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Research Article

# Modeling and optimization of dynamic-mechanical properties of hybrid polymer composites by multiple nonlinear neuro-regression method

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## ABSTRACT

The purpose of this research is to improve the dynamic-mechanical properties of the polypropylene filled by artichoke stem (AS) particles and wollastonite (W) in different weight fractions. The effect of weight ratios of fillers in polypropylene was mathematically modeled using the data obtained as a result of the experimental work. In the modeling phase, multiple nonlinear neuro-regression analysis was used. In this context, proposed linear and nonlinear models have been examined by performing $R^2_{training}$, $R^2_{adjusted}$, $R^2_{testing}$, and boundedness check. The models that satisfy these four criteria were selected as the objective functions for the optimization phase. Finally, Modified Differential Evolution Algorithm was used to obtain maximum storage modulus and loss modulus by adjusting weight percent ratio of artichoke stem particle and wollastonite. The experimental results and the modeling optimization results showed that when the polypropylene-artichoke stem particle-wollastonite hybrid polymer composite was used instead of other non-hybrid polymer composite, the storage modulus and the loss modulus improved by approximately 40%.

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## INTRODUCTION

The utilization of natural fibers as filler/reinforcement material in polymers is increasing day by day due to the advantages of being renewable resources, having low density, non-toxic properties, and being available at low prices. Natural fibers are an alternative to synthetic fibers in construction structures, the automotive industry, and daily use materials in applications that do not require high strength. In addition to these advantages, the usage of natural fiber fillers is limited because of their insufficient thermal properties. In order to improve the thermal properties of natural fiber-filled polymer composites, it is aimed to produce hybrid polymer composites by reinforcing polymer with mineral fillers. Hybrid composites can be obtained by combining two or more filler types with the same structure. By combining the properties of two materials, a more suitable composite material can be produced at the desired level. The use of hybrid polymer composites is aimed to provide many

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features that are important in engineering design, such as reducing material weight and production cost, increasing strength and thermal properties of materials, and providing easy recycling of materials.

In recent years, the relevant studies have increased for the useful recycling of materials that can be found easily in nature and evaluated as waste. One of the main purposes of these studies is to reduce the effects of the damage caused by these wastes to the environment. Polymer matrix composites are reinforced with organic and inorganic fillers such as sugarcane bagasse, cotton stalk, wheat straw, sandalwood, poplar sawdust, wood flour/talc, artichoke stem/wollastonite to reduce production costs and minimize possible harm to the environment [1–5]. Lee et. al. [4] prepared wood flour and talc-filled polylactic acid (PLA) composites. As they report, loading wood flour and wood flour/talc mixture into raw PLA results in a small decrease in the composites' glass transition and crystalline temperatures. Also, wood flour, talc, and silane in the composites cause a successively larger decrease in the composite crystallinity. The addition of talc and silane to PLA/wood flour composites improved the tensile modulus. Sever and Yilmaz [5] combined artichoke particles with wollastonite filler to improve the thermal performance in polypropylene (PP) based polymer composites. 3%, 5%, and 7% weight wollastonite were added to the artichoke–PP matrix compared with artichoke–PP composites containing 10 wt% artichoke particles. The test results can be summarized as follows; the storage modulus of artichoke–PP composites increased with increasing artichoke content. The hybrid composites had a higher storage modulus than composites containing 10 wt% artichoke particles. The hybrid composite containing 7 wt% of artichoke particles and 3 wt% wollastonite showed the highest storage modulus value. The initial decomposition temperature of the hybrid composite containing 3 wt% of artichoke and 7 wt% wollastonite had the highest value among all composites. Goyanes et al. [6] investigated the dynamic-mechanical properties of epoxy composites filled with quartz powder. They report that the glass transition temperature increased with filler content and the dynamic-mechanic modulus also increased with quartz powder percentages. The data obtained from experimental works are supported by statistical analysis, mathematical modeling, and optimization studies [7, 8]. Although there have been many studies on the design, modeling, and optimization of synthetic fiber-reinforced polymer composites [9, 10, 13], there are limited studies regarding natural fiber-reinforced polymer composites [11, 12, 14–16]. In recent years, the usage of flax, jute, kenaf fibers stands out regarding modeling and optimization of natural composites in the literature. In this regard, Savran and Aydin [11] handled the maximization of natural frequency problems for carbon-glass epoxy and carbon-flax epoxy hybrid composites. Then they discussed the usability of natural flax fiber instead of glass fiber in natural frequency problems. The robustness and reliability of the results were tested using three different optimization methods: Modified Differential Evolution Algorithm (MDEA), Simulated Annealing, and Nelder Mead. They have reached that the usage of flax fiber in the hybrid structure instead of glass fiber provides 8.5% natural frequency increment and 21–24% cost reduction. Megahed et al. [17] studied the cost-weight-frequency problem. The minimum weight and cost of non-hybrid and hybrid composites are considered objective under the lower frequency limit constraint. Carbon, glass, and flax fibers were utilized as reinforcement and epoxy as matrices in non-hybrid and hybrid structures. The effect of the hybridization on the weight and cost performance of the beam was investigated under frequency constraint using Particle Swarm Algorithm. Results denoted that hybridization of carbon and flax fibers was the best design compared with hybrid carbon-glass structure and non-hybrid epoxy-based carbon, glass, flax structures regarding lightweight, low cost, and higher fundamental frequencies. Öndürücü et al. [18] investigated the critical buckling loads of jute and glass fiber composite subjecting to seawater experimentally. They found that natural fiber-reinforced composites exposed to seawater have lower buckling strength than kept in room conditions. Chaudhuri et al. [19] investigated the effect of biodegradation in both soil and pure microbial culture media on the tensile strength behavior of HDPE/jute composites using a central composite design. Jute fiber loading and treatment time were considered as independent factors. The optimal conditions for the biodegradation of the HDPE/jute composites were evaluated Response Surface method. According to results, two-factor interaction (2FI) and linear models were found appropriate to define mathematically the experimental results related to tensile strength behavior of HDPE/jute composite. Optimum design parameters were determined as % 30 and 6 months for fiber loading and treatment time, respectively. Rao et al. [20] considered modeling and optimization of keratin-based hair fiber composite in terms of Young's modulus and Poisson's ratios. They preferred response surface methodology to form an empirical model regarding Young's modulus and Poisson's ratios. ANOVA was applied to test the importance of independent design variables and interactions of these. Optimum levels for design variables fiber length and fiber weight fraction were determined utilizing the grey Taguchi method. The results indicated that Young's modulus and Poisson's ratios optimized by the Grey Taguchi method were gained as 4.13 GPa and 0.22, respectively. Corresponding factor levels related to optimum results were %20 and 30 mm for fiber weight ratio and fiber length, respectively. Yaghoobi and Fereidoan [21] utilized Box–Behnken and Response Surface method to model and optimize tensile strength and modulus values of Polypropylene–Kenaf fiber bio-composite. The second-order polynomial model was consistent with experimentally observed data regarding strength and modulus properties. While the studies related to natural composites are widespread in the literature, agricultural waste and mineral-filled hybrid composites are limited.

