Dataset	CS		TC	
		RMSE	R^2	RMSE	R^2
(a)	Validation	0.6329	0.9970	0.0226	0.9964
	Test	1.2728	0.9922	0.0381	0.9921
(b)	Validation	0.5669	0.9975	0.0203	0.9971
	Test	0.7239	0.9975	0.0149	0.9988

Despite the constraints posed by the limited real dataset in scenario (a), the MLP model delivered reliable predictions for both compressive strength (CS) and thermal conductivity (TC) across the training, validation, and test datasets. However, the predictive performance improved markedly in scenario (b), where synthetic data augmentation was employed during training. This enhancement was consistently reflected across all datasets, demonstrating the effectiveness of integrating synthetic data to overcome the limitations of a small real dataset.

The evaluation of the MLP model was conducted using an independent test set comprising 8 data points. Figure 3(a) and Figure 3(b) depict the CS predictions for scenarios (a) and (b), respectively, while Figure 4(a) and Figure 4(b) illustrate the TC predictions. For CS, Figure 3(a) shows that scenario (a) produced results reasonably aligned with the x=y line, although several predictions deviated, with errors exceeding 0.18. Scenario (b), as shown in Figure 3(b), displayed significantly improved alignment with the x=y line, reducing prediction errors substantially. This enhancement is evident in the metrics, with scenario (b) achieving an R^2 value of 0.9975 and an RMSE of 0.7239, a noticeable improvement over scenario (a).

The results of TC predictions are shown in Figure 4(a) and Figure 4(b). In scenario (a), some predictions deviated from the ideal line, with a maximum error of 0.05, as indicated in Figure 4(a). In contrast, scenario (b), presented in Figure 4(b), reduced these errors by 50%, with a maximum deviation of 0.025. The performance metrics for scenario (b) further highlight this improvement, with an R^2 value of 0.9921 and an RMSE of 0.0381, underscoring the benefits of incorporating synthetic data into the model training.

Overall, the results confirm that augmenting the training dataset with synthetic data enhances the predictive accuracy of the MLP model for both compressive strength and thermal conductivity. The incorporation of synthetic data not only minimizes errors across the test dataset but also strengthens the model's generalization capabilities, offering a robust solution for scenarios constrained by limited real data availability.

