Designing Polymer Nanocomposites for Optimizing and Predicting Using Machine Learning Algorithms

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This research presents a hybrid Machine-Learning (ML) approach for predicting the thermal conductance of Polymeric Nanocomposites (P-NCs). Artificial Neural Networks (ANN) and Particle Swarm Optimization (PSO) are employed to calculate the correlation between the input and output variables. The ANN is used to model the combination. At the same time, the PSO algorithm enhances the accuracy of predictions by conducting an optimized search for a global minimum. The input criteria for the selection process include the fibers' and matrix's thermal conductance, capital resistance, volume percentage, and dimension ratio. The findings demonstrate that the PSO enhances the prediction capability of this hybrid system, surpassing conventional neural systems.

Keywords: Polymer Nanocomposites, Machine Learning, Optimisation, Prediction.

1. Introduction

Nanocomposite Materials (NCM) research is presently receiving significant interest due to its possible influence on contemporary society. The creation of nanofillers in polymers, aimed at enhancing specific and visible properties, is now a research subject in several disciplines. The area has made significant progress overall. Several study subdivisions are still in their early stages. NCMs have enhanced mechanical, electrical, and thermal characteristics compared to conventional composites, including fillers such as glass, carbon, or aramid fiber [1]. The final product's constitution changes based on the production process. The matrix, composed of thermoplastic polymers, distributes loads evenly throughout the inserted nano-reinforcing surface [4]. Introducing Nanoparticles (NP) into a material is a widely used method to enhance the strength and durability of the polymeric matrix [2].

The nanofillers are categorized into three primary types according to their distinctive features. Carbon-based nanomaterials' remarkable physical, electrical, and visible characteristics, such as graphene layers and Carbon Nanotubes (CNT), have introduced novel prospects for tissue technology [3]. This field is crucial for advancing biological alternatives that can repair or substitute entire or partial tissue [13]. Graphene Films (GF) and CNT are the most prevalent carbon-based nanostructures [18]. GF and CNT are highly esteemed for their favorable characteristics. CNTs possess a chemical composition and physical arrangement, providing a milieu similar to a biological extracellular matrix.

Within this particular setting, nanocomposites exhibiting three distinct phases have been detected: phase split up, incorporated, and removed. The nanofiller hinders the polymer from intercalating, forming a composite material with clearly distinguishable phases. This material has some distinctive qualities that are similar to composites [10]. Introducing a solitary elongated polymer chain amongst nanofillers makes it possible to create an incorporated architecture that leads to a well-organized incorporated morphology. If the nanofiller is wholly and evenly distributed throughout an ongoing polymer matrix, the result will seem as if it has been removed.

Due to the intricate nature and extensive computational requirements, researchers have been seeking alternate methods to use finite element and molecule dynamical models to analyze the behavior of materials in various situations. The objective is to get a feasible solution, which is the reason for doing this task. Machine Learning (ML) is a branch of Artificial Intelligence (AI) that has seen significant expansion in the past decade, primarily because of its focus on extracting heretofore undiscovered patterns from vast databases [5].

2. Related Works

Multiple methodologies exist to predict the material properties of composites. Okafor et al. introduced the systematic approach of the rule-of-mixture, which enables the prediction of the characteristics of composites supplemented with fibers [6]. Tendera et al. used a unique theoretical model to determine the efficient thermal conductance of NCM enhanced with NP [19]. Wu et al. constructed a model of nano-clay architecture by formulating a theory that describes the behavior of efficient particles [8]. Patro et al. calculated the heat relaxation duration, electrical conductivity, and heat retention for NCM-containing CNTs with varying volume percentages [9]. Markarian et al. developed a two-phase, randomized composite material framework capable of simulating various thermal and mechanical characteristics using the Finite Element Methods (FEM) [20]. Badjian et al. conducted molecular dynamics calculations to investigate the impact of carbon nanobud on the mechanical characteristics and heat conductance of cross-linked epoxy polymers [11].