The present paper examined the production of AS and W-filled PP hybrid and non-hybrid composite materials. The storage and loss modules of the composite materials were obtained by dynamic-mechanical analyses. Multiple nonlinear neuro-regression method was used in the modeling of the experimental results. In order to express the physical process most accurately, essential mathematical functions consisting of polynomial and trigonometric expressions, Bessel special functions and hybrid functions containing these three mathematical expressions were used. The models that most accurately describe the physical process were chosen as the objective function for the optimization phase. Based on Modified Differential Evolution Algorithm (MDEA), the maximum values that the storage modulus and loss modulus can take under different boundary conditions are tried to be determined.

The originality of this study can be summarized as (i) the present paper has been considered both experiment and modeling-optimization process simultaneously. Thus, both mathematical models that accurately describe the experimental results were presented. It was allowed to improve the storage and loss modulus of the materials through the optimization process, (ii) modeling of the experimental results, polynomial, trigonometric, special functions, and hybrid models consisting of their combinations were used. The proposed models were compared with each other considering the success criteria, (iii) in the literature, polynomial models are frequently preferred during the modeling phase and $R^2$ is used alone as a success criterion in evaluating the model. However, it has been shown that polynomial models and the $R^2$ success criterion are not sufficient to accurately describe experimental or simulation results in this study, (iv) in the modeling process, a new method called neuro-regression has been proposed, which includes a combination of the Artificial Neural Network (ANN) approach and regression together. Thus, the present study fills a gap in the literature regarding the modeling and optimization of agricultural waste–mineral-filled polymer hybrid composites.

## MATERIALS AND METHODS

### Experimental Procedures

In this research, cellulosic-based artichoke stem particles (AS), mineral-based wollastonite (W), and hybrid AS-W particles were used to improve the dynamic-mechanical properties of polypropylene (PP) (Table 1). The PP-copolymer (PP, LG Chem M 1500, Korea) used in this study has a melt flow index of 16 g/10 minutes (230 °C/2.16 kg) and a density of 0.9 g/cm$^3$. Artichoke stems were supplied from the products left as agricultural waste from an artichoke plant field in İzmir, Turkey. To make artichoke stems suitable for composite production, stems were broken into small pieces then ground with a laboratory-type grinder. Then, artichoke stem particles were passed through 60 and 140 mesh sieves (Retsch RS200, Germany). Particle sizes in the range of 100 µm-250 µm were used to produce composites. Wollastonite mineral (Tremin 939-300 needle-shaped, untreated, density=2.85 g/cm$^3$ and Mohs hardness=4.5) was obtained from Kaolin Industrial Minerals, İstanbul.