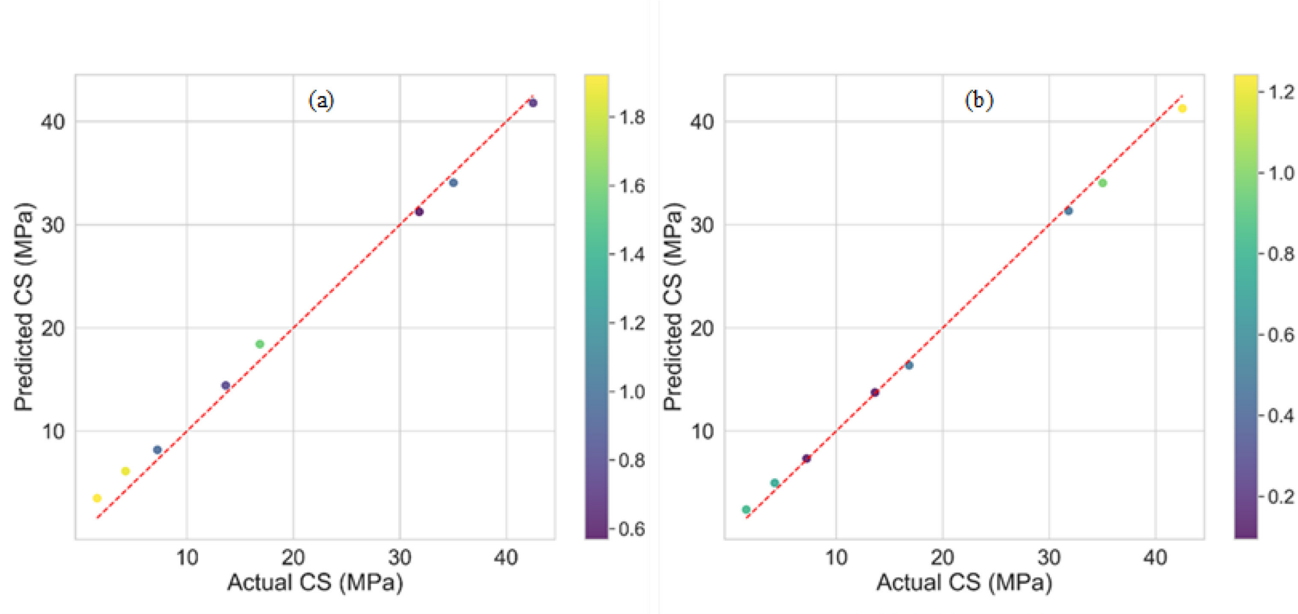


Figure 3. Comparison of compressive strength predictions on the test dataset under two training scenarios: (a) MLP trained solely on real data and (b) MLP trained on a hybrid dataset combining 1,000 synthetic data points with real data.

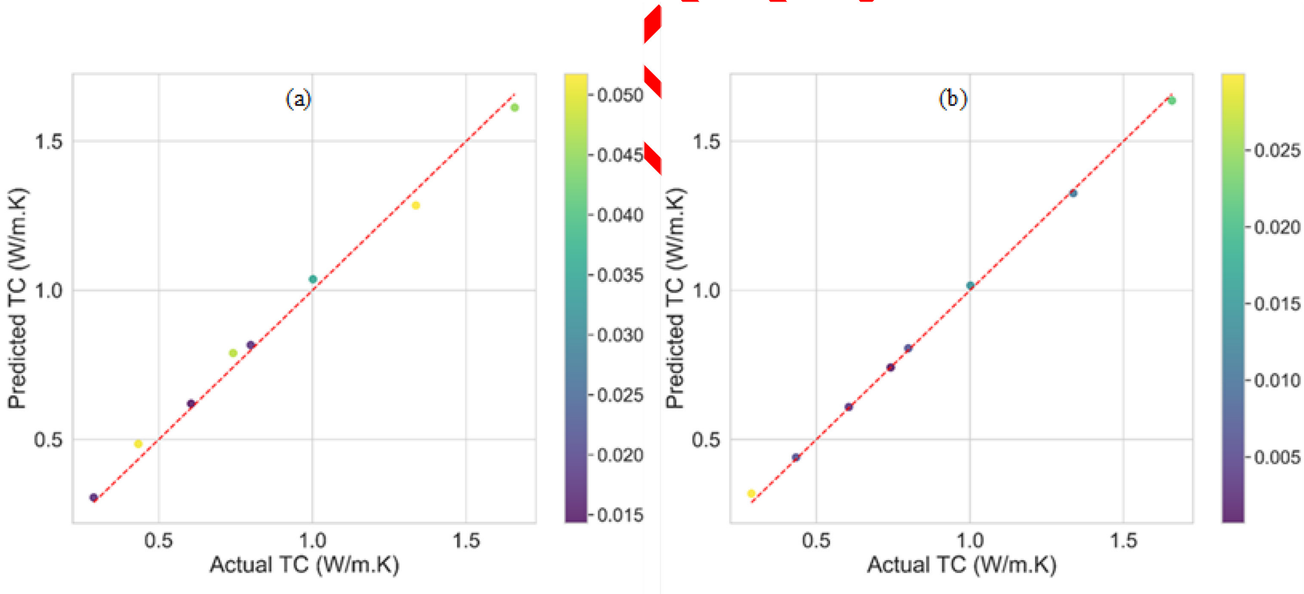


Figure 4. Comparison of thermal conductivity predictions on the test dataset under two training scenarios: (a) MLP trained solely on real data and (b) MLP trained on a hybrid dataset combining 1,000 synthetic data points with real data.

Figure 5 and Figure 6 illustrate the correlation between the actual test dataset values and the predictions generated by the Multilayer Perceptron (MLP) model. These visual comparisons provide a clear understanding of the model's ability to forecast compressive strength and thermal conductivity. In Figure 5(a) and Figure 6(a), the model is trained exclusively on the real dataset, while Figure 5(b) and Figure 6(b) present the model's performance when trained with an augmented dataset containing 1,000 synthetic data points alongside the real dataset.

For compressive strength predictions, Figure 5(a) demonstrates a generally strong agreement between predicted and actual values, though deviations are evident, with errors ranging from 0.57

to 1.92 MPa. When synthetic data is included in the training, as shown in Figure 5(b), the model's performance significantly improves, particularly for compressive strength values between 7 MPa and 31 MPa. The incorporation of synthetic data leads to more consistent predictions and a marked reduction in error magnitude.

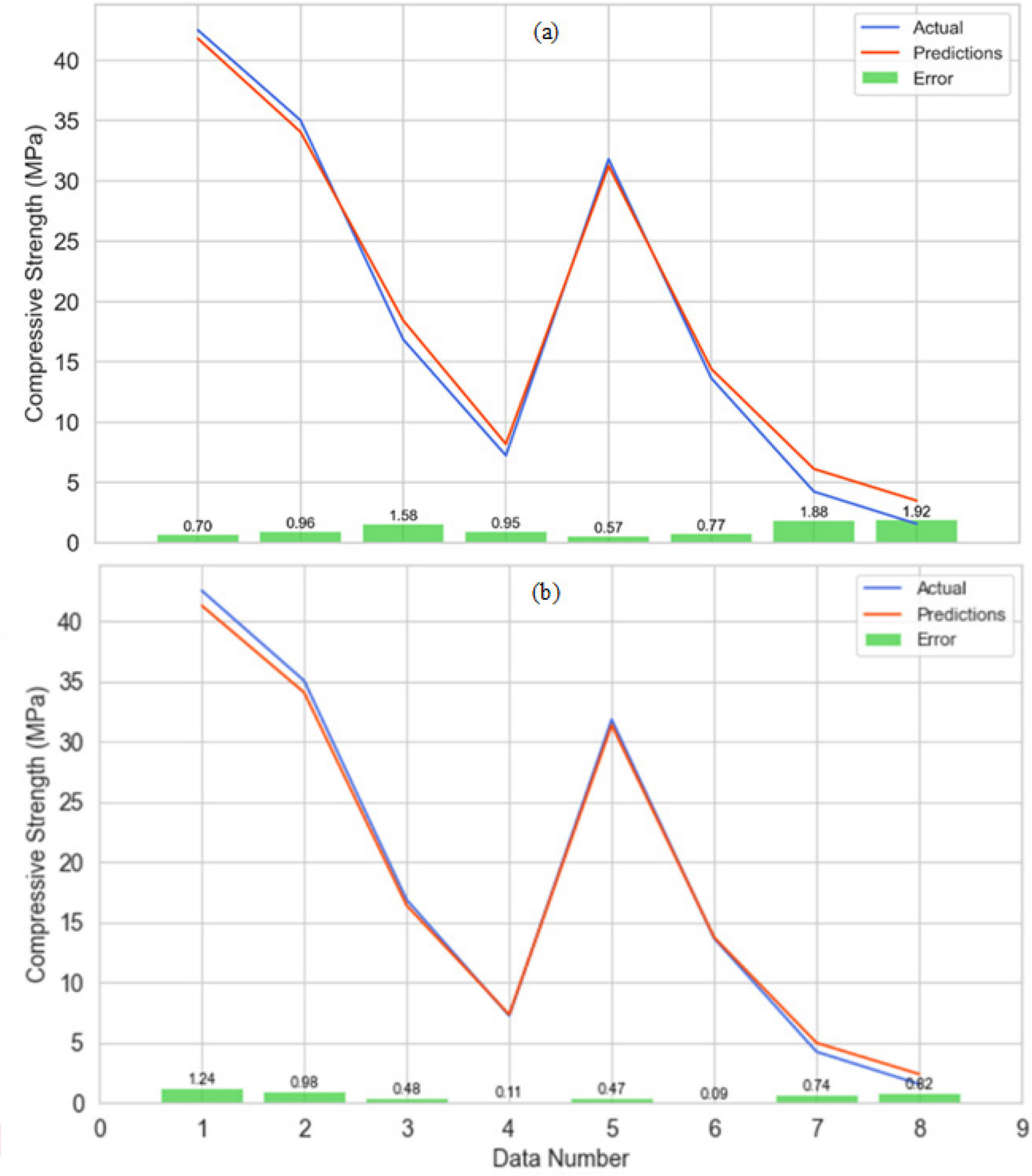


Figure 5. Prediction performance comparison for compressive strength on the test dataset under two training conditions: (a) MLP trained solely on real data and (b) MLP trained on a hybrid dataset combining 1,000 synthetic data points with real data.

Thermal conductivity results reveal even greater improvements. Figure 6(a) highlights the model's capability to closely approximate actual values, with approximately half of the data points showing errors up to 0.05 W/m.K. Figure 6(b) demonstrates the superior accuracy achieved by incorporating synthetic data, with only two data points exhibiting minor errors of 0.02 and 0.03 W/m.K. These results underscore the enhanced predictive reliability gained through data augmentation.

Overall, the comparison of actual versus predicted values across both scenarios clearly indicates that integrating synthetic data enhances the MLP model's performance. The augmented dataset improves the model's accuracy and minimizes prediction errors, particularly in scenarios with limited real data availability. These findings validate the effectiveness of the proposed data augmentation approach in strengthening the model's generalization capabilities.

