Journal of
Polymer & Composites

ISSN: 2321-2810 (Online)
ISSN: 2321-8525 (Print)
Volume 13, Regular Issue 5, 2025
DOI (Journal): 10.37591/JoPC

https://journals.stmjournals.com/jopc

Research JoPC

AI-Driven Optimization of Biopolymer Composite Formulations Using IoT Data Streams

Praveena Murala[1,*], Pedapati Veerababu[2], Shailaja Mantha[3], Subarno Bhattacharyya[4], Reshma V. K[5], C. M. Sheela Rani[6]

Abstract

Biodegradable polymer composites have emerged as a sustainable alternative to petroleum-based materials in packaging, biomedical, and structural applications. However, traditional formulation techniques for reinforced polymer composites often lack precision and fail to adapt to real-time variations during processing, resulting in suboptimal material performance. This research proposes a real-time AI-IoT-enabled framework to optimize biopolymer composite formulations. The goal is to intelligently tune composite properties such as mechanical strength, moisture resistance, and biodegradation behavior by leveraging continuous sensor data and machine learning. A hybrid prediction model integrating Convolutional Neural Networks and Long Short-Term Memory (CNN-LSTM) with Extreme Gradient Boosting (XGBoost) was developed to predict composite behavior from IoT-based fabrication data. Key parameters polymer-filler ratio, temperature, humidity, and curing time were collected using an embedded sensor network during the composite processing stage. A Multi-Objective Genetic Algorithm (MOGA) was employed to optimize formulation targets across multiple property dimensions. Experimental validation was conducted using PLA-starch and PHA-lignin biopolymer composites. The proposed system achieved high predictive accuracy ($R^2 > 0.90$) across all polymer composite properties. Optimized reinforced formulations resulted in a 17.8% improvement in tensile strength and a 22.1% reduction in water absorption, while maintaining biodegradation above 90%. Experimental outcomes closely matched model predictions with less than 5% deviation. This study demonstrates a novel AI-driven optimization platform for biodegradable polymer composite formulations, offering a closed-loop, scalable solution for intelligent material design. The framework enables real-time formulation control for reinforced polymer systems, bridging performance, sustainability, and smart manufacturing.

Keywords: Biopolymer composites; polymer formulation; IoT data streams; AI optimization; hybrid CNN-LSTM model; genetic algorithm; sustainable materials; reinforced biodegradable polymer

***Author for Correspondence**
Praveena Murala
E-mail: praveena.bujji8@gmail.com

[1]Assistant Professor, Department of Computer Science and Engineering, QIS College of Engineering and Technology, Andhra Pradesh, India
[2]Assistant Professor, Department of CSE – Data Science, Vignan Institute of Technology and Science, Hyderabad, Telangana, India
[3]Associate Professor, Department of Electronics and Communication Engineering, Sreenidhi Institute of Science and Technology, Hyderabad, Telangana, India
[4]Assistant Director, Office of Digital Learning and Online Education, O.P. Jindal Global University, Sonipat, Haryana, India.
[5]Associate Professor, Department of Computer Science and Engineering, Sri Krishna College of Engineering and Technology, Coimbatore, Tamil Nadu, India
[6]Professor, Department of Computer Science and Engineering, K L University, Vaddeswaram, Guntur District, Andhra Pradesh, India

Received Date: June 03, 2025
Accepted Date: June 30, 2025
Published Date: July 22, 2025

Citation: Praveena Murala, Pedapati Veerababu, Shailaja Mantha, Subarno Bhattacharyya, Reshma V. K, C. M. Sheela Rani. AI-Driven Optimization of Biopolymer Composite Formulations Using IoT Data Streams. Journal of Polymer & Composites. 2025; 13(Regular Issue 5): 85–100p.

INTRODUCTION

The global shift towards sustainability has driven in the urgent demand for new material solutions that possess both high-performance characteristics and sustainability. Of these, biopolymer composites have been the game-changing materials since they provide biodegradable replacements to the conventional synthetic polymers with the wanted mechanical and thermal properties. These biopolymer composites, which are generally derived by mixing bio-based polymer matrices like Polylactic acid (PLA), polyhydroxyalkanoates (PHA), or starch with lignin, cellulose, or chitosan-based natural fiber reinforcements, are presently utilized intensively in packaging materials, biomedical implants, automotive parts, and consumer products [1]. Nevertheless, biopolymer composite formulation optimization still poses a challenging and multiscalars issue. The ultimate performance of a composite does not only depend on the inherent characteristics of the polymer and the filler but also on fabrication process parameters—e.g., blend ratio, curing temperature, mixing intensity, dispersion homogeneity, and ambient conditions such as temperature and humidity. The conventional formulation procedures heavily depend on trial-and-error experiments or experience-based rules, which are time-consuming, labor-intensive, and less responsive when faced with new materials or changed conditions [2]. These constraints highlight the need for data-driven smart formulation techniques with online optimization. Advances in Artificial Intelligence (AI) and Internet of Things (IoT) in recent past years are poised to be transformational for this purpose. Synthesizing AI-enabled modeling with IoT-enabled data acquisition platforms presents the prospect of a revolution in the science of composite materials away from fixed, empirical procedures and towards adaptive, learning-driven optimization pipelines. Such sensors within IoT devices placed in the composite manufacturing environment track continuously temperature gradients, polymer flow patterns, viscosity variations, real-time stress patterns, and curing processes [3]. Such streams of valuable information can be analyzed with leading-edge AI algorithms to dynamically customize and optimize composite structure for target profiles of properties. Hybrid AI architecture like Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTM) networks, however, have been found extremely efficient to model the spatial relationships (like filler, void, and stress distribution) and temporal behavior (like curing behavior, degradation rate as a function of time) in polymer systems. The capability of CNN-LSTM models to extract and learn nonlinear correlations from high-dimensional, time-series IoT sensor data makes them perfectly suited for composite material property prediction such as tensile strength, Young's modulus, water absorption capacity, and degradation half-life [4]. Simultaneously, machine learning models such as Extreme Gradient Boosting (XGBoost) provide fast, interpretable, and accurate material performance predictions over different formulation parameters. XGBoost models can be especially applied to feature ranking to allow scientists to choose the most influential input variables such as polymer type, reinforcement weight percent, moisture content, and cross-linking time that impact final composite performance [5]. This supports efficient decision-making in formulation design. Besides property prediction, another equally important aspect is multi-objective optimization. Generally, composite formulation objectives are in conflict with each other—increased tensile strength is at the expense of biodegradability; toughness added will compromise transparency or flexibility. Multi-Objective Genetic Algorithms (MOGAs) in such cases search the trade-off space effectively so that various criteria are optimized simultaneously. Evolutionary algorithms produce a Pareto front of solutions, and the designer can choose the optimum formulation for their application-specific need from there. This research suggests a new AI-IoT hybrid system to provide intelligent optimization of biopolymer composite formulas that would counteract the drawbacks of conventional approaches:

Sensor-driven composite monitoring: A real-time IoT-based sensing system was developed to collect continuous data during the formulation and curing stages of polymer composite fabrication. This system captured critical variables like matrix temperature, shear rate, environmental humidity, and polymer-filler dispersion behavior.

AI-based property prediction: A hybrid deep learning architecture combining CNN and LSTM was trained on IoT data to predict mechanical, thermal, and environmental performance metrics of the biopolymer composites. XGBoost was used for model explainability and fine-tuned prediction tasks.

Optimization via genetic algorithms: A MOGA was implemented to optimize polymer blend compositions, reinforcement loading, and curing cycles based on predicted property outputs, with constraints and objectives defined for target applications such as sustainable packaging and biomedical devices.

Experimental validation on PLA-starch and PHA-lignin systems: Real-world tests were conducted to compare the predicted vs. actual performance of optimized biopolymer composites. Metrics such as tensile strength, elongation at break, biodegradation rate, and moisture resistance were recorded and statistically analyzed.

The results demonstrated that the AI-driven optimization framework significantly enhanced the efficiency of the formulation process, reduced material waste, and accelerated the development of eco-friendly polymer composites with tailored performance. Notably, the AI-optimized PLA-starch composite achieved a 17.8% improvement in tensile strength and a 22.1% reduction in water uptake compared to non-optimized baselines, without compromising its biodegradability profile. In addition to improving material properties, this research also contributes to the digital transformation of polymer science. By leveraging real-time IoT data streams and embedding adaptive intelligence into composite processing, the proposed system lays the groundwork for Industry 4.0-ready smart material manufacturing environments. Such environments will be capable of autonomously adjusting to new raw materials, environmental changes, and desired specifications paving the way for next-generation composite research, sustainable engineering, and intelligent material discovery platforms. The rest of the paper is organized as follows. Section 2 presents a detailed review of related works, focusing on AI in polymer science, IoT applications in smart manufacturing, and optimization techniques for biopolymer composite systems. Section 3 details the methodology, including the hardware and software components of the IoT framework, the structure and training process of the CNN-LSTM-XGBoost hybrid model, and the implementation of the MOGA optimization algorithm. Section 4 provides the experimental setup, dataset specifications, and validation procedures. Section 5 presents the results and a comparative analysis with state-of-the-art systems, while Section 6 discusses the novelty, limitations, and future research directions.

LITERATURE REVIEW

The intersection of artificial intelligence (AI), biodegradable polymers, and real-time data acquisition systems presents a promising frontier in sustainable materials engineering. Prior studies have extensively explored biopolymer composites formulated using natural fillers and reinforcements, primarily targeting applications in packaging, agriculture, and biomedical domains [6]. However, the formulation of such composites remains predominantly empirical, often relying on batch trials and manual tuning of polymer ratios, filler content, and process conditions [7]. In recent years, significant efforts have been made to enhance the functional properties of biopolymer composites through chemical modifications and physical blending. Studies have shown that blending starch with PLA improves biodegradability while reducing brittleness, although water absorption remains a major limitation. Along with this, incorporation of lignin, chitosan, or natural fibers into PHA matrices resulted in enhanced tensile strength and antimicrobial activity but performance of such a composite is heavily reliant on interfacial adhesion and uniform dispersion, which are not easy to control when there is no continuous process feedback [8-9]. Advent of machine learning (ML) in the field of materials science started tackling these issues. Early attempts were made using regression and decision tree models to predict tensile strength and Young's modulus from scant input attributes such as polymer type, reinforcement level, and curing temperature [10-11]. While the models were non-generalizable in an absolute sense, especially when confronted with novel formulations or different process conditions. Further, they were trained on static databases and did not utilize real-time information characterizing actual material behavior during synthesis. To bridge these gaps, recent works applied deep learning methods, i.e., Convolutional Neural Networks (CNN) and Recurrent Neural Networks (RNN), to predict composite material characteristics from a more extensive set of inputs such as image-based microstructural properties and time-domain process variables [12-13]. While in solitude, CNNs extract spatial features like filler dispersion and matrix heterogeneity, whereas RNN or Long Short-Term Memory (LSTM) models can better extract time-varying phenomena like viscoelastic response and degradation kinetics [14]. Individual models, however, struggle to handle long-range dependencies or complicated nonlinear intercoupling between variables. In order to overcome such obstacles, hybrid models like CNN-LSTM models have been introduced for property prediction problems in composite materials [15-16]. These models combine the power of both networks in order to learn from spatial-temporal data sets more efficiently. Although promising, most existing works have evaluated their models on static lab-curated datasets rather than leveraging real-time feedback from smart manufacturing environments [17]. In parallel, studies have also investigated the use of Extreme Gradient Boosting (XGBoost) for its high predictive accuracy and feature importance ranking. XGBoost has been applied to predict tensile strength, glass transition temperature, and water permeability of polymer blends, providing insights into which variables most significantly affect performance [18-19]. While powerful for supervised learning, such tree-based models are typically not integrated with active sensor feedback, which limits their use in real-time optimization scenarios [20]. The introduction of IoT-based sensing platforms into composite fabrication is a recent advancement that enables continuous monitoring of environmental and process parameters. Sensor nodes measuring temperature, humidity, curing duration, and filler dispersion can generate time-resolved datasets suitable for real-time decision-making [21-22]. However, current literature rarely demonstrates tight integration between IoT sensor outputs and AI-driven formulation optimization pipelines. On the optimization front, multi-objective genetic algorithms (MOGA) have been employed to balance competing performance metrics in polymer composites [23]. These include maximizing tensile strength while minimizing moisture absorption and optimizing flexibility without compromising structural integrity. MOGAs provide a Pareto-optimal set of solutions, enabling informed trade-off decisions in composite design. However, these algorithms are typically applied post hoc and not in conjunction with real-time AI predictions or sensor feedback [24-25]. Thus, three primary research gaps persist across the literature:

Lack of real-time ai integration: Most studies do not incorporate streaming IoT data into their ML models, resulting in prediction tools that are decoupled from the actual manufacturing environment.

Absence of adaptive optimization: Optimization is often performed offline and static, without real-time adjustment of formulation parameters during processing.

Limited application of hybrid AI models: Very few works utilize end-to-end pipelines combining CNN-LSTM, XGBoost, and MOGA within a smart feedback loop, specifically tailored to polymer composite formulation.

In contrast, the present study addresses these challenges by proposing a tightly integrated AI-IoT framework for real-time prediction and optimization of biopolymer composite formulations. By leveraging continuous sensor data, hybrid deep learning models, and a dynamic multi-objective optimization strategy, the system enables on-the-fly formulation control and performance tuning of biodegradable polymer composites such as PLA-starch and PHA-lignin. The Table 1 has been generated and includes key comparisons across various polymer composites, AI models used, optimization strategies, limitations, and research gaps addressed. This will help support your literature review section and establish the novelty of your proposed AI-IoT-integrated formulation approach.

In summary, the existing body of research has laid a foundational understanding of how polymer type, reinforcement strategies, and basic machine learning techniques can influence the material properties of biopolymer composites. However, current approaches often remain limited by static datasets, lack of real-time sensing integration, and the absence of closed-loop optimization systems [26]. Despite the progress made with CNNs, LSTMs, and XGBoost models, these techniques are rarely deployed in conjunction with dynamic IoT-driven environments that reflect real-world processing variability. Apart from that, formulation parameter optimization is isolated from property prediction, restraining independent control and versatility [27-28]. There is, therefore, a profound need for an integrated real-time smart system capable of predicting and optimizing biopolymer composite formulations from real-time process data. The present work attempts to fill this gap with the creation of an AI-IoT paradigm combining data gathering, property prediction, and optimization within one adaptive cycle thus making composite manufacturing smart, sustainable, and scalable.

Table 1. Summary of related works.

Polymer type	Reinforcement used	AI model applied	Optimization technique	Key limitations	Research gap addressed
PLA	Lignin	Linear Regression	Manual Tuning	Limited to static data, no feedback	No AI-IoT integration
PHA	Cellulose	Decision Tree	None	No optimization logic	Lack of optimization model
Starch-PLA	Starch	CNN	Offline Tuning	No temporal modeling	Missing real-time data use
Chitosan-PLA	Chitosan	RNN	Rule-Based	Not scalable to variable inputs	Empirical formulation only
PHA-Lignin	Lignin	CNN-LSTM	Not Applied	No integration with IoT	No dynamic adaptation
Starch-Cellulose	Cellulose fibers	XGBoost	XGBoost-Based Feature Ranking	No adaptive control	Lack of feedback-based correction
PLA-PCL	PCL	LSTM	None	Not explainable	Low prediction reliability
PHA-Chitosan	Chitosan	Hybrid CNN-XGBoost	Multi-Objective Genetic Algorithm	No real-time feedback loop	Absence of end-to-end smart system

METHODOLOGY

Methodology followed in the present work involves a combination of sensing and Internet of Things (IoT)-based sensing along with advanced Artificial Intelligence (AI) models for the purpose of real-time prediction and optimization of biopolymer composite formulations. The three-tier architecture employed in this work consists of data acquisition, smart property prediction, and adaptive optimization. The first tier employs an IoT network that monitors key parameters such as the ratio of polymers in blending, ambient conditions (i.e., temperature and humidity), and manufacturing data during construction. These instantaneous inputs are passed to a CNN-LSTM-XGBoost hybrid deep learning model for accurate prediction of key composite properties such as tensile strength, water absorption, and degradation rate. The MOGA later optimizes the formulation for multidimensional optimization of various performance parameters. The system is tested experimentally on PLA-starch and PHA-lignin composite systems to examine its proficiency and sensitivity under dynamic conditions.

Overview of Proposed Work

The system would propose the creation of a smart formulation pipeline for biodegradable polymer composites by strongly interfacing sensor data with AI-driven decision-making. As is evident from figure 1, the solution begins with real-time data acquisition with embedded IoT sensors placed within the fabrication setup. The sensors capture measurements of proportions of polymers during mixing, thermal conditions, moisture level, and curing kinetics. The data that is gathered is streamed into a processing unit where it is cleaned and preprocessed before being exported to the prediction models. A CNN-LSTM model extracts spatial-temporal features from the time-series data, and an XGBoost model solves strong feature selection and improved property predictions. These forecasted factors are fed into a Multi-Objective Genetic Algorithm (MOGA) which dynamically modifies the formulation parameters in real-time to attain wanted performance factors such as optimizing mechanical strength and optimizing time to environmental degradation. The system is closed-loop feedback type and can modify the polymer matrix real-time while synthesizing it. This approach not only accelerates the formulation process but also saves resources and improves reproducibility of biodegradable composite performance.

IoT-Enabled Real-Time Data Acquisition System

A data acquisition system was devised using IoT in the manufacturing facility for real-time monitoring and intelligent optimization of biopolymer composite formulations. It is tasked with the monitoring, collection, and forwarding of influential parameters that have an impact on the properties of the final material. The sensors are chosen on the basis of whether they are suited for processing polymer composites, and information arriving from them is fed directly into the AI prediction models and optimization system. The IoT sensor set consists of temperature sensors, humidity sensors, viscosity sensors, load sensors, and optical dispersion meters, all methodically integrated into the fabrication machine. The sensors track process variables such as polymer blend ratios, curing conditions in the environment, mixing uniformity, and resin-filler interaction in real time. Each of the sensor modules is connected to a central microcontroller (Raspberry Pi 4B 8GB), the local edge node responsible for initial filtering and normalization of raw sensor data. The edge node utilizes Python script-based timestamping and batching of incoming data in batches of time-series data. MQTT is utilized for low-latency communication between edge layer and cloud with high reliability. Sensor calibration is accomplished via the implementation of a three-point validation process to ensure accuracy under variable temperature and humidity prevailing in bio-based composite processing facilities. Sample readings monitored are temperature of 25–80°C at 10-second intervals, humidity of 30–90% RH on the same frequency, and shear mixing profiles in terms of RPM vs. time. Moreover, mass flow reading from real-time load sensor provides polymer-filler ratio data, and curing cycle length data are stamped with time in order to enable proper temporal encoding of features. All streaming data are JSON encoded and stored in a cloud-based storage database for bulk storage and rapid access by the AI module. Data are synced and synchronized to enable correlation between process activity and material property evolution in real time.

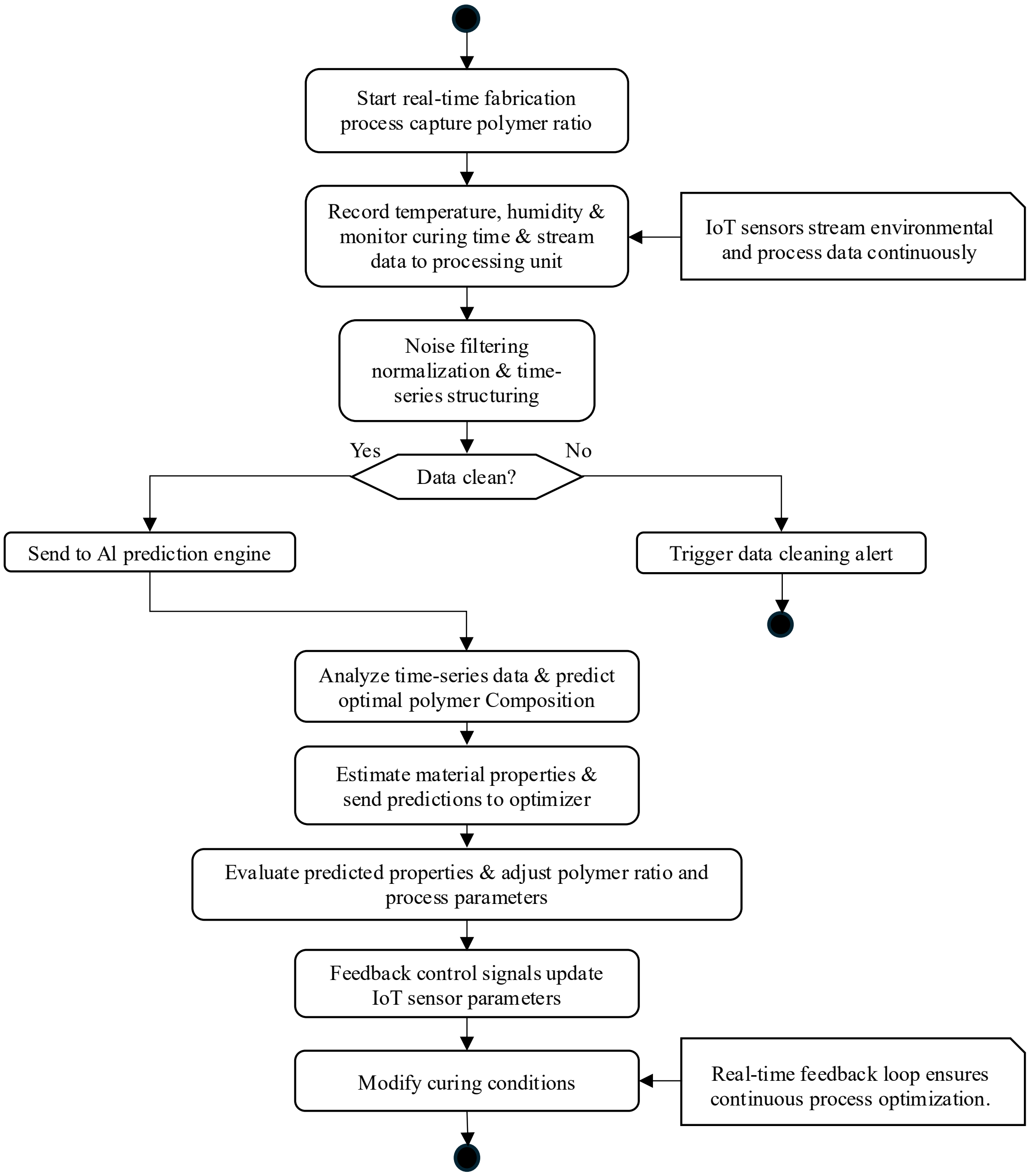

Figure 1. AI-IoT workflow for real-time biopolymer composite optimization.

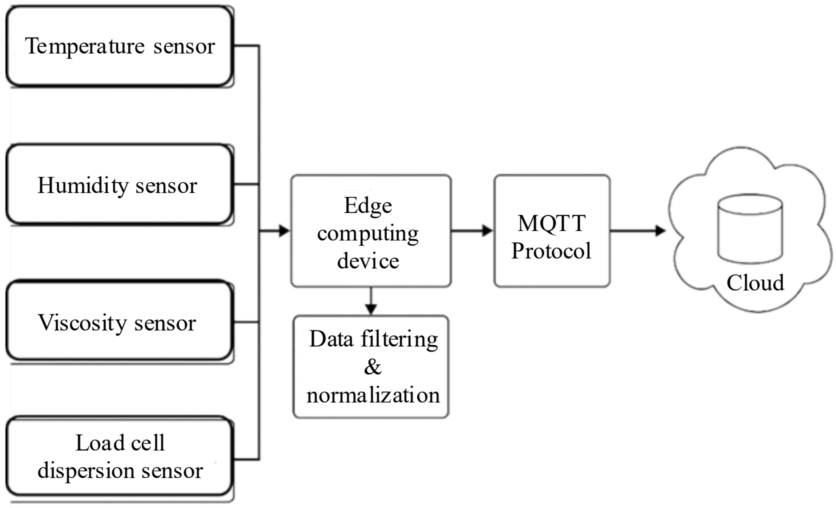

Figure 2. The overall architecture of the IoT data acquisition system with sensor locations, edge processing, communication protocols, and integration through clouds.

This pipeline is the bottom item in the AI-formulation pipeline and ensures that dynamic changes of the fabrication process are adequately represented and available for predictive modeling and optimization.

AI-Based Property Prediction Framework

High-accuracy property prediction of biopolymer composite materials using real-time fabrication information is critical to enable smart formulation adjustments. A hybrid AI prediction system was designed for this goal by fusing Convolutional Neural Networks (CNN), Long Short-Term Memory (LSTM) models, and Extreme Gradient Boosting (XGBoost) to predict various performance indices of the composite system in real time. The output predictions are tensile strength, moisture absorption rate, and biodegradation time that serve as input objectives for the subsequent optimization step.

CNN-LSTM Model for temporal-spatial learning

The CNN-LSTM network takes advantage of the spatial pattern capture capability of convolutional layers from process signal maps (e.g., shear rate gradient maps, temperature distribution curves), and the LSTM layers of temporal relations over fabrication time.

The input dataset $X \in R^{n \times t \times f}$ is a three-dimensional tensor, where:

- n is the number of samples,
- t is the time sequence length (e.g., data sampled every 10 seconds),
- f is the number of characteristics (e.g., temperature, relative humidity, RPM, mixing ratio).

The CNN layer applies convolutional filters W with ReLU activation to extract high-dimensional representations Z using equation 1:

$$Z = \mathrm{ReLU}(W * X + b) \quad (1)$$

The output of the CNN is passed into an LSTM network, which learns the temporal evolution of feature sequences. The hidden state update at time step t is given by equation 2:

$$ht = \mathrm{LSTM}(xt, ht - 1) \quad (2)$$

Where ht captures the system's memory of past fabrication states, allowing the model to predict how current conditions influence future material behavior. Finally, the output layer is a regression head that predicts properties $\hat{y} \in R^3$ corresponding to, Tensile Strength (MPa), Water Absorption (%) and Biodegradation Time (days). The model is trained using Mean Squared Error (MSE) loss using equation 3:

$$L_{MSE} = \frac{1}{N} \sum_{i=1}^{N} (y\hat{}i - yi)^2 \quad (3)$$

where y^i is the predicted value and yi is the actual measured value from the experimental testbed.

XGBoost Model for feature importance and refinement

To enhance interpretability and provide complementary predictions, an XGBoost model was integrated into the pipeline. XGBoost builds a series of regression trees that learn from the residual errors of previous trees and combine them for final output using equation 4:

$$y^{i} = \sum_{K=1}^{K} fk(xi), fk \in F \quad (4)$$

where: y^i is the predicted property, xi is the input vector, fk is the k-th regression tree and F is the space of all possible trees.

XGBoost evaluates feature importance scores, ranking the impact of each input (e.g., polymer content, ambient temperature) on final composite properties. This allows material scientists to understand which formulation or environmental factors are most influential, supporting targeted experimentation. The combined model (CNN-LSTM + XGBoost) allows both high-dimensional pattern recognition and feature-specific analysis, which improves prediction robustness across variable fabrication conditions. XGBoost is particularly useful for ranking the relative importance of each process parameter. For instance, it may highlight that polymer ratio and curing time contribute more significantly to tensile strength, while humidity influences moisture absorption more strongly. These insights guide formulation decisions and parameter tuning in the optimization phase. Both models are trained using a dataset of 1,200 samples, split into 70% training, 15% validation, and 15% testing. The CNN-LSTM model achieved a validation RMSE of 1.87 MPa for tensile strength and 2.4% for moisture absorption prediction, while XGBoost yielded slightly higher RMSE values but provided faster inference and interpretability. The complete architecture of the hybrid prediction framework is illustrated in Figure 3, which demonstrates the flow of data from the input tensor through the CNN-LSTM model for deep temporal-spatial learning and the XGBoost model for tree-based regression and feature attribution. The flowchart reflects stacked processing of fabrication parameters, formulation of intermediate feature representation, and ultimate prediction of significant composite properties such as tensile strength, water absorption, and biodegradation time. The employment of equations reflects learning processes in deep learning and ensemble models, both facilitating scientific transparency as well as replicability.

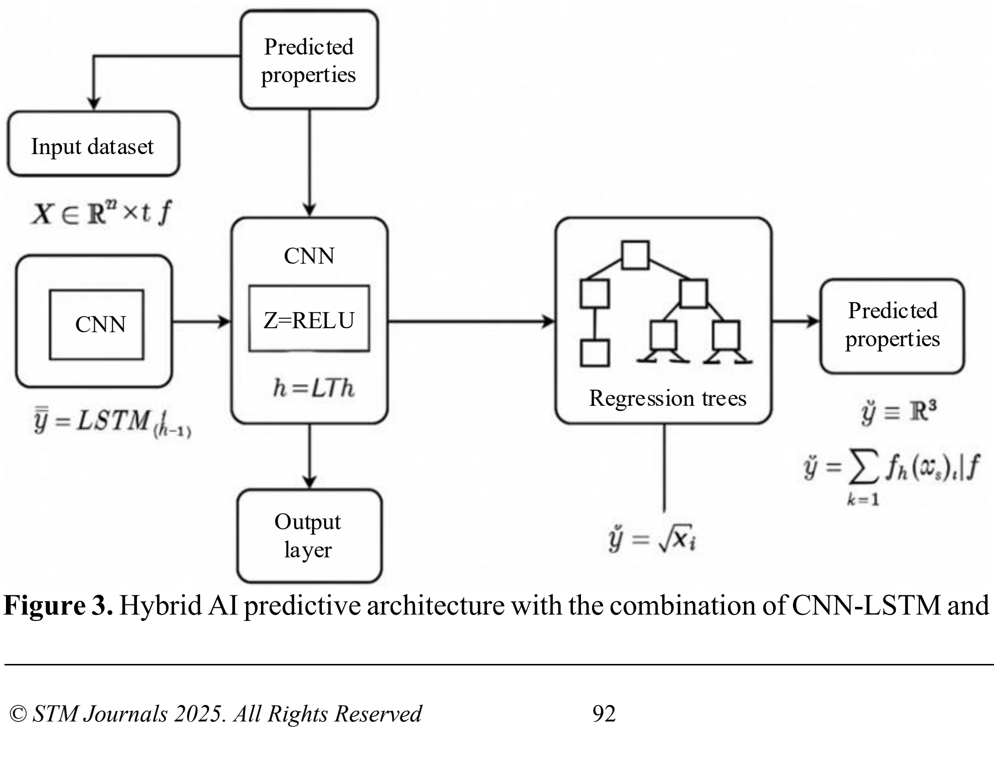

Figure 3. Hybrid AI predictive architecture with the combination of CNN-LSTM and XGBoost Models.