The production of hybrid and non-hybrid polymer composites was produced using a laboratory-scale high-speed thermokinetic mixer and a laboratory-type heated-cooled hydraulic press (Gülnar Machine, Turkey). These materials' dynamic-mechanical properties (storage modulus and loss modulus) were obtained using a dynamic-mechanic analyzer (DMA Q800, TA Instruments Inc., USA). Analyses were performed using a single-point holder at a temperature range of 40-140°C. The heating rate was determined as 3°C/min, and analyses were performed.

### Modeling

Regression analysis is one of the statistical methods used to describe the mathematical relationship between dependent (output) and independent (input) variables in a problem. With regression analysis, mathematical models that most accurately express the results of experimental or simulation studies are tried to be put forward. The most important criterion used as a statistical evaluation criterion of model success is $R^2$, called the "determination coefficient". This parameter, which shows how consistent the actual values obtained from experiments or simulations and the values predicted by the mathematical model, take values between 0 and 1. The $R^2$ parameter is close to 1 indicates that the proposed mathematical model correctly describes the physical process regarding experimental or simulation results. Mathematical models with an $R^2$ value of 0.85-1 statistically are considered successful.

In the present study, a hybrid method that takes advantage of regression and artificial neural networks has been used in the modeling phase. In this approach, all data is divided into 80% for training and 20% for testing. The training process aims to minimize the error between the experimental and predicted values by adjusting the regression models and their coefficients. The model's prediction ability is measured in the testing phase by asking input parameter values that it has never seen before. The performance of the models is measured according to the values received by $R^2$ during the training and testing phase. Here, $R^2$ is expressed as:

$$R^2 = \frac{SSE}{SST} \tag{1}$$

$$R^2_{adjusted} = 1 - \left(\frac{n-1}{n-k-1}\right) x(1 - R^2) \tag{2}$$

where

$$SSE = \sum(y_i - f_i)^2 \quad (3)$$

$$SST = \sum(y_i - \underline{y})^2 \quad (4)$$

Where, $y_i$, $f_i$, $\underline{y}$, $n$ and $k$ are expressed as observed values, predicted values by the model, mean of observed values, total sample size and number of independent variables, respectively. SSE and SST are named as sum of square error and sum of square total error.

The model, which is successful at these stages, is finally subjected to a boundedness check, and it is evaluated how realistic the results are. The model that passes all the tests is chosen as the objective function in optimization. Modified Differential Evolution Algorithm (MDEA), one of the stochastic methods, was used in the optimization phase. This algorithm is robust, population-based, fast, and very successful in finding the global optimum. While some of the experimental data used in the study were taken from the study by Sever and Yılmaz [5], some of them were produced within the scope of this study. Separated data for training and testing purposes are given in Table 1.

**Optimization**

Optimization is a process based on obtaining the best designs by maximizing or minimizing the value of the parameter chosen as the objective function, under specified constraints arising from the inherent of the problem or included by the expert regarding the studying issue. Generally, optimization algorithms are divided into two groups as deterministic and stochastic, according to the method they follow in the solution phase. In cases where the objective function consists of simple mathematical expressions and can be differentiated, the solution can be reached by using deterministic methods. However, engineering problems inherently contain high nonlinearities, limiting the use of deterministic methods.

The solution of such problems with deterministic methods may involve difficulties both in modeling and in the solution process related to the nature of the problem. Depending on the design variables and data types, the difficulty of the problems may increase. On the other hand, stochastic methods do not need derivative information and can show high performance even under challenging problems where the design parameters can take values under certain constraints. Therefore it is much more common to use than deterministic methods.

Modified Differential Evolution Algorithm (MDEA) is one of the population-based stochastic optimization techniques based on genetic algorithms in terms of operation and options, which can give effective results in problems involving both discrete and continuous data.