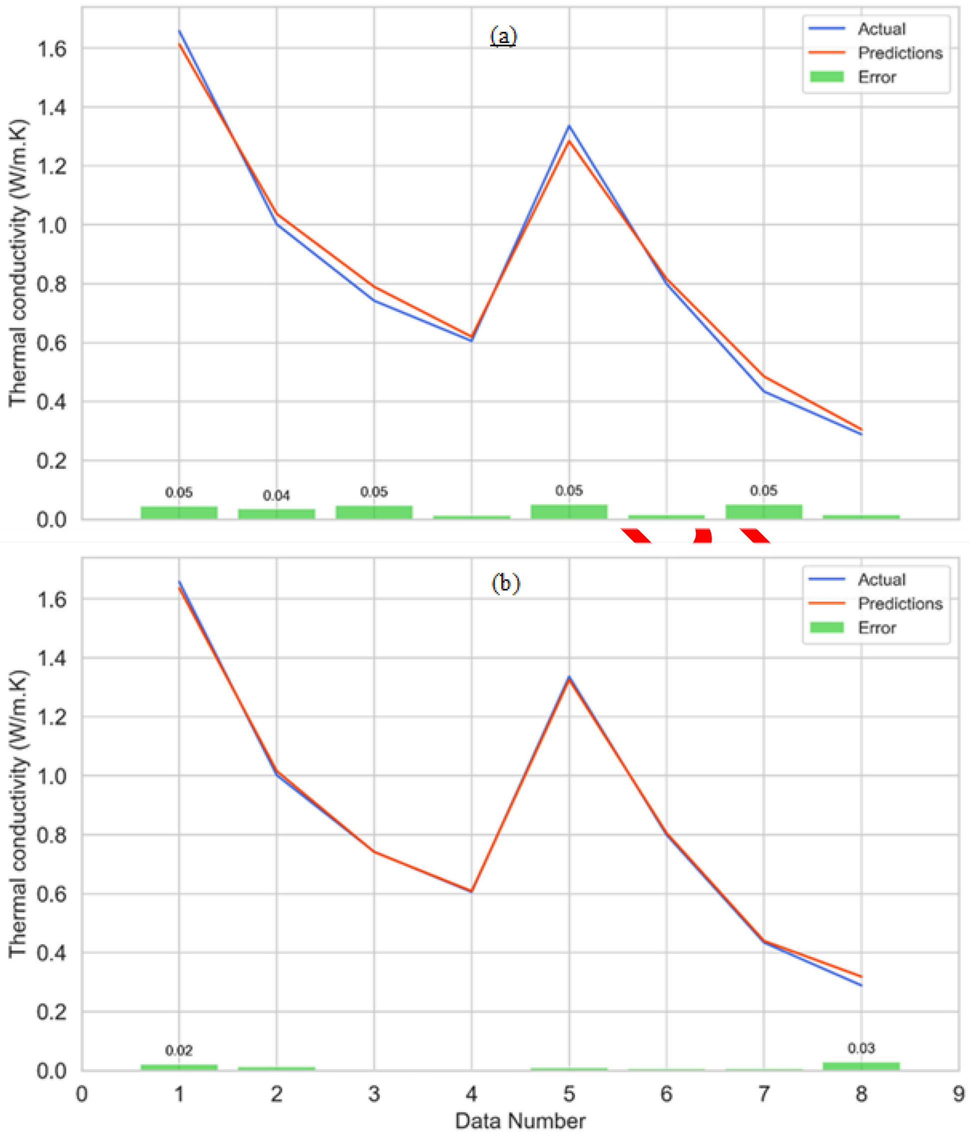


Figure 6. Prediction performance comparison for thermal conductivity on the test dataset under two training conditions: (a) MLP trained solely on real data and (b) MLP trained on a hybrid dataset combining 1,000 synthetic data points with real data.

CONCLUSIONS

This study introduced an innovative approach to training a multilayer perceptron (MLP model by leveraging data augmentation techniques. Specifically, a generative adversarial network (GAN) was utilized to generate synthetic datasets, which allowed the MLP to be trained on a combination of real and artificial data. The methodology was demonstrated using a limited dataset of concrete mixtures incorporating phase change materials (PCM) and nano-silica aerogel, focusing on predicting both thermal conductivity and compressive strength.

Two training scenarios were examined in this study: (a) using only the real dataset for MLP training and (b) pretraining the MLP with 1000 synthetic data points followed by real data. The results revealed a substantial improvement in prediction accuracy and error reduction when synthetic data was incorporated into the training process. This underscores the reliability of the CopulaGAN synthesizer for generating high-quality synthetic data and highlights the robustness of MLP models when trained on hybrid datasets. Scenario (a) achieved RMSE and R^2 values of 1.2728 and 0.9922 for compressive strength, and 0.0381 and 0.9921 for thermal conductivity. In contrast, scenario (b) achieved significantly better results, with RMSE and R^2 values of 0.7239 and 0.9975 for compressive strength, and 0.0149 and 0.9988 for thermal conductivity.

Building upon earlier work by the authors, this research extends the predictive capabilities of the MLP model, adapting it to include compressive strength alongside thermal conductivity, while demonstrating its flexibility with a smaller, augmented dataset. The findings underscore the potential of data augmentation to overcome the limitations of data scarcity, a common challenge in machine learning applications for materials science.

In addition to achieving significant accuracy improvements, this study highlights the broader applicability of the proposed methodology to other energy-efficient construction materials. By combining real and synthetic data, the MLP model offers an adaptable and scalable framework for predicting multiple material properties. However, further research could expand this work by incorporating additional input variables such as temperature, aggregate characteristics, and mineral composition. Furthermore, expanding the dataset and validating the model using independent or experimental data could enhance its generalizability and robustness.

Ultimately, this study demonstrates the transformative potential of integrating synthetic data into predictive modeling workflows, enabling reliable predictions even with limited datasets. By addressing these challenges, the proposed methodology provides a valuable tool for advancing the development of sustainable and energy-efficient building materials.

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NOMENCLATURE

Abbreviations	
AAg	Aerogel aggregate content
ANN	Artificial neural network
C	Cement content
DL	Deep learning
DNN	Deep neural network
GAN	Generative adversarial network
ML	Machine learning
MLP	Multilayer perceptron
PAg	PCM aggregate content
S	Sand content
Sp	Superplasticizer content
W	Water content
Symbols	
Coefficient of determination	R^2
Compressive strength - CS	[MPa]
Density - D	ρ [kg/m³]

Root mean squared error	$RMSE$
Thermal conductivity - TC	k [W/m.K]

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