Liu et al. used a data-driven computational homogenized technique based on Artificial Neural Networks (ANN) to forecast the fluctuating anisotropy conductivity of Polymeric Nanocomposites (P-NCs) [12]. Nag et al. used ANN to determine P-NC’s strain-sensing behavior from CNT [21]. Das et al. utilize Deep ANN and a universal optimization method to analyze the physical behavior of 2D graphene nanocomposites [14].

Fang et al. used Particle Swarm Optimization (PSO) to optimize the hyper-parameters and accurately forecast the crack closure percentages [15]. Garud et al. used a PSO - Genetic Algorithm (GA) in conjunction with an ANN to predict the settings of solar space heating technology [22]. Wu et al. used a hybrid optimization to assess the injection molding procedure for bi-aspheric lenses [17]. PSO significantly enhances the precision of neural network forecasts [16]. This research presents a hybrid approach that combines PSO and neural networks to forecast the spatiotemporal thermal conductance of CNT-augmented P-NCs accurately [7].

3. Proposed Polymeric Nanocomposite

The research emphasizes P-NCs typically produced using the Chemical Vapor Deposition (CVD) procedure. The polyurethane resin is a cycloaliphatic polyamine, whereas the catalyst consists of zeolite-supported chrome and iron. The production of single-walled CNT involves using ethyl alcohol via CVD. The filler has a realistic size of 1 μm. They consider the interface impedance between the fillings and the matrix, as shown in Figure 1.

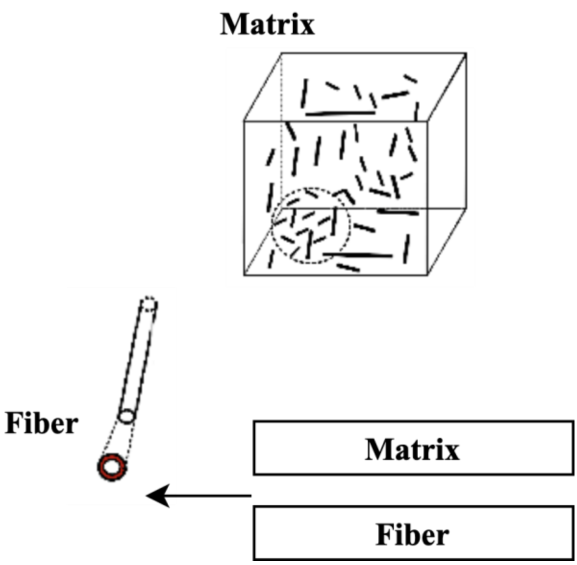

Figure 1. Architecture of the Polymeric Nanocomposite Design

The research uses an existing Python script to extract data from a text file generated by a C++ application. This data is then used to create the finite element differentiation of the Representative Volumetric Element (RVE). The fillings are positioned inside the RVE to avoid overlapping, depending on the input variables' provided Probability Density Forms (PDFs). The technique guarantees that the RVE adheres to the regularity of the architecture. Any missing fillers on either side of the RVE are present on the opposing side of the RVE modeling. Figure 2 provides a summary of the flowchart for the stochastic modeling technique.

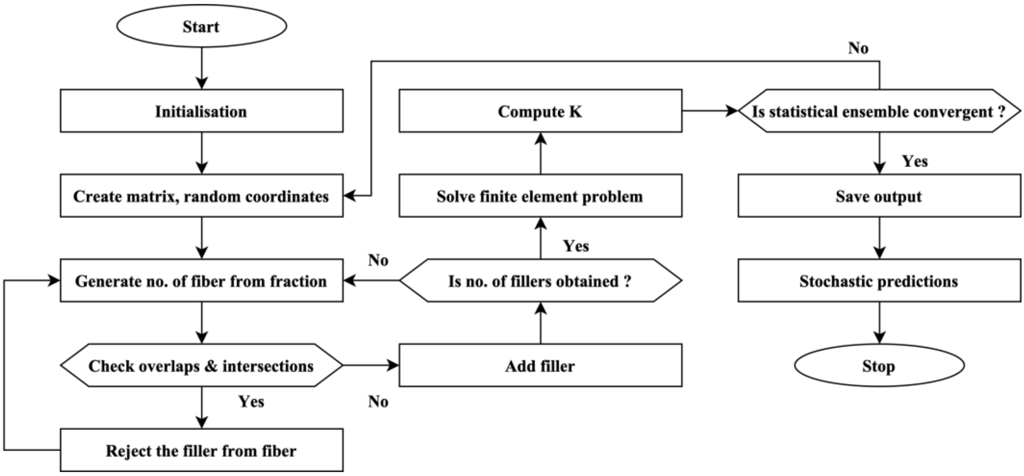

Figure 2. Workflow of the proposed fabrication method for Polymeric Nanocomposites