> *"The DE algorithm in Mathematica contains a population of m points, {$\theta_1$, $\theta_2$,…, $\theta_j$,…, $\theta m$}. The amount of m should be higher than the total design variables. The iteration process starts with a generation of a new population randomly from the points. The real scaling factor rsf defines $\theta_{rsf} = \theta_w + rsf.(\theta_u - \theta_v)$, $i_{th}$*

**Table 1.** Training and testing data used for modeling and optimization

| | Experiment Number | Material | Weight ratio of Artichoke (%) "$x_1$" | Weight ratio of Wollastonite (%) "$x_2$" |
|---|---|---|---|---|
| Training | 1 | PP [4] | 0 | 0 |
| | 2 | PP-20AS [4] | 20 | 0 |
| | 3 | PP-30AS [4] | 30 | 0 |
| | 4 | PP-10W | 0 | 10 |
| | 5 | PP-30W | 0 | 30 |
| | 6 | PP-7W-3AS [4] | 3 | 7 |
| | 7 | PP-5W-5AS [4] | 5 | 5 |
| | 8 | PP-10W-10AS | 10 | 10 |
| | 9 | PP-14W-6AS | 6 | 14 |
| | 10 | PP-6W-14AS | 14 | 6 |
| | 11 | PP-15W-15AS | 15 | 15 |
| | 12 | PP-21W-9AS | 9 | 21 |
| | 13 | PP-9W-21AS | 21 | 9 |
| Testing | 14 | PP-10AS [4] | 10 | 0 |
| | 15 | PP-20W | 0 | 20 |
| | 16 | PP-3W-7AS [4] | 7 | 3 |

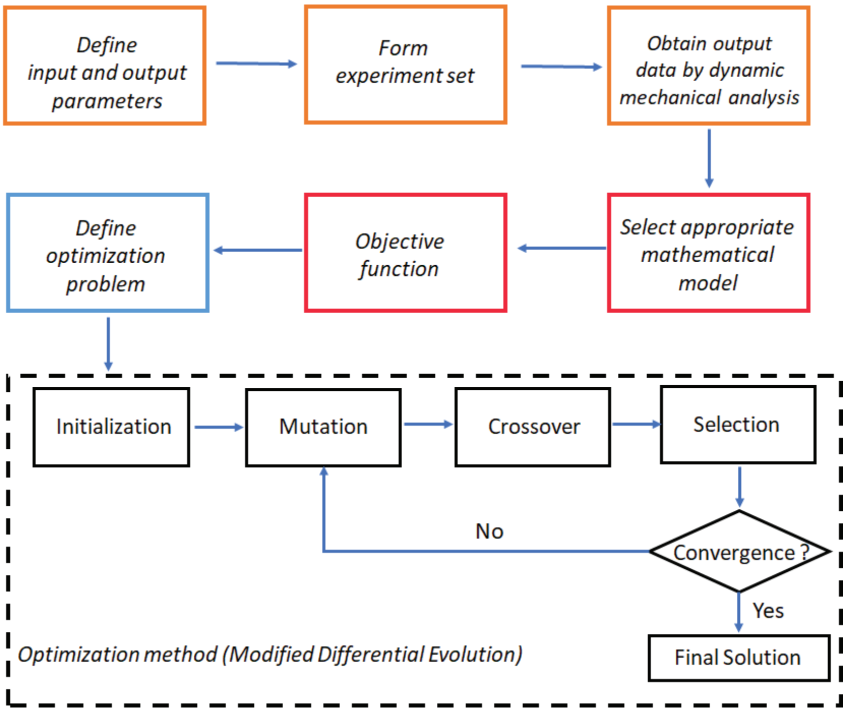



**Figure 1.** Flowchart of design, modeling and optimization processes.

*iteration points can be acquired from the earlier population. Next, in order, a new $\theta$ is set by recruiting the $j_{th}$ coordinate from $\theta_{rsf}$ with probability P. It can be adjusted by the preference "CrossProbability". In that phase, if the constraint $f(\theta_i) > f(\theta_{new})$ is valid, then $\theta_i$ is held instead of $\theta$ recent in the population. The final iteration process decided when the difference between two lastly generated points compared and if the newest points have lower tolerances provided by the parameters."[22].*

The procedure followed in the manufacturing, modeling and optimization stages is given in Figure 1.

## RESULTS AND DISCUSSION

In this study, experimentally obtained storage modulus and loss modulus behavior were modeled by multiple neuro-regression analyses. The optimization studies were carried out to maximize the storage and loss modulus by using models that passed the determined success criteria. In the considered optimization problems, the weight ratios of wollastonite mineral and artichoke stem particles were chosen as input parameters, while storage and loss moduli were chosen as output parameters.

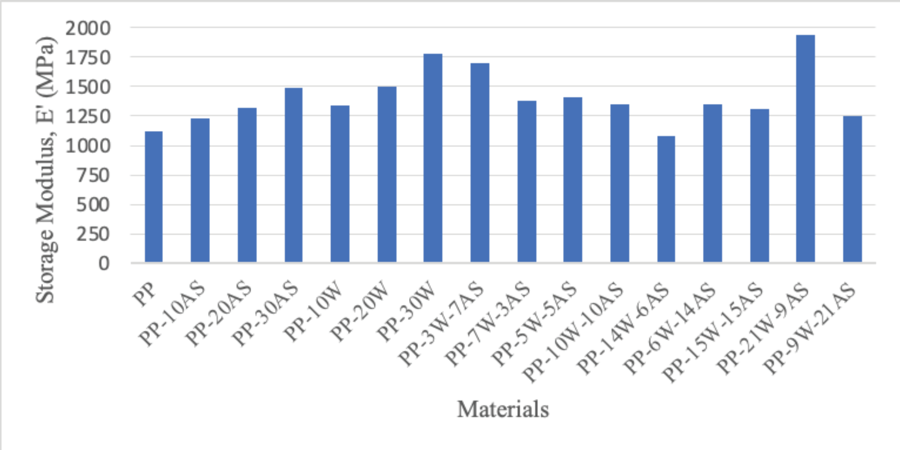
Figure 2 shows the storage and loss modulus values obtained from experimental work. It is seen an increasing trend when compared to raw PP material. Notwithstanding, the PP-21W-9AS hybrid structure showed the best result with 1942.09 MPa value in storage modulus and 103.05 MPa value in loss modulus. The PP-21W-9AS hybrid composite structure was determined to increase the modulus values by approximately 40% compared to the raw PP material.

### Modeling and Optimization Results for Storage Modulus

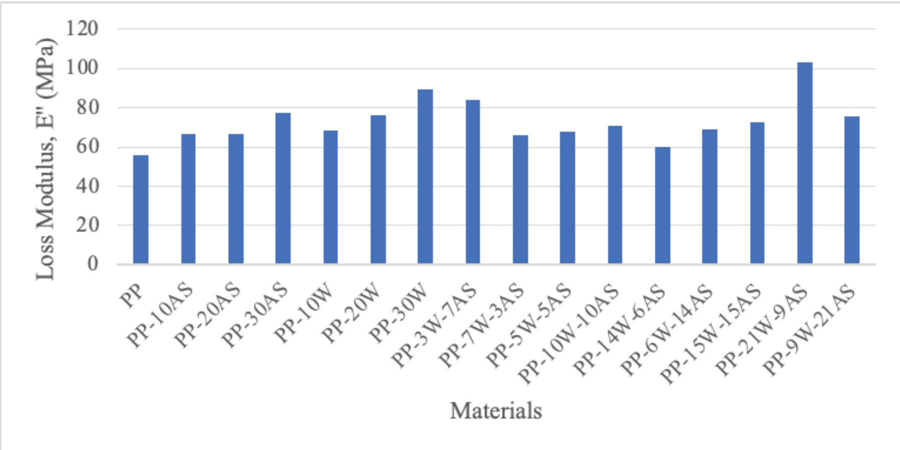
The proposed mathematical models to determine relationship between weight ratio of materials and storage modulus are given in Table 2.

The values of the parameters used in evaluating the success of regression models are given in Table 3. The criterion for the model to express the data well is that the values of the "$R^2_{training}$" and "$R^2_{adjusted}$" parameters are as close to 1 as possible. When the results are evaluated, only in terms of $R^2_{training}$ and $R^2_{adjusted}$, it is seen that all models except the linear model have values in the range of 0.9-1 and are in well fit with the experimental data. However, considering only these two success criteria leads to error because these two parameters only give information about how well the model expresses the data. In the "Testing" stage, the model is asked to predict the values of the outputs corresponding to the inputs it has never encountered before. At this stage, when the results given in Table 3 are examined, it is seen that only the hybrid model gives acceptable results. However, fulfilling the testing criteria does not mean that the model is applicable.

Another success criterion, the "boundedness check" of the model, should also be done. In this step, it is checked whether the maximum and minimum results of the model under defined input parameters constraints are realistic. The only model satisfying these four criteria mentioned above is the Poly-trigonometric multiple nonlinear model




**(a)**




**(b)**

**Figure 2.** (a) Storage modulus (E') and (b) Loss Modulus (E") values from dynamic-mechanical analyses (DMA).

**Table 2.** Multiple regression models type related to storage modulus

| Name | Models |
|---|---|
| Multiple Linear (ML) | $Y = 1146.6 + 6.1241x_1 + 18.86x_2$ |
| Third order multiple nonlinear (TON) | $Y = 1115.4 - 93.185x_1 + 8.4623x_1^2 - 0.16433x_1^3 + 214.11x_2 + 0.31823x_1x_2 - 0.42098x_1^2x_2 - 25.971x_2^2 + 0.64713x_1x_2^2 + 0.65282x_2^3$ |
| Fourth order multiple nonlinear (FON) | $Y = 1115.4 + 162.71x_1 - 1.0661x_1^2 - 0.72053x_1^3 + 0.019633x_1^4 + 176.83x_2 - 83.727x_1x_2 + 4.4085x_1^2x_2 - 0.047097x_1^3x_2 - 10.15x_2^2 + 6.4478x_1x_2^2 - 0.21778x_1^2x_2^2 - 0.8836x_2^3 - 0.081355x_1x_2^3 + 0.034997x_2^4$ |
| Second order trigonometric multiple nonlinear (SOTN) | $Y = 2855.7 - 4342.3Cos(x_1) + 14140.Cos(x_1)^2 + 5036.Cos(x_2) - 22160.Cos(x_1)Cos(x_2) + 5585.1Cos(x_2)^2 + 4757.9Sin(x_1) + 46626.Cos(x_1)Sin(x_1) - 16201.Cos(x_2)Sin(x_1) - 12743.Sin(x_1)^2 - 2716.5Sin(x_2) + 18814.Cos(x_1)Sin(x_2) - 46045.Cos(x_2)Sin(x_2) + 13717.Sin(x_1)Sin(x_2) + 530.04Sin(x_2)^2$ |
| Poli trigonometric multiple nonlinear (PTN) | $Y = 1126.84 + 17.89Cos(x_1) - 60.74Cos(x_2) + 6.923Sin(x_1) - 3.40Sin(x_2) + 43.94x_1 - 4.159x_1^2 + 0.1554x_1^3 - 0.0017x_1^4 + 43.46x_2 + 21.65x_1x_2 - 0.99x_1^2x_2 + 0.01026x_1^3x_2 - 4.447x_2^2 - 3.218x_1x_2^2 + 0.078x_1^2x_2^2 + 0.2339x_2^3 + 0.092x_1x_2^3 - 0.0036x_2^4$ |

**Table 3.** Fitting performance and boundedness of neuro-regression models for storage modulus

| Model | $R^2_{training}$ | $R^2_{adjusted}$ | $R^2_{testing}$ | Max. value (MPa) | Min. value (MPa) |
|---|---|---|---|---|---|
| ML | 0.41 | 0.29 | -0.83 | 1712.33 | 1146.55 |
| TON | 0.92 | 0.91 | -16.49 | 1948.11 | 204.40 |
| FON | 1 | 1 | -57.02 | 2111.64 | -1144.05 |
| SOTN | 1 | 1 | -78447 | 97868 | -49386.5 |
| PTN | 0.94 | 0.93 | 0.95 | 2244.57 | 1000.82 |

(PTN), which consists of polynomial and trigonometric expressions. For this reason, this model was chosen as the objective function in the optimization phase.

Figure 3 shows the experimental results of the storage modulus and the proposed hybrid model (PTN) to express them mathematically. The red points show the experimental results, and the yellow one represents the model surface in terms of the percent weight ratios of artichoke ($x_1$) and wollastonite ($x_2$) parameters. When Figure 3 is examined, it is seen that the model is well fit with the experimental results. The graphical result here confirms the success of the mathematical model with high $R^2$ values previously given in Table 3.

The graph given in Figure 4.a shows the difference between the values predicted by the PTN model, which successfully met all the success criteria and the observed values obtained as a result of the experiments. In cases where the observed and predicted values are the same, the points on the graph are expected to be on the line. As the distance of the points to the line increases, the error rate between the observed and predicted values increases. The train adjusted and test $R^2$ coefficients of the PTN model in Table 3 are in the range of 0.9-1, and the distribution of the points in Figure 4.a is very close to the line. In this case, we can deduce that the error rates are low and acceptable.

Figure 4.b shows the ratio of the error resulting from the difference between the estimated by the PTN model and actual values obtained by the experiment to the standard error of this error value for each output value. The point scattering ranges from +3 to -3, indicating that the errors are statistically acceptable. The storage modulus, one of the output parameters within the scope of the study, provides the success criterion related to the distribution of errors.

Table 4 shows the obtained maximum storage modulus when the design parameters are considered under continuous and integer constraints as two different scenarios. When the results were examined, it was seen that these two different scenarios did not make a significant difference in the storage modulus values. While the maximum storage modulus was found to be 2245.84 MPa, the input parameters $x_1$ and $x_2$ took the values of 2.80% and 27.20%, respectively.

Experimental results showed that a maximum storage modulus of 1942.09 MPa is obtained by using hybrid PP-21W-9AS material containing 21% wollastonite and 9% artichoke stem particles. As a result of the optimization, this value was 2244.57 MPa with 13% improvement.

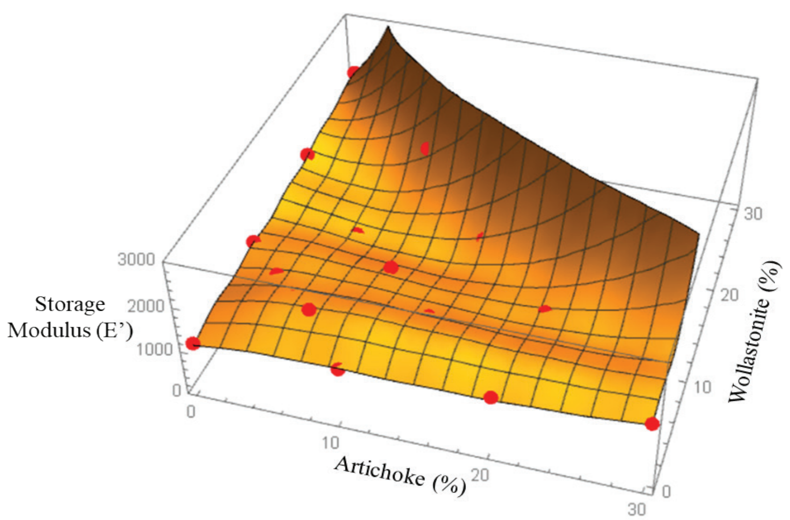
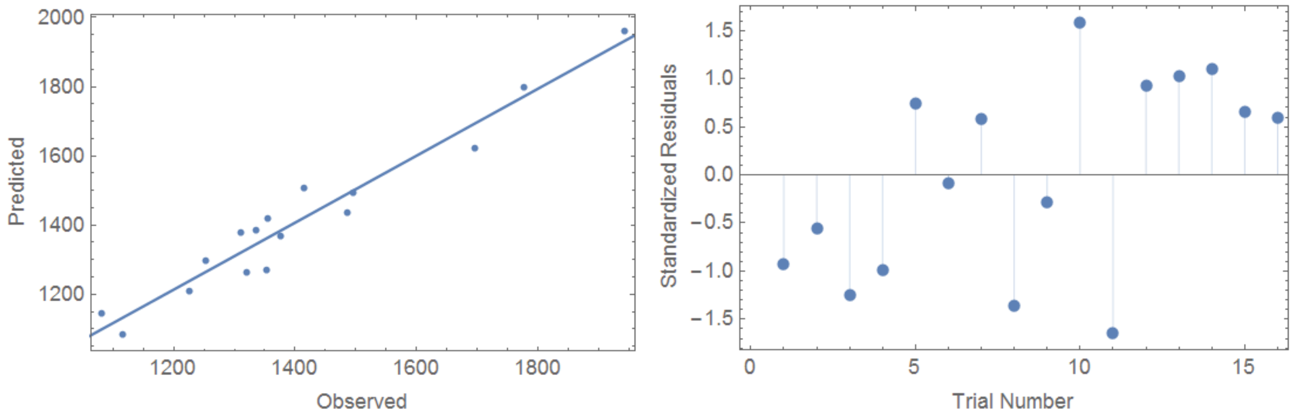



**Figure 3.** 3D plot representation of comparison between experimental and PTN model results on storage modulus.




**(a)** **(b)**

**Figure 4.** (a) Plots of predicted versus observed values (b) standardized residuals.

**Table 4.** Optimization results for storage modulus

| Objective | Objective function | Constraints | Storage Modulus (MPa) | Suggested design |
|---|---|---|---|---|
| Max. Storage Modulus | PTN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$, $\{x_1, x_2\} \in$ Integers | 2244.57 | $x_1=3$, $x_2=27$ |
| | PTN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$, | 2245.84 | $x_1=2.80$, $x_2=27.20$ |

**Table 5.** Multiple regression models type related to loss modulus

| Name | Models |
|---|---|
| Multiple Linear (ML) | $Y = 54.64 + 0.6049x_1 + 1.187x_2$ |
| Fourth order multiple nonlinear (FON) | $Y = 55.86 + 10.89x_1 - 0.08606x_1^2 - 0.04784x_1^3 + 0.001313x_1^4 + 8.119x_2 - 5.471x_1x_2 + 0.2944x_1^2x_2 - 0.003008x_1^3x_2 - 0.3337x_2^2 + 0.4234x_1x_2^2 - 0.01442x_1^2x_2^2 - 0.05455x_2^3 - 0.005965x_1x_2^3 + 0.00193x_2^4$ |
| Second order trigonometric multiple nonlinear (SOTN) | $Y = 22.21 + 2.048Cos(x_1) + 10.32Cos(x_1)^2 - 6.684Cos(x_2) + 13.Cos(x_1)Cos(x_2) + 15.92Cos(x_2)^2 - 2.478Sin(x_1) + 46.78Cos(x_1)Sin(x_1) - 12.18Cos(x_2)Sin(x_1) + 35.66Sin(x_1)^2 + 17.4Sin(x_2) - 28.42Cos(x_1)Sin(x_2) + 7.86Cos(x_2)Sin(x_2) - 15.75Sin(x_1)Sin(x_2) + 47.57Sin(x_2)^2$ |
| Special function based multiple nonlinear (SFN) | $Y = 118.5 + 16.79\,J_{x_1}(11) - 59.72\,J_{x_2}(0) - 17.29\,j_5(x_1) - 38.78\,j_5(x_2) - 0.5942x_1 + 0.0758x_1^2 - 0.001184x_1^3 - 10.33x_2 - 0.1815x_1x_2 + 0.002777x_1^2x_2 + 0.6357x_2^2 + 0.01119x_1x_2^2 - 0.0107x_2^3$ |
| Poli trigonometric multiple nonlinear (PTN) | $Y = 65.07 - 4.744Cos(x_1) - 4.467Cos(x_2) + 17.33Sin(x_1) - 11.56Sin(x_2) + 6.779x_1 - 0.712x_1^2 + 0.01752x_1^3 - 3.237x_2 - 0.2883x_1x_2 + 0.01169x_1^2x_2 + 0.4263x_2^2 + 0.004704x_1x_2^2 - 0.0099x_2^3$ |

**Modeling and Optimization Results for Loss Modulus**

The proposed mathematical models to define phenomena regarding the loss module are given in Table 5.

The values of the success parameters used in the evaluation of the regression models are given in Table 6. It is clearly seen that the two models that meet all success criteria are SFN and PTN.

In Table 5, Spherical Bessel function of the first kind, denoted , is defined by

$$j_v(z) = \sqrt{\frac{\pi}{2\,z}}\,J_{v+\frac{1}{2}}(z) \tag{5}$$

where $j_v(z)$ is a Bessel function of the first kind and, in general, z and v are complex numbers

In Figure 5, experimental results and proposed hybrid models (a. SFN and b. PTN) to express them mathematically are shown as red points and yellow surface, respectively, on the same graph. Both models showed well fit with experimental results.

Other models were eliminated because (i) the linear model could not satisfy the testing criterion, (ii) the 2nd-degree trigonometric model could not fulfill the boundedness check criteria, and (iii) the 4th-degree polynomial model could not satisfy both testing and boundedness check criteria. Hybrid models (SFN, PTN) fulfilling the success criteria were chosen as objective functions for optimization.

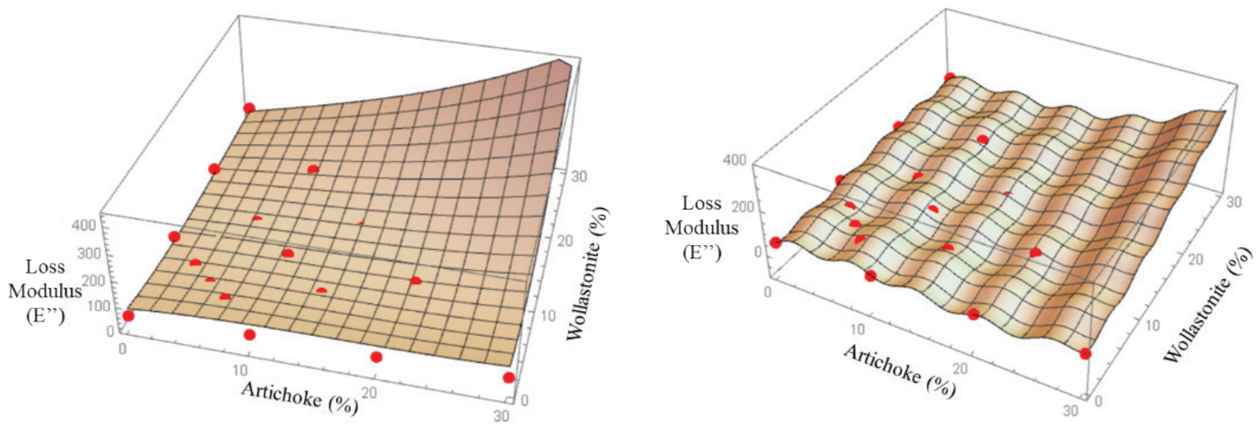
Figure 6 shows the relationship between the values predicted by the SFN and PTN models, which successfