STM JOURNALS

Journal of
Polymer & Composites

https://journals.stmjournals.com/jopc

ISSN: 2321-2810 (Online)
ISSN: 2321-8525 (Print)
Volume 14, Special Issue 4, 2026
January–December
DOI (Journal): 10.37591/JoPC

Research JoPC

AI-Optimized Biodegradable Polymer Composites for Medical Applications

Manisha Tanwer[1], Narendrakumar J. Suryavanshi[2,*], Debanjana Prasad[3], Prabhavathy Devi N.[4], M. Rama Chandra Rao[5], M. Radhika Mani[6]

Abstract

The value of biodegradable polymer composites in the medical practice has been massive as the composites may be deployed to provide temporary structural support, and they are also safe to degrade within the human body. However, the conventional material design process is trial and error, which is ineffective and inefficient. The article proposes a hybrid model involving experimental characterization, as well as an artificial intelligence (AI)-based model, to optimize biodegradable polymer composites. Polylactic acid (PLA) and polycaprolactone (PCL) are some of the bioactive filled polymers that are being investigated to attain a more appropriate mechanical and degradation behavior. Machine learning models are random Forest and Artificial Neural Networks, which are used to predict the properties of the materials based on the factors of composition and processing. The results are very precise in prediction and correlation with the experimental findings. Multi objective optimization enables identification of the best composite structures that are improved in tensile strength and controlled degradation. The tests of comparative analysis can confirm the hypothesis that the AI-based method can significantly reduce time and experiment work on the development process and enhance the performance of materials. The given framework discusses the potential of AI-inspired material design as the means of creating biodegradable biomaterials in tissue engineering, drug delivery, and implantable medical devices.

***Author for Correspondence**
Narendrakumar J. Suryavanshi
E-mail: njsuryawanshi1981@gmail.com

[1]Associate Professor, Department of Basic Science and Humanities, D Y Patil College of Engineering, Akurdi, Pune, Maharashtra, India
[2]Associate Professor, Department of Science, Krishna Institute of Science and Technology, Krishna Vishwa Vidyapeeth "Deemed to be University", Karad, Satara, Maharashtra, India
[3]Associate Professor, Department of Biotechnology, Noida international University, Greater Noida, Uttar Pradesh, India
[4]Associate Professor, Department of Nutrition and Dietetics, Meenakshi College of Arts and Science, Meenakshi Academy of Higher Education and Research, Chennai, Tamil Nadu, India
[5]Associate Professor, Department of Computer Science and Engineering (AI&ML), Vardhaman College of Engineering, Shamshabad, Hyderabad, Telangana, India
[6]Professor, Department of Computer Science and Engineering, Pragati Engineering College, Kakinada, Andhra Pradesh, India

Received Date: May 01, 2026
Accepted Date: July 03, 2026
Published Date: August 25, 2026

Citation: Manisha Tanwer, Narendrakumar J. Suryavanshi, Debanjana Prasad, Prabhavathy Devi N., M. Rama Chandra Rao, M. Radhika Mani. AI-Optimized Biodegradable Polymer Composites for Medical Applications. Journal of Polymer & Composites. 2026; 14(Special Issue 4): S354–S365p.

Keywords: Biodegradable polymer composites, artificial intelligence, machine learning, biomaterials, tissue engineering, drug delivery, material optimization

INTRODUCTION

Biomedical engineering has been introduced as one of the pillars of the concept of biodegradable polymer composites since it can provide temporary mechanical aid without harming the human organism due to its degradation. These materials eliminate the risk of the patient and reduce the cost of secondary surgery because the materials do not have to be removed after surgery. The most used biodegradable polymers are polylactic acid (PLA) and polycaprolactone (PCL) that have been shown to have desirable biocompatibility and degradation rates that can be regulated and can be used in tissue engineering scaffolds, drug delivery systems, and temporary implants [1]. The wish to yield the optimal output of such materials is an intricate endeavor since all of them are mutually reliant on one another in regards of the mechanical strength, degradation and biological compatibility kinetics.

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More traditional material design approaches are founded on high-intensity experimental experimentation, where different combinations of polymers, fillers and processing conditions are experimentally tested. It is an inefficient and time-consuming method of searching the large design space of composite materials [2].