This research utilizes a hybrid methodology that combines an ANN with PSO. Figure 2 depicts the flow chart of the suggested method. The particles' positions are determined randomly in the first phase. Afterwards, the system is trained using the PSO technique. The particle location information acquired at the beginning of this procedure is linked to the original weights and biases. Once the PSO method finishes the data training, the Back Propagation Neural Network (BPNN) proceeds with the training. The ideal value trajectory of the backpropagation method, which computes the weights and deviation gradients, differs from the universal optimal variable of the PSO. The outcomes of searching for simultaneous ideal values are likely to encounter conflicts. The perfect approach involves using PSO to swiftly search the global optimum value to produce the target regions, followed by the BPNN for precise computations with small-scale and fine-grained accuracy inside those candidate regions. This dual optimization guarantees that the present local optimum solution is the universal solution in most circumstances.

The use of the suggested framework is estimated using the following steps: The process involves three main steps: (i) normalizing all the data, (ii) selecting an appropriate and optimal hybrid approach, and (iii) implementing an efficient hybrid structure. This research analyzes the influence of the main factors on the model and emphasizes the importance of accurately selecting these variables. During the training stages, a 5-fold Cross-Validation (CV) is used. Hence, the information is randomly divided into five categories, each comprising five components. The first category, the training information, shall consist of 80% and is utilized to train the systems. The second set, known as the testing information, consists of the remaining 20% of the data and is employed to assess the effectiveness of the algorithms. The testing data needs to be distinct from the training information.

The research enhances the performance by introducing noise to its output samples throughout the training phase. This noise helps to smooth the results and improve the network's capability. The ANN model is accessed in MATLAB. Using the code, this programming software implements the suggested method.

4. Simulation Analysis and Results

The RVE that the research utilized had a final size of 200 nanometers. The research enhances the network structure before training the simulations. The number of synapses in an ANN model's input and output layers is predetermined and corresponds to the number of input and output variables, accordingly. The number of concealed layers and neurons is adjustable and contingent upon the magnitude of the information. The research evaluates 20 distinct networks, including one concealed layer with varying neurons ranging from 1 to 20. To mitigate the issues of excess fitting or underestimating during the training procedure, maximizing the use of the data source is essential. The research uses a 5-fold CV in each training model. The performance analysis over different sizes of P-NCs is shown in Figure 3.

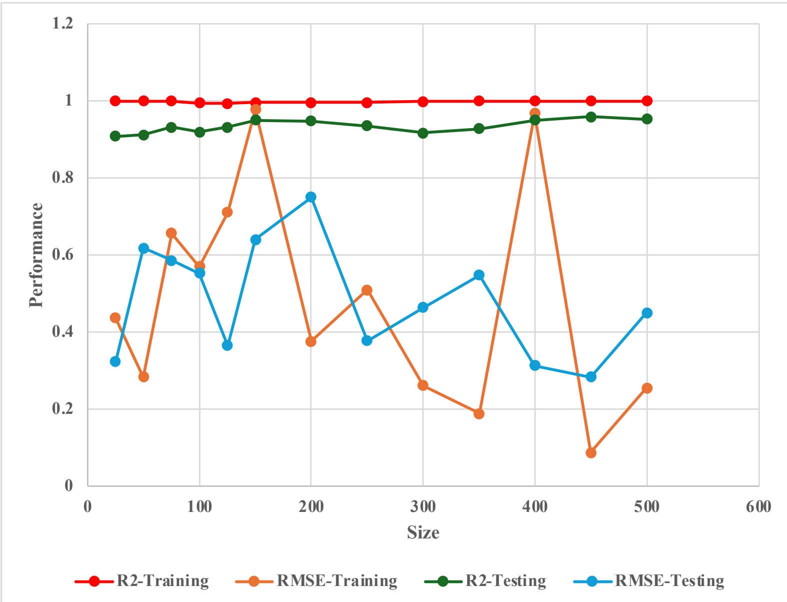

Figure 3. Performance analysis over different size

Once the ANN structure has been repaired, the variables of the hybrid model must be established. These parameters include the starting weight, acceleration steady, and swarm population density. The potential variables of the PSO system are chosen based on prior research. The research selects a range from swarm population figures as the values for the variables. Root Mean Squared Error (RMSE) is a performance metric in this variable adjustment. The ANN is trained using five input variables: the conductance of the fiber, the conductance of the matrix, the connection resistance, the volume percentage, and the aspect ratios. These variables are employed to predict the efficient conductance of the composites.

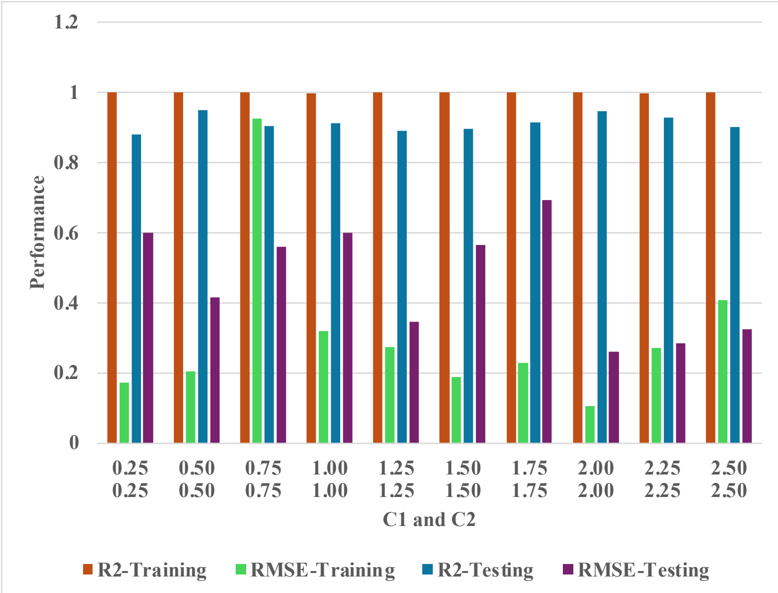

Figure 4. Performance analysis over different C1 and C2

The individual ANN model achieved a precision of 97.2% in the training dataset and 90.3% in the testing dataset. However, the combined model significantly enhanced its precision to 99.3% and 94.7% in both sets. The training duration for the ANN is 31.3 seconds, whereas the suggested method is 67.3 seconds. While the training of the proposed system is more extensive than the simple ANN training, it remains much less compared to the Central Processing Unit (CPU) expenses for the finite element system. The top and lower limits of the training batch data are established. The research inputs the samples from the Latin Hypercube Sampling (LHS) method into the pre-existing and trained suggested method to acquire forecasting information using the combined network approach.

5. Conclusion and Discussions

The primary objective of this research was to examine the predictive capacity of ANN and the suggested approach. The study used RVE-based FEM to forecast the efficient heat conductivity of P-NCs. The research has chosen five input variables: fiber conductance, matrix conductance, Kapitza impedance, volume percentage, and aspect proportion. Two hundred specimens from the database were utilized to train the algorithm. The research determined that the ideal number of neurons in the concealed layers is 20. The complete ANN structure is a 5 x 20 x 1 configuration. The suggested design identified the optimal values for the population dimension (C1, C2) and the starting weights - 430, (3.1, 3.1), and one, respectively. The research used two statistical measures, R2 and RMSE, to analyze the network's efficiency quantitatively. The hybrid technique demonstrated superior performance compared to the ANN. The LHS method created random input data inside the prediction region. The forecasted information has an R2 value of 98% and an RMSE value of 0.083. The information is predicted within a few moments with adequate precision, significantly reducing the computational expense of the simulation. The findings demonstrate that this mixed approach significantly impacts forecasting the efficiency of P-NCs.

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