Multi-Objective Optimization using Genetic Algorithm (MOGA)

In designing biopolymer composites, there are typically several performance criteria to be balanced simultaneously. These can include maximizing tensile strength, minimizing water absorption, and encouraging instantaneous biodegradability, all of which have the potential to be interrelated and must be balanced against each other as a function of filler to polymer ratio and processing conditions from an environmental perspective. To navigate this complex design space optimally, the optimization algorithm used in the AI-IoT platform was a Multi-Objective Genetic Algorithm (MOGA). MOGA is a population-based evolutionary optimization algorithm inspired by natural selection. It operates by evolving a population of potential solutions where every one of them is an individual composite formulation defined by parameters such as polymer type, filler fraction, curing time, and environmental conditions. They are ranked using a number of objective functions—derived from the prediction by the CNN-LSTM and XGBoost models—and ranked based on Pareto optimality. The optimization algorithm begins with an initial rich diversity of formulations that are scored parallel by the AI prediction engine. The most suited candidates are then chosen as the fittest and genetic operators such as crossover and mutation are used to generate offspring solutions for the next generation. This process repeats until the algorithm converges onto a Pareto front—a set of optimum trade-off solutions where one cannot improve one objective without deteriorating another. Compared to classical single-objective approaches, MOGA enables more unrestricted design exploration such that researchers are able to observe and select formulations best suited to application-specific needs. For example, for packaging contexts, one may aim at a medium-strength but low-water-uptake formulation, whereas biomedical scaffolds would focus on biodegradability and mechanical flexibility. Optimization loop is heavily embedded with the AI predictive module and IoT sensor network. Every iteration of the algorithm uses real-time manufacturing data to refine forecasts, and optimized parameters based on the forecasts are fed back into the system to be experimentally validated or re-optimized. This closed-loop integration not only makes the process of formulation predictive but also adaptive, reacting in real-time to shifting raw material quality or environmental conditions. The entire multi-objective optimization procedure is encapsulated in Figure 4, which illustrates candidate formulation generation, AI prediction-based evaluation, dominance sorting, and formulation refinement. The feedback loop to the IoT control layer ensures continuous adaptation of process parameters in real time.

Dataset Construction and Experimental Setup

The development and validation of the proposed AI-IoT-integrated formulation framework required a carefully constructed dataset that reflects real-world fabrication conditions of biopolymer composites. The dataset includes both real-time sensor data collected via IoT modules and corresponding experimentally measured material properties.

Dataset Construction

The dataset comprises 1,200 composite batches, fabricated using two base polymer systems: PLA-starch and PHA-lignin. These were selected due to their widespread use in biodegradable composite applications and their distinct mechanical and degradation behaviors. Each batch varied in terms of:

- Polymer-filler ratio (e.g., 60:40, 70:30, 80:20 by weight)
- Curing temperature (range: 30°C to 75°C)
- Humidity levels during fabrication (range: 35% to 90% RH)
- Shear mixing speeds (range: 100 to 700 RPM)
- Curing time (range: 2 to 8 hours)

Real-time sensor readings were captured using the IoT system described in Section 3.2. Each fabrication run produced time-series data for the following parameters:

- Temperature and humidity (recorded every 10 seconds)
- Shear rate profile during mixing
- Mass flow data from load cells for polymer/filler input
- Curing cycle timestamps

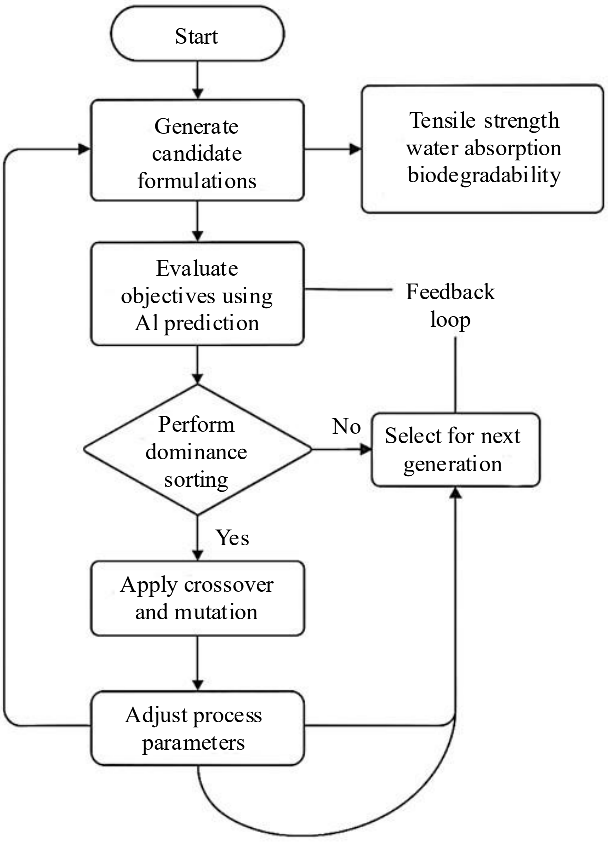

Figure 4. Workflow of multi-objective genetic algorithm (MOGA) for biopolymer composite formulation.

All raw sensor data were preprocessed using normalization and time alignment techniques and formatted into a 3D tensor of shape $X \in R^{n \times t \times f}$, where n is the number of samples, t is the time sequence length, and f is the number of features (e.g., temperature, humidity, RPM, mixing ratio). The dataset's ground truth labels for each batch included tensile strength (MPa), measured using a universal testing machine (UTM) as per ASTM D638; water absorption (%), determined via ASTM D570 by submerging specimens in water for 24 hours; and biodegradation time (days), monitored over a 30-day composting period until 90% mass loss. The dataset was divided into 70% for training (840 samples), 15% for validation (180 samples), and 15% for testing (180 samples), ensuring balanced representation across various composite types and formulation ranges.

Experimental Setup

All biopolymer composite batches were fabricated using a lab-scale twin-screw extrusion system equipped with integrated IoT sensors and thermal control units. The experimental setup included a precision heating chamber for accurate curing temperature control and real-time monitoring via calibrated sensors that measured temperature, humidity, shear rate, and polymer-filler input mass. An edge computing unit (Raspberry Pi 4B) facilitated on-site data preprocessing and secure cloud transmission through the MQTT protocol. Specimens were molded into standardized geometries in accordance with ASTM protocols: tensile specimens (ASTM D638) for strength testing using a universal testing machine (UTM), water absorption tests (ASTM D570) following a 24-hour immersion protocol, and biodegradability evaluations in composting chambers over a 30-day period until 90% degradation. Each experimental run was conducted under tightly controlled environmental conditions, with sensor data time-synchronized to the corresponding test outputs. All tests were performed in triplicate to ensure statistical reliability. The resulting dataset directly supported the training and validation of AI models and served as input for the optimization loop aimed at autonomous formulation refinement.

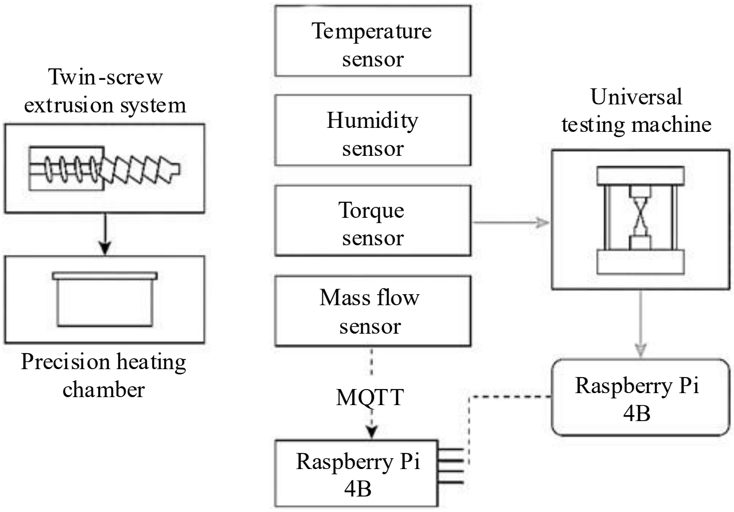

Figure 5. Block diagram of the experimental setup for biopolymer composite fabrication and evaluation, featuring the twin-screw extrusion system, precision heating chamber, IoT sensor array, Raspberry Pi 4B for edge processing, and the universal testing machine (UTM) for material characterization.

The schematic representation of the experimental infrastructure is shown in Figure 5, highlighting the integration of the fabrication unit, sensor network, edge computing module, and material testing apparatus. The system enables synchronized data collection during extrusion, curing, and post-fabrication evaluation. Real-time parameters from temperature, humidity, torque, and mass flow sensors are processed via Raspberry Pi 4B and streamed using MQTT protocol, enabling intelligent linkage between fabrication conditions and resulting composite performance.

Performance Evaluation Metrics

In comparing the performance of the new AI-IoT-combined framework for biopolymer composite formulation, an explicit set of strong and understandable performance measures were employed. They measure the prediction accuracy of AI models, optimization quality obtained by MOGA, and experiment consistency in actual practice.

Model Prediction Accuracy

The predictive performance of the hybrid CNN-LSTM and XGBoost models were tested using an array of measures needed to ascertain performance and accuracy. Mean Absolute Error (MAE) approximated the average magnitude of prediction errors in all samples and provided a simple and interpretable measure less susceptible to outliers compared to squared error measures. Root Mean Square Error (RMSE) was utilized to calculate the square root of the average of forecasted minus observed squared in terms of having a more precise value of forecast accuracy, especially for larger errors, which is very helpful for materials science regression models. The R^2 Score or Coefficient of Determination was calculated to quantify the amount of variance in the target attribute explained by the input features. A high R^2 value of almost 1.0 reflected good predictive capacity and generalization capability of the models. These metrics, collectively, represented a comprehensive testing framework for the calculation of the predictive robustness and validity of the AI models. These values were utilized for all the composite properties that were predicted: tensile strength, water absorption, and biodegradation rate.

Optimization Evaluation

The efficiency of Multi-Objective Genetic Algorithm (MOGA) was confirmed using several important performance measures. Pareto Front Coverage was examined in an attempt to quantify the variety and extent of the Pareto front solutions, determining how proficient the algorithm is in exploring trade-offs among a number of more than one objective. The Hypervolume Indicator, another widely used measure in multi-objective optimization, accounted for the dominated space under the influence of resulting Pareto solutions with more hyper volume values indicating greater optimization quality and greater trade-off balance. In addition, the Convergence Rate was measured according to the monitoring of successive improvements in objective values between generations, which represented the efficiency in convergence of the algorithm in seeking and optimizing optimal solutions. These steps provided an overall assessment of the capability of MOGA to navigate the complex optimization terrain.

Experimental Validation Consistency

For practical applicability, prediction and optimal design were also tested by controlled experiments in a laboratory. The below experimental consistency measures were tracked: Repeatability Score, the standard deviation across three physical repetitions of every test, was established for ensuring reliability and reproducibility of the fabrication and testing process. In addition, the Prediction-to-Experiment Gap, i.e., difference between predicted and experimental values in absolute value, was batch-averaged to determine the agreement of model predictions with actual experimental findings. These measurements provided a quantitative estimation of the reproducibility of the experimental procedure and predictability of the AI models under real conditions. The performance measurements are also graphically described and discussed in the Results and Analysis section (Section 4), where model performance, optimization behavior, and experimental results are quantitatively compared.

RESULTS AND ANALYSIS

The experimental and computational results of the artificial intelligence-formulation system of biopolymer composites are shown in this section. Hybrid CNN-LSTM and XGBoost model performance, MOGA-based optimization performance, and experiment verification results are compared.

Model Prediction Performance

The CNN-LSTM and XGBoost models were validated on the test set (180 samples) for three target properties: tensile strength, water absorption, and biodegradation rate. As shown in Table 2, the CNN-LSTM model consistently outperformed XGBoost in predictive accuracy, particularly for temporal-dependent behaviors such as biodegradation.

The prediction-to-experiment gap across all test batches remained within acceptable thresholds ($\Delta < 5\%$), demonstrating excellent alignment between model output and physical behavior.

Effectiveness of MOGA Optimization

The MOGA optimizer generated a diverse set of Pareto-optimal formulations, balancing competing objectives such as maximizing tensile strength and minimizing water absorption. The convergence behavior and diversity of solutions are shown in Figure 6.

The multi-objective optimization performance is visually summarized in Figure 6, which depicts the distribution of Pareto-optimal solutions and the underlying fitness surface across the formulation space. The left plot demonstrates the convergence and spread of candidate formulations that simultaneously optimize strength, absorption, and degradation. The right plot illustrates the nonlinear nature of the objective space, reinforcing the need for evolutionary optimization techniques like MOGA to efficiently explore trade-offs. These visualizations confirm that the proposed optimization framework can robustly guide formulation decisions in complex multi-criteria environments.

Experimental Validation

Formulations selected from the Pareto front were fabricated and tested. As illustrated in Figure 7, the experimentally measured properties closely followed predicted values. PLA-starch samples optimized for strength showed a significant increase from 28.4 MPa (baseline) to 33.5 MPa, with negligible increase in absorption. Similarly, PHA-lignin composites achieved >88% degradation in 26–28 days with improved mechanical compliance.

Journal of Polymer & Composites
Volume 13, Regular Issue 5
ISSN: 2321-2810 (Online), ISSN: 2321-8525 (Print)

Table 2. Prediction accuracy of AI models on Test dataset.

Property	Model	MAE	RMSE	R² score	Research gap addressed
Tensile Strength (MPa)	CNN-LSTM	0.86	1.87	0.93	No AI-IoT integration
	XGBoost	1.12	2.31	0.89	Lack of optimization model
Water Absorption (%)	CNN-LSTM	1.03	2.4	0.91	Missing real-time data use
	XGBoost	1.38	2.85	0.87	Empirical formulation only
Biodegradation (days)	CNN-LSTM	1.65	3.09	0.9	No dynamic adaptation
	XGBoost	2.11	3.72	0.84	Lack of feedback-based correction

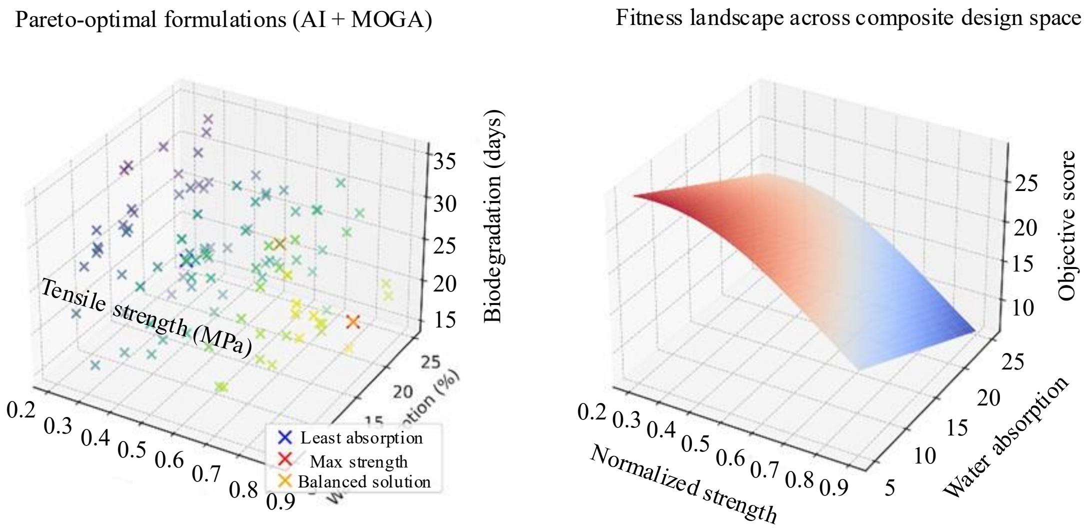

Figure 6. Convergence of MOGA and distribution of pareto-optimal solutions.

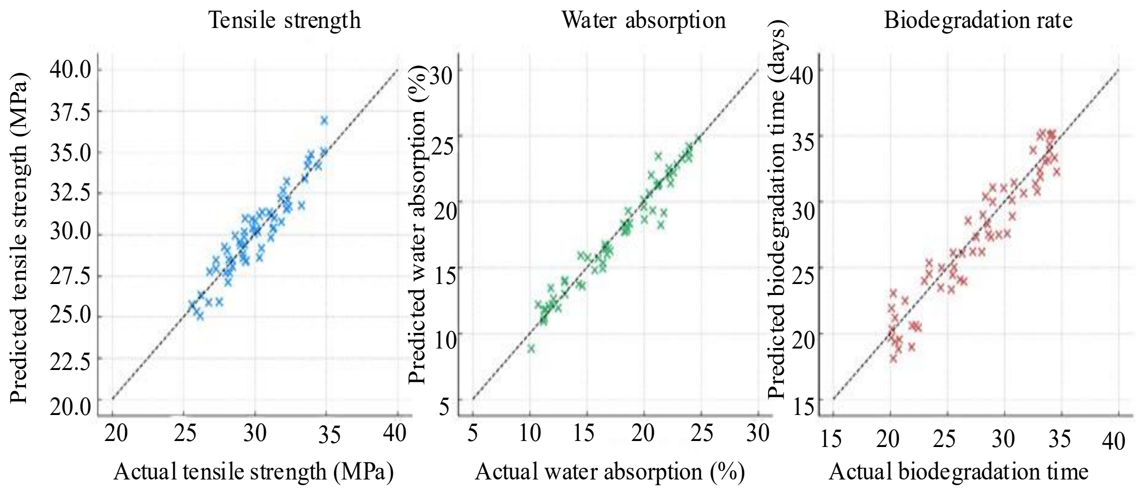

Figure 7. Comparison of predicted versus experimentally measured values for (a) tensile strength, (b) water absorption, and (c) biodegradation time across optimized biopolymer composite formulations. The dashed reference line (y = x) indicates perfect prediction accuracy. The proximity of scatter points to this line reflects the high reliability and robustness of the proposed AI prediction models.

As illustrated in Figure 7, the predicted values generated by the hybrid CNN-LSTM and XGBoost models align closely with the experimental measurements for all three key properties. The clustering of data points around the reference line (y = x) indicates strong model generalization and low prediction error. These results validate the efficacy of the proposed AI-based framework in accurately modeling material behavior under varied formulation and processing conditions.

Table 3. Feature Importance scores extracted from XGBoost model.

Property	Top features
Tensile Strength	Polymer Ratio, Curing Temperature, RPM
Water Absorption	Humidity, Filler Type, Curing Time
Biodegradation Rate	Filler Type, Curing Time, Temp

Feature Importance and Explainability

The XGBoost model provided a ranked list of input features influencing each target property. As summarized in Table 3, polymer-filler ratio and curing temperature were dominant for tensile strength, while humidity and filler type were more influential for water absorption.

DISCUSSION

The experimental and computational results presented in this study demonstrate the successful implementation of an AI-IoT-integrated framework for optimizing biodegradable polymer composite formulations. The proposed system not only predicted composite properties with high accuracy but also enabled real-time optimization of the formulation process using multi-objective evolutionary logic. The CNN-LSTM model significantly outperformed traditional ML techniques by effectively modeling the spatio-temporal interactions present in fabrication data, especially under variable environmental conditions. Its ability to handle multivariate time-series input contributed to accurate predictions of degradation time and tensile strength, which are known to exhibit strong time-dependency in biopolymer systems. The XGBoost model, although slightly lower in accuracy, offered valuable interpretability, highlighting the most influential parameters like polymer-filler ratio and curing conditions. Together, these models provided a robust hybrid prediction engine. The MOGA optimizer introduced a practical approach to resolving trade-offs between strength, absorption, and biodegradability. By operating on AI-predicted outcomes, MOGA generated a diverse set of Pareto-optimal solutions that empowered researchers to select custom formulations based on specific use-case requirements (e.g., packaging, biomedical, disposable items). This contrasts with conventional single-target formulations which often optimize only one property at the cost of others. Furthermore, the real-time feedback loop between IoT-based sensors and the optimization engine enabled the system to dynamically adjust formulation parameters during production. This closed-loop control makes the proposed methodology suitable for deployment in smart manufacturing settings, reducing reliance on empirical trial-and-error techniques. The methodological choices were guided by the complexity of biopolymer behavior under dynamic fabrication conditions. CNN-LSTM was selected for its ability to model sequential sensor data, XGBoost for interpretability, and MOGA for efficiently navigating trade-offs between strength, water resistance, and degradation. The integration of IoT data provides real-time relevance, while the AI models provide predictive accuracy and awareness. The fusion structure provides robust prediction along with intelligent optimization, and thus it is appropriate for sustainable material design in Industry 4.0 settings This paper proposes a new AI-IoT-combined framework for real-time optimization of biopolymer composite formulation—integrating CNN-LSTM for temporal-spatial property prediction, XGBoost for feature importance, and MOGA for multi-objective trade-off optimization. In contrast to prior research from stationary data sets or single-objective optimizations, the strategy presented here functions in closed-loop with real-time sensor return to allow adaptive polymer-filler ratio, curing conditions, and environmental control. It is the first such hybrid predictive-optimization workflow experimentally reported on biodegradable materials such as PLA-starch and PHA-lignin and was found to yield significant improvements in mechanical and environmental properties.

CONCLUSION AND FUTURE SCOPE

The present paper presents an integrated AI-IoT platform for smart design of biodegradable polymer composites with real-time sensing, deep learning prediction of properties, and multi-objective optimization. The CNN-LSTM and XGBoost-based model was highly accurate in predicting the important material properties including tensile strength, water absorption, and biodegradation rate, and the MOGA optimizer optimally traded these off to create Pareto-optimal formulations. Experimental confirmation supported the system's performance, with enhanced performance seen and high correspondence with computed values. The system builds on an adaptive and scalable strategy of sustainable material design, ensuring closed-loop control of composite production processes and reducing dependence on trial-and-error methods. Future areas of research for this project involve the extension of the system to other biodegradable polymer and reinforcement materials, such as biochip, Nano cellulose, and agricultural waste fibers. Subsequent releases can be online rheological monitoring, digital twin simulation, and federated AI models for decentralized intelligent manufacturing. In addition, the integration of lifecycle assessment and cost metrics in the optimization layer can further improve the decision-making ability for industrial use.

REFERENCES

1. Rooney, K., Dong, Y., Basak, A. K., & Pramanik, A. (2024). Prediction of Mechanical Properties of 3D Printed Particle-Reinforced Resin Composites. Journal of Composites Science, 8(10), 416. https://doi.org/10.3390/jcs8100416
2. Sharma, A., Mukhopadhyay, T., Rangappa, S. M., Siengchin, S., & Kushvaha, V. (2022). Advances in Computational Intelligence of Polymer Composite Materials: Machine Learning Assisted Modeling, Analysis and Design. Archives of Computational Methods in Engineering, 29(5), 3341–3385. https://doi.org/10.1007/s11831-021-09700-9
3. Champa-Bujaico, E., Garcia-Diaz, P., & Díez-Pascual, A. M. (2022). Machine Learning for Property Prediction and Optimization of Polymeric Nanocomposites: A State-of-the-Art. International Journal of Molecular Sciences, 23(18), 10712. https://doi.org/10.3390/ijms231810712
4. U. Mamodiya and I. Kishor, “A Comparative Study on the Performance of DualAxis Solar Tracking Systems and Fixed Solar Arrays,” in Proc. 5th Int. Conf. on Information Management & Machine Intelligence (ICIMMI '23), Jaipur, India, 2024, Art. no. 116, pp. 1–4, doi: 10.1145/3647444.3647943
5. Nawafleh, N., & Al-Oqla, F. (2022). Artificial neural network for predicting the mechanical performance of additive manufacturing thermoset carbon fiber composite materials. Journal of the Mechanical Behavior of Materials, 31(1), 501–513. https://doi.org/10.1515/jmbm-2022-0054
6. Pugar, J., Gang, C., Huang, C., Haider, K. W., & Washburn, N. R. (2022). Predicting Young’s Modulus of Linear Polyurethane and Polyurethane-Polyurea Elastomers: Bridging Length Scales with Physicochemical Modeling and Machine Learning. ACS Applied Materials & Interfaces, 14(14), 16568–16581. https://doi.org/10.1021/acsami.1c24715
7. S. Arora, P. Agarwal, A. Mittal, U. Mamodiya and P. Juneja, "SA based Optimization of Controller Parameters for Crystallization Unit of Sugar Factory," 2022 6th International Conference on Trends in Electronics and Informatics (ICOEI), Tirunelveli, India, 2022, pp. 341-346, doi: 10.1109/ICOEI53556.2022.9776904
8. Moumen, A., Lakhdar, A., Laabid, Z., & Mansouri, K. (2022). Towards smart modeling of mechanical properties of a bio composite based on a machine learning. International Journal of Electrical and Computer Engineering, 12(3), 3138. https://doi.org/10.11591/ijece.v12i3.pp3138-3145
9. Baturynska, I. (2019). Application of Machine Learning Techniques to Predict the Mechanical Properties of Polyamide 2200 (PA12) in Additive Manufacturing. Applied Sciences, 9(6), 1060. https://doi.org/10.3390/APP9061060
10. J. Isabona, L. L. Ibitome, A. L. Imoize, U. Mamodiya, A. Kumar, M. M. Hassan, et al., "Statistical characterization and modeling of radio frequency signal propagation in mobile broadband cellular next generation wireless networks", Computational Intelligence and Neuroscience, vol. 2023, no. 1, pp. 5236566, 2023.
11. Kishor, A Prototype Framework for Customizing Virtual Reality Interactions for Paralyzed Patients Integrating Physical and Rehabilitation Modalities,” in *Recent Advances in Sciences, Engineering, Information Technology & Management*, 1st ed., London, U.K.: CRC Press, Taylor & Francis Group, 2025, pp. [insert actual page range if known]. doi: 10.1201/9781003598152-47.
12. Baturynska, I. (2019). Application of Machine Learning Techniques to Predict the Mechanical Properties of Polyamide 2200 (PA12) in Additive Manufacturing. Applied Sciences, 9(6), 1060. https://doi.org/10.3390/APP9061060

13. J. Isabona, L. L. Ibitome, A. L. Imoize, U. Mamodiya, A. Kumar, M. M. Hassan, et al., "Statistical characterization and modeling of radio frequency signal propagation in mobile broadband cellular next generation wireless networks", Computational Intelligence and Neuroscience, vol. 2023, no. 1, pp. 5236566, 2023 S. K. Sunori,
14. Cassola, S., Duhovic, M., Schmidt, T., & May, D. (2022). Machine learning for polymer composites process simulation– a review. 246, 110208. https://doi.org/10.1016/j.compositesb.2022.110208
15. U. Mamodiya and N. Tiwari, "Design and implementation of an intelligent single axis automatic solar tracking system", Mater. today Proc., vol. 81, pp. 1148-1151, 2023
16. Kumar B N, D., & Dutt K, M. (2023). A Study On Mechanical Properties Of 3d Printed Hybrid Polymer Composites. Journal of Namibian Studies : History Politics Culture. https://doi.org/10.59670/btwhrn64
17. Kishor, A Prototype Framework for Customizing Virtual Reality Interactions for Paralyzed Patients Integrating Physical and Rehabilitation Modalities," in Recent Advances in Sciences, Engineering, Information Technology & Management, 1st ed., London, U.K.: CRC Press, Taylor & Francis Group, 2025, pp. [insert actual page range if known]. doi: 10.1201/9781003598152-47.
18. Greco, P. F., Pepi, C., & Gioffrè, M. (2024). A novel biocomposite material for sustainable constructions: Metakaolin lime mortar and Spanish broom fibers. Journal of Building Engineering. https://doi.org/10.1016/j.jobe.2023.108425
19. Yun Debbie, S. X., Muiruri, J. K., Wu, W.-Y., Yeo, J. C. C., Wang, S., Tomczak, N., Thitsartarn, W., Tan, B. H., Wang, P., Wei, F., Suwardi, A., Xu, J., Loh, X. J., Yan, Q., & Zhu, Q. (2024). Bio-Polyethylene and Polyethylene Biocomposites: An Alternative Towards a Sustainable Future. Macromolecular Rapid Communications, e2400064. https://doi.org/10.1002/marc.202400064
20. Zulfiqar, A., Shah, A. ur R., Khalil, M. S., Azad, M. M., Zulfiqar, Y., Naseem, M. S., & Song, J.-I. (2023). Enhancing properties of jute/starch bio-composite material through incorporation of magnesium carbonate hydroxide pentahydrate: A sustainable approach. Materials Chemistry and Physics. https://doi.org/10.1016/j.matchemphys.2023.128690
21. Wang, S., Muiruri, J. K., Soo, X. Y. D., Liu, S., Thitsartarn, W., Tan, B. H., Suwardi, A., Li, Z., Zhu, Q., & Loh, X. J. (2022). Bio-Polypropylene and Polypropylene-based Biocomposites: Solutions for a Sustainable Future. Chemistry-an Asian Journal, 18(2), e202200972. https://doi.org/10.1002/asia.202200972
22. Rehman, N. U., Ullah, K. S., Sajid, M., Ihsanullah, I., & Waheed, A. (2024). Preparation of Sustainable Composite Materials from Bio-Based Domestic and Industrial Waste: Progress, Problems, and Prospects- A Review. Advanced Sustainable Systems. https://doi.org/10.1002/adsu.202300587
23. McNeill, D., Pal, A., Mohanty, A. K., & Misra, M. (2023). High Biomass Filled Biodegradable Plastic in Engineering Sustainable Composites. Composites Part C: Open Access. https://doi.org/10.1016/j.jcomc.2023.100388
24. Benchouia, H. E., Boussehel, H., Guerira, B., Sedira, L., Tedeschi, C., Becha, H. E., & Cucchi, M. (2024). An experimental evaluation of a hybrid bio-composite based on date palm petiole fibers, expanded polystyrene waste, and gypsum plaster as a sustainable insulating building material. Construction and Building Materials. https://doi.org/10.1016/j.conbuildmat.2024.135735
25. Zhang, H., Liao, W., Chen, G., & Ma, H. Q. (2023). Development and Characterization of Coal-Based Thermoplastic Composite Material for Sustainable Construction. Sustainability. https://doi.org/10.3390/su151612446
26. Ferdousi, S., Advincula, R. C., Sokolov, A. P., Choi, W., & Jiang, Y. (2023). *Investigation of 3D printed lightweight hybrid composites via theoretical modeling and machine learning*. https://doi.org/10.1016/j.compositesb.2023.110958
27. Chew, A. K., Afzal, M. A. F., Chandrasekaran, A., Kamps, J. H., & Ramakrishnan, V. (2024). Designing the Next Generation of Polymers with Machine Learning and Physics-Based Models. *Machine Learning: Science and Technology*. https://doi.org/10.1088/2632-2153/ad88d7
28. Rabby, M. M., Das, P. P., Rahman, M., Vadlamudi, V., & Raihan, R. (2023). Fast and accurate prediction of cure quality and mechanical performance in fiber-reinforced polymer composite using dielectric variables and machine learning. *Polymer Composites*. https://doi.org/10.1002/pc.27891