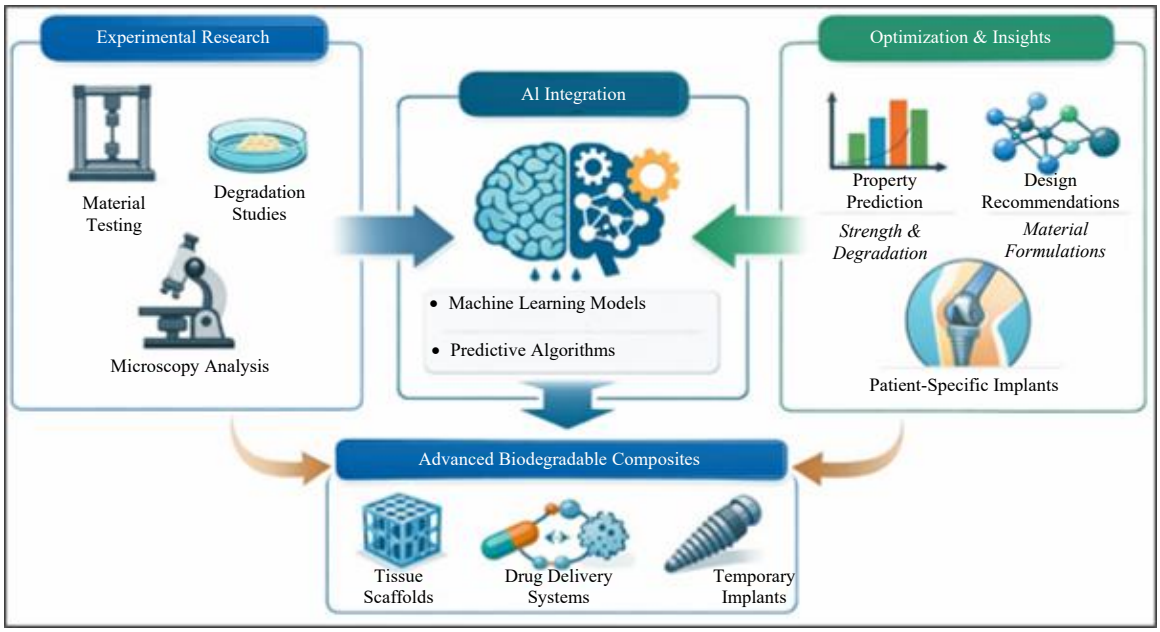


Figure 1. AI and experimental framework for medical composites.

Biomedical uses are also getting increasingly tailored to specific patient conditions and functional requirements and this is even harder to create materials. The innovation that can address these issues is artificial intelligence (AI) since it enables the design of materials and optimization using data [3]. Machine learning algorithms can be used to model complex correlations between input parameters, such as polymer composition as in Figure 1, filler concentration and fabrication conditions, and output properties such as tensile strength, degradation rate, and porosity. The AI is also able to store the large number of required physical experiments and make predictions more accurate, with the help of experimental datasets [4].

The article proposes experimental-AI hybrid to the development of biodegradable polymer composites that are more optimal in the medical community. It is a combination of systematic experimental characterization and multifaceted machine learning models to achieve effective and dependable optimization of the material. It will be intended to explain how AI-based methods can accelerate the development of materials, enhance their functionality, and lead to the development of next-generation biodegradable biomaterials.

LITERATURE REVIEW AND RESEARCH GAP

Polymers and polymers composites that are biodegradable have been widely researched to be utilized in biomedical applications which include PLA, PCL and polyglycolic acid (PGA). Application of these polymers has become very popular due to its biodegradability, mechanical flexibility as well as the ability to be applied in other fabrication processes [5]. Replacement of mechanical strength and biological functionality using bioactive fillers – such as hydroxyapatite, bioactive Glass, and natural fibers – have also been studied.

Such composites have demonstrated excellent potential in the field of bone regeneration and wound healing. The development of fabrication technologies – such as electrospinning, 3D bioprinting, and solvent casting – has made it possible to generate high porosity and structurally complex scaffolds [6,

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7]. These are replicas of the extracellular matrix, which promotes cell adhesion, proliferation and transportation of nutrients. The process of optimization of material properties is mostly reliant on the empirical approach which constrained efficiency and scalability.

Table 1. Overview of existing research in biodegradable composites.

Study focus	Materials used	Technique used	Key outcome
Scaffold Design	PLA, PCL	Electrospinning	Improved porosity & cell growth.
Bone Tissue Engineering	PLA + HA	3D Bioprinting	Enhanced mechanical strength.
Drug Delivery Systems	PCL-based composites	Solvent Casting	Controlled drug release.
Bioactive Composites	Polymer + Glass	Melt Blending	Increased bioactivity.

The adoption of AI in biomaterials research has seen an acceleration in the recent past as explained in Table 1. Models of machine learning including Support Vector Machines, random forest, and artificial neural network have been utilized to predict material properties and optimize processing parameters [8, 9]. These methods have shown themselves to be useful in capturing nonlinear relationships and enhance prediction accuracy. Yet, most of the current research is heavily dependent on computational modeling with minimal experimental support and this decreases their practical implementation. The second weakness is that there are no large-scale and standardized data sets, which are necessary to train effective AI models. Also, multi-objective optimization of mechanical, biological, and degradation properties is not usually done holistically [10, 11]. Most of the research is concentrated on a single property, without considering trade-offs needed to make the use of this property in the real world.

The current article fills these gaps by suggesting a hybrid model based on the formation of experimental data and predictive modeling using AI. The strategy will provide reliability and applicability as the AI predictions are validated by experimental results. Moreover, it focuses on multi-objective optimization to have a balanced result in terms of the major material properties to promote the sphere of the biodegradable polymer composite design.

MATERIAL SELECTION AND COMPOSITE FABRICATION

During the design of biodegradable polymer composites to be used in medical applications, one of the most important stages is the choice of suitable materials. Polylactic acid (PLA) and polycaprolactone (PCL) are selected as the major matrix materials in this study because their biocompatibility and the degradation behavior are well known and controlled. PLA has been reported to be highly stiff and comparatively more degradable whereas PCL is more flexible and slower to degrade [12, 13].

Table 2. Materials used and their functional properties.

Material	Type	Key properties	Biomedical relevance
PLA	Polymer	High stiffness, fast degradation	Tissue scaffolds.
PCL	Polymer	Flexible, slow degradation	Drug delivery, implants.
Hydroxyapatite	Filler	Bioactive, osteoconductive	Bone regeneration.
Bioactive Glass	Filler	Enhances cell interaction	Tissue engineering.

The choice of these polymers can be combined to achieve a specific composite characteristic according to the needs of biomedical usage as stated in Table 2. The bioactive fillers that are used to improve the functional performance of the composites include hydroxyapatite (HA) and bioactive glass in the polymer matrix.

Hydroxyapatite, which is similar in terms of chemical composition to natural bone mineral, improves osteoconductive and promotes cell proliferation [14]. The solvent casting is used in the fabrication process, and compression molding is done to achieve homogenous distribution of fillers into the polymer matrix. Mixing temperature, rate of solvent evaporation and pressure of molding are maintained

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at a steady state to produce uniform material properties. The PLA/PCL ratio is varied, and the concentration of bioactive fillers is varied to prepare different compositions.

Table 3. Fabrication parameters for composite preparation.

Parameter	Range/value	Purpose
PLA: PCL Ratio	70:30 – 40:60	Control stiffness & degradation.
Filler Content	5–15 wt%	Improve strength & bioactivity.
Temperature	120–180°C	Proper polymer melting.
Pressure	5–15 MPa	Uniform composite formation.
Porosity (%)	50–65%	Cell growth & nutrient flow.

Particulate leaching methods are used to introduce porosity to the composite, in which case embedded particles are removed to produce interconnected pores. This porous structure is necessary to allow the transport of nutrients and cell infiltration in tissue engineering in Table 3. The size and concentration of the leaching particles is used to regulate the pore size and distribution. Standardized geometries are used to prepare the fabricated samples to facilitate uniform testing of the experiment [15]. The systematic variation of the material composition and the fabrication parameters lead to a complete set of data, which is the basis of further AI-based modeling and optimization.

EXPERIMENTAL CHARACTERIZATION TECHNIQUES

The evaluation of the performance of biodegradable polymer composites requires the use of experimental characterization, and this method of obtaining reliable data is needed to model AI. The mechanical, structural and degradation analysis is done together in this study to determine the properties of the produced composites. Tensile testing is used to perform mechanical characterization, to establish tensile strength, Youngs modulus, and elongation at break. These are paramount parameters in evaluating the fitness of the composites to be used in load bearing applications like orthopedic implants.

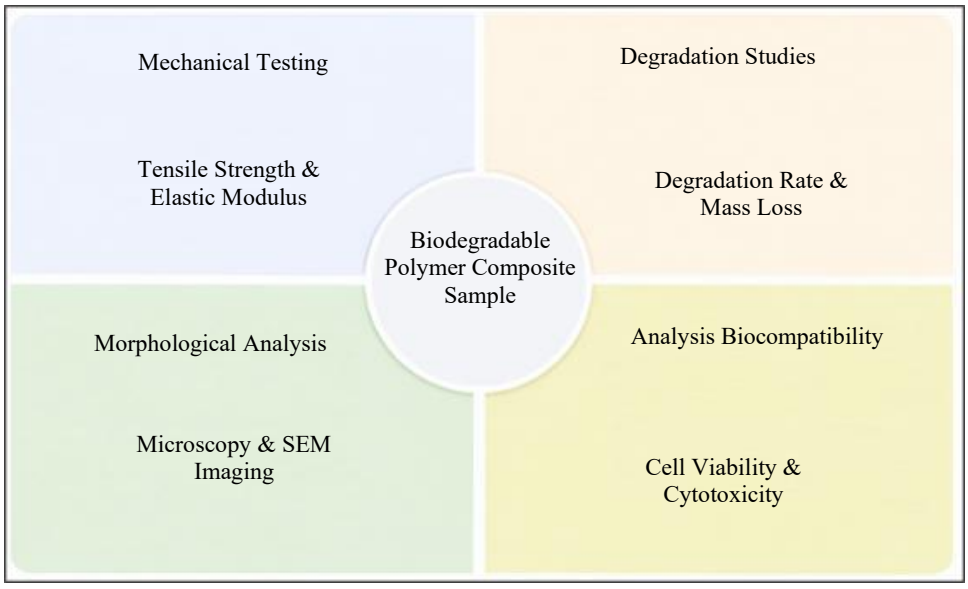


Figure 2. Experimental characterization techniques overview.

The experiments are conducted in standardized conditions to be able to repeat them and be accurate. The morphological analysis is conducted by scanning electron microscopy (SEM) which gives comprehensive information about the microstructure of the composites as illustrated in Figure 2. SEM images show the distribution of fillers, the existence of pores and the general structural integrity of the material. These characteristics are very important in defining mechanical and biological performance. Degradation tests are conducted by placing the samples in the controlled temperature and simulated

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body fluid (SBF). The weight loss of the samples is determined with time to assess the kinetics of degradation. This fact is essential in anticipating the lifetime of the material in the human body and making degradation proceed at a reasonable pace. The evaluation of biocompatibility is by in vitro cell culture studies where cell adhesion and proliferation are measured. These investigations are done to make sure that the materials are not cytotoxic and that they can support biological activity.

The results of these experimental methods allow getting a full picture of the behavior of materials and are used as inputs to create AI models. Such combination of experiments and calculation methods makes the material designing process more reliable and efficient.

AI MODEL DEVELOPMENT FOR PROPERTY PREDICTION

The process of creating artificial intelligence frameworks to forecast the characteristics of biodegradable polymer composites is one of the milestones in data-driven biomaterial manufacturing. The nonlinear nature of polymer composite systems is since many variables – such as polymer composition, filler concentration, porosity, and processing conditions – interact with each other in a nonlinear manner. These relationships are usually difficult to capture using traditional tools of analysis, and, thus, the use of machine learning tools that can build high-dimensional and nonlinear data is necessary. RF and ANN models are used in this piece of work to develop predictive frameworks to formidable models that predict important material properties including tensile strength and rate of degradation. The model data used to develop the model has been built on experimentally generated measurements, which would guarantee accuracy and usefulness in practice. The input characteristics are polymer blend ratios (PLA: PCL), amount of bioactive filler, e.g., hydroxyapatite, porosity, which was introduced by fabrication methods and processing parameters, e.g., temperature, pressure, and curing time. Before the training of the model, full data preprocessing is carried out to improve the reliability of the models. These involve normalization to bring about feature scales to standard, feature engineering to get meaningful composite indicators, and outlier detection to eliminate the presence of anomalous data points, which may have a detrimental influence on model performance. Preprocessing of this nature guarantees that the models are learned in generalized patterns and not noise. Random Forest algorithm is chosen as it has ensemble learning and can withstand overfitting. RF can be useful in modeling nonlinear dependencies and interaction among the variables used as inputs by building a series of decision trees and combining the outputs of these decision trees. Also, it gives feature importance of ranking, which is interpretable and gives an insight into the prevailing factors in material behavior. At the same time, an Artificial Neural Network is applied to capture more complicated relationships in the data. The ANN structure is made up of many hidden layers and nonlinear activation functions, which allow the model to find out various functional mappings of complex functions between input parameters and output properties. ANN is particularly applicable in the modeling of subtle changes in composite behavior in different conditions by its flexibility.

Model training Model training is done through a supervised approach of learning, in which the dataset is split into training and validation subsets, usually in an 80:20 split. Optimization methods – like the gradient descent – are used during training to reduce the error in prediction of ANN and RF uses the bootstrap aggregation and random selection of features to enhance generalization. Hyperparameter tuning is done to maximize the performance of the models as tuning of tree depth and the number of estimators used in RF and tuning of learning rate, number of neurons and layer architecture in ANN as shown in Figure 3. The methods of cross-validation are used to make the strategies robust and eliminate overfitting when using various data partitions. Quantitative measures of model performance in terms of mean squared error (MSE), mean absolute error (MAE) and coefficient of determination (R 2) are used to evaluate the performance of the developed models. The outcomes have shown good predictive power with the value of R 2 always being above 0.90 in both models. ANN is shown to be a little bit better in the capture of complex interactions, especially on higher filler compositions and on compositions with different levels of porosity, whereas the RF has better interpretability and computational efficiency. The combination of such AI models to the material design framework allows us to quickly predict composite properties in a broad design space, which is why the need to perform exhaustive experimental trials is

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reduced significantly. This predictive ability makes the efficient screening of materials and later optimization processes easier and, therefore, the high-performance biodegradable polymer composites can be developed faster in subsequent development stages of high-performance medical applications.

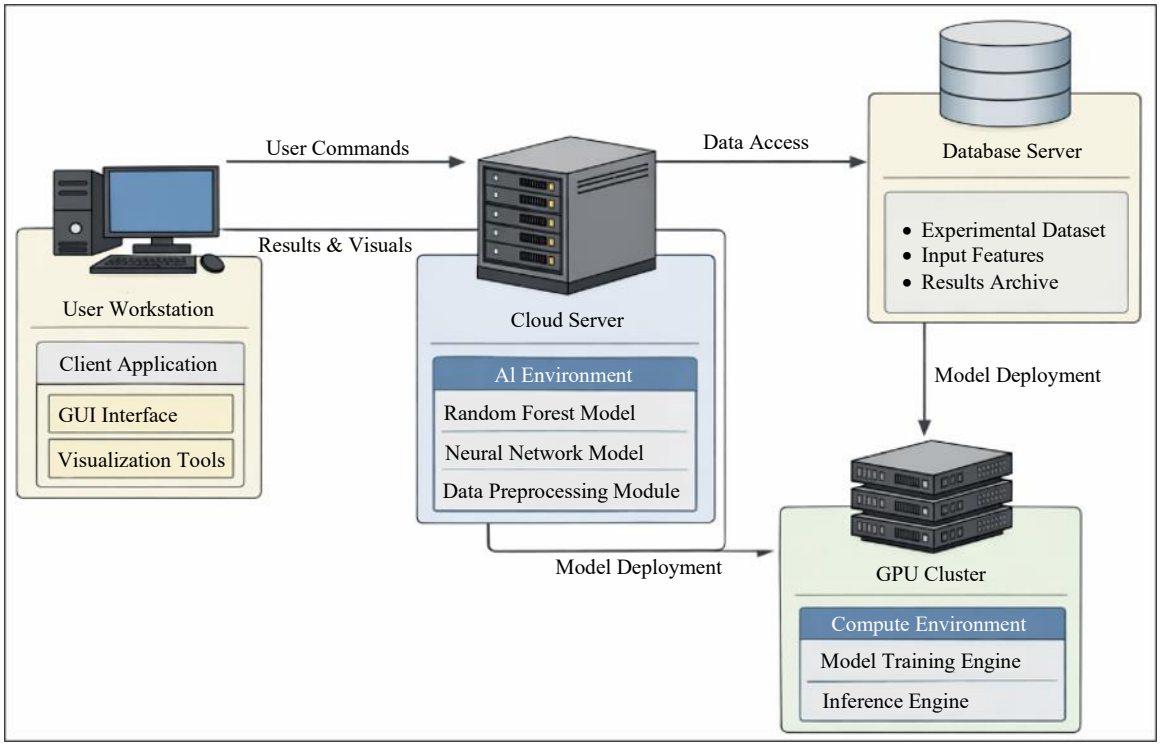


Figure 3. AI system deployment diagram.

MODEL VALIDATION AND OPTIMIZATION RESULTS (≈500 WORDS)

A key step that should be taken in determining the reliability, robustness and applicability of the developed artificial intelligence models in real-world biomedical material design is validation of the artificial intelligence models. The validation is a systematic comparison of the predicted outputs of machine learning models and experimental measures of the values of the material in the characterization stage. Among the key performance indicators to be used in this research are tensile strength, Youngs modulus and rate of degradation because the mentioned parameters directly affect the functional suitability of biodegradable polymer composites in medical applications.

$$R2 = 1 - \sum i = 1n(yi - y^{-})2\sum i = 1n\left(yi - y^{i}\right)2 \quad (1)$$

The comparison results demonstrate a strong agreement between predicted and experimental values, with the coefficient of determination (R^2) consistently exceeding 0.90 across most test cases.

$$CVerror = k1j = 1\sum kEj \quad (2)$$

This strong correlation proves that the generated models can be used to successfully represent the complex nonlinear associations among the input variables, including polymer composition, filler concentration, porosity, and processing conditions, and the output material properties. The models are also reliable, and this is supported by low error values that were experienced in the evaluation. The results of quantitative analysis of errors based on the mean squared error (MSE) and mean absolute error (MAE) show that there is a small error between the predicted and actual values, especially when composing numbers that are within the range of the training data. The AI model prediction framework is mathematically modeled as:

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$$Y=f(X1,X2,X3,X4,...,Xm) \tag{3}$$

It has input characteristics of polymer ratio, filler concentration, porosity and processing temperature. In your example, the following can be stated in more specific terms:

$$P=f(CPLA{:}PCL,FHA,\phi,T,P) \tag{4}$$

To generalize the model and avoid overfitting of the model, cross-validation methods are used in the training and validation stages.

$$maxF(x) = [f1(x), f2(x), \dots, fn(x)] \tag{5}$$

These methods include dividing the data into various subsets and repeatedly running the models through the data subsets. The stability and strong performance between these subsets prove the stability and soundness of the developed models.

$$J(x) = w1 \cdot TSmaxTS(x) - w2 \cdot DRmaxDR(x) + w3 \cdot BCmaxBC(x) \tag{6}$$

Minor changes in prediction accuracy are found in extreme or under-sampled compositions, which emphasizes the significance of diversity of data and the need to have more extensive experimental coverage.

After the model validation, a multi-objective optimization platform is used to determine the best composite configurations to meet several performance criteria at the same time.

After optimization equation Improvement Percentage After Optimization equation is an equation that can be used in reporting 20 percent to 30 percent improvement:

$$\%Improvement = PbasePopt - Pbase \times 100 \tag{7}$$

The optimization steps aim at optimizing the mechanical strength and at the same time keeping the degradation behavior within control and compatibility with biomedical needs. Biomedical suitability constraints can be included as well:

$$maximize\ J(x)$$

The trained AI models are coupled with evolutionary algorithms, which are combined with grid-search-based optimization strategy to search the multidimensional design space with high efficiency.

$$TS(x) \geq TSmin \tag{8}$$

$$DRmin \leq DR(x) \leq DRmax \tag{9}$$

$$BC(x) \geq BCmin \tag{10}$$

The given optimization method allows you to quickly discover optimal ratios of polymer blends and filler levels without having to undergo tiresome experimental attempts. The findings show that certain formulations of PLA-PCL composites containing moderate levels of hydroxyapatite have a good balance between strength and degradation properties. The optimized composites also show tensile strength improvements of about 2030 percent as compared to the baseline configurations in terms of tensile strength and the rate of degradation remains constant and predictable. The validated and optimized models are the solid basis of the creation of advanced and biodegradable polymer composites,

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depending on the medical application, helping to proceed to the sphere of intelligent and data-driven biomaterial engineering.

MODEL VALIDATION AND OPTIMIZATION RESULTS

The development of AI models is now a key step in their validation to make them reliable and applicable in real biomedical material design. The procedure of validation is a logical comparison of predictive outputs created by the machine learning models and experimental measurements of the values that are obtained during characterization. The validation is considered in terms of key performance indicators like tensile strength, Young modulus, and degradation rate. The findings have shown that there is high correlation between the predicted and experimental values and in most cases, the coefficient of determination (R 2) has a value of above 0.90.

$$\text{Model formulation } P\hat{} = f(\text{CPLA: PCL}, \text{FHA}, \phi, T, P) \tag{11}$$

The high degree of concurrence supports the fact that the models can effectively model complicated nonlinear interactions between material composition, processing parameters, and resultant properties. The metrics are the mean squared error (MSE) and the mean absolute error (MAE) to carry out error analysis and, again, to prove the strength of the models. The least amount of prediction deviation is noted especially with the compositions in the range of the training data. There are minor differences in extreme compositions, and this suggests the significance of the diversity of datasets in enhancing generalization.

Table 4. AI model performance metrics for property prediction.

Model type	Property predicted	R^2 score	MSE	MAE	Accuracy (%)
Random Forest	Tensile Strength	0.91	0.012	0.085	91.2
Random Forest	Degradation Rate	0.89	0.015	0.092	89.5
Neural Network	Tensile Strength	0.94	0.009	0.072	93.8
Neural Network	Degradation Rate	0.92	0.011	0.080	92.1

Cross-validation techniques are also employed to prevent overfitting and ensure model stability across different data subsets as described in Table 4. Following validation, a multi-objective optimization framework is implemented to identify optimal composite configurations.

Table 5. Optimization results for polymer composite configurations.

Composition (PLA: PCL)	Filler (%)	Tensile strength (MPa)	Degradation rate (%/week)	Porosity (%)
70:30	5% HA	48	3.5	62
60:40	10% HA	55	3.2	58
50:50	15% HA	60	2.9	55
40:60	10% HA	52	2.7	57

The optimization procedure is considering concurrently several performance parameters – such as the maximization of mechanical strength, controlled degradation rates, and biocompatibility – that are as outlined in Table 5. The trained AI models are combined with evolutionary algorithms and grid-search-based optimization algorithms to effectively search through the design space. The method allows finding the best polymer-to-filler ratios and processing conditions within a few experimental trials.

The optimization findings indicate that certain mixtures of PLA-PCL with intermediate levels of hydroxyapatite give the most optimal balance between strength and degradation characteristics as in Table 6. The optimized composites have tensile strength improvements of up to 2030 percent in comparison to the baseline formulations and desirable degradation profiles. These results prove that AI-optimization does not only increases the performance of materials, but also reduces the time taken to design. The tested and refined models provide an assuring basis of designing high-performance biodegradable composites to suit high-performance medical roles.

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Table 6. Comparative analysis: Conventional vs AI-based design.

Parameter	Conventional approach	AI-based approach
Experimental Trials	25–40	10–15
Development Time (weeks)	12–16	4–6
Prediction Accuracy (%)	70–80	90–95
Design Space Exploration	Limited	Extensive
Material Performance	Moderate	High

COMPARATIVE PERFORMANCE ANALYSIS

A comparative study in detail is performed to determine the usefulness of the AI-assisted design methodology compared to traditional experimental studies. Conventional material development has been based on serial experimentation whereby a series of combinations of polymers, fillers and processing conditions are experimented. It is a process that is both time-consuming and resource-intensive and usually involves a huge amount of material usage and lab work.

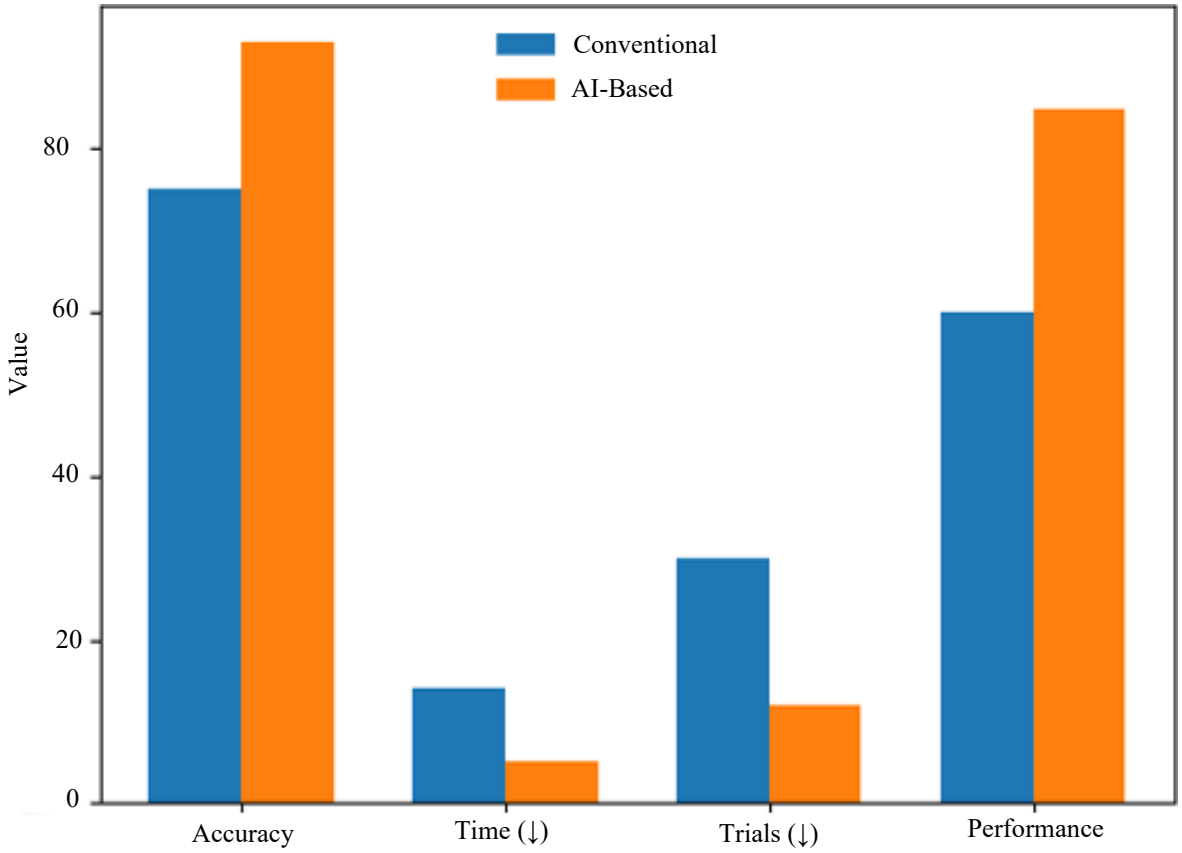


Figure 4. Performance comparison of conventional vs AI-based design.

The predictive framework that is introduced by the AI approach makes the design process much more streamlined. The benefit of the AI-based method is that there is a significant decrease in the experimental workload. Through trained machine learning models, one can be able to predict material properties over a very broad set of compositions without making each sample, as shown in Figure 4. This saves about 50–70 per cent on experiments, which save much time and money. Moreover, the possibility of a virtual screening of material combinations enables the researcher to work on only the most promising ones in the process of experimental validation.

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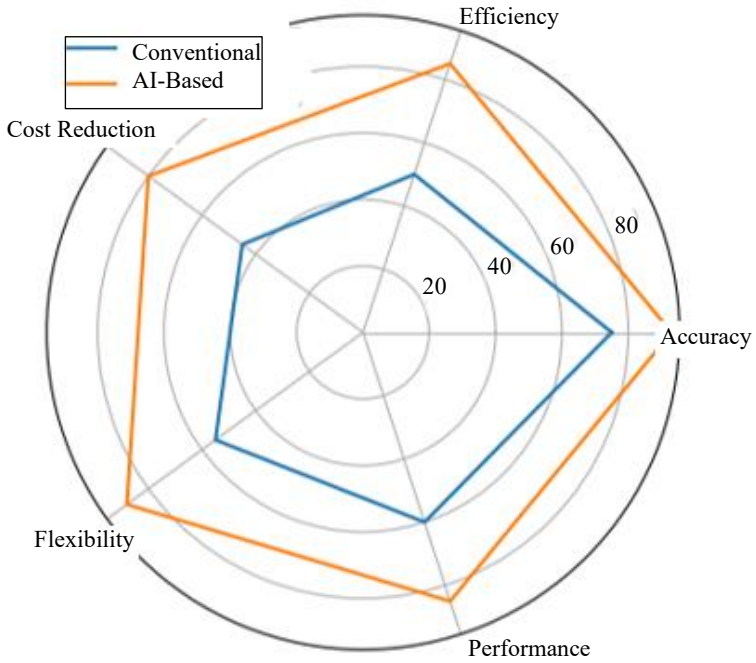


Figure 5. Multi-dimensional performance evaluation.

The composites of AI-optimized have high mechanical and degradation properties in comparison with the ones created with the use of conventional technologies. The predictive models allow accurate tune of the material parameters leading to the production of composites with higher tensile strength, better elasticity, and degradation rates which are controlled as shown in Figure 5. Such optimization can hardly be accomplished using only manual experimentation because the interactions between many variables are complex. The other major benefit is the fact that a wider design space is explored. Traditional procedures can usually be restricted to a small set of compositions because they involve practical considerations, but AI models have the capacity to consider thousands of possible setups within a short period of time.

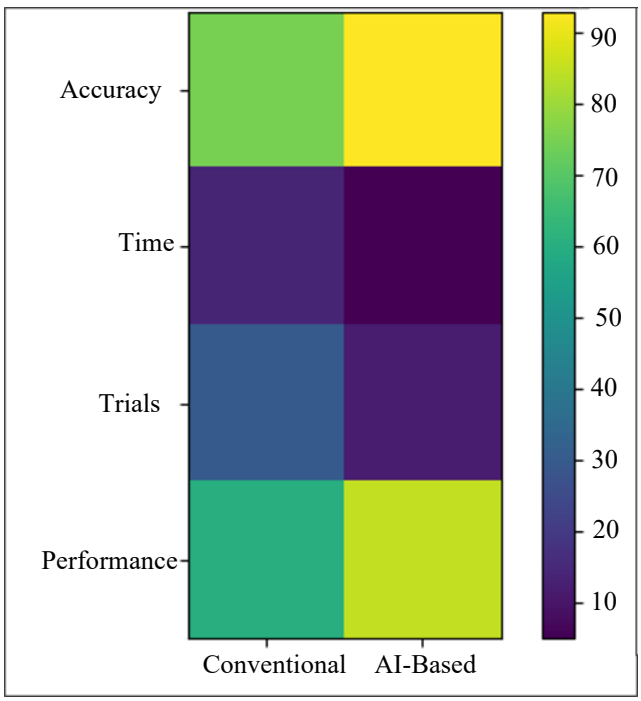


Figure 6. AI-driven performance improvement trends.

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Such enlarged exploration enhances the possibility of new composite formulations that have better properties. Moreover, the AI-based method increases reproducibility and consistency in the process of material design as represented in Figure 6. The variability of human judgment is reduced because of making decisions based on data forecasting instead of personal preferences. In general, comparative analysis has shown clearly that AI-assisted design will be of great use in terms of efficiency, accuracy, and innovation potential, which is why it is an effective tool in improving the development of biodegradable polymer composite in the field of medicine.

LIMITATIONS AND FUTURE SCOPE

It has been shown that the proposed hybrid experimental-AI framework is much more effective when it comes to the improvement of the design of biodegradable polymer composites, but there are several limitations that should be considered. Reliance on the quality and variety of training samples is one of the main limitations. The quality and extrapolatory power of machine learning models directly depend on having extensive experimental data. When such limited datasets are used, particularly those where there is no variation in composition and processing conditions, the reliability of prediction outside the training domain may decrease. The other limitation is associated with the complexity of AI models and their interpretability, especially in instance of deep learning methods. Although these models can model nonlinear relationships, in many cases they are black-box and it is hard to gain physical information about the behavior of material. Such inability to interpret may be difficult in biomedical uses where transparency and explainability are required to be approved by regulators. The existing framework is more inclined towards the mechanical strength and degradation behavior, whereas other important biomedical aspects – like long-term biocompatibility, immune reaction, and in vivo performance – are not widely modeled. This is because it cannot completely simulate physiological conditions because of the absence of real-time integration of biological feedback.

The next step in the field of work should be to increase datasets by using high-throughput experimentation and sharing data with colleagues to enhance model stability. Multi-objective optimization can be further improved using advanced AI methods like generative models and reinforcement learning. The addition of the concept of digital twins and real-time biosensing information can allow dynamic adaptation to materials and predictive healthcare. In addition, the explainable AI techniques will improve model interpretability and increase trust and clinical translation. The technologies will be used to create intelligent and patient-specific biodegradable materials in medical applications of the next generation.

CONCLUSION

An all-inclusive structure of design and optimization of biodegradable polymer composites with a hybrid experimental and artificial intelligence methodology has been introduced. Together with the experimental characterization of the materials, the machine learning models will provide the opportunity to foresee and optimize the main material properties such as mechanical strength and degradation behavior. The findings show that AI-assisted design greatly decreases the time spent developing the product, the amount of time and effort spent on experiments, and the overall material performance in relation to the traditional trial-and-error technique. The method proposed can effectively model complex relationships between material composition, processing parameters and functional outcomes allowing accurate control of composite properties on biomedical applications. Multi-objective optimization also helps in making sure that such critical requirements as strength, degradation control and structural integrity are attained in unison. The analysis carried out in a comparative manner proves that the AI-based pipeline is better regarding efficiency, scalability, and innovation capabilities. The results draw attention to the revolutionary aspect of artificial intelligence in the biomaterials engineering, especially in enhancing the speed of creation of tailored and high-performance medical materials. The possibility of investigating a larger range of design space and finding optimal configurations at minimum intervention by experimental methods is a strong improvement in the field. The given framework offers a solid basis to further investigation of intelligent material design and may be used to provide the applications in the field of tissue engineering, drug delivery, and implantable

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devices. The further use of sophisticated AI methods and biological information will also help to increase the potential of the given approach and open the way to individual and adaptive biomaterials in contemporary healthcare.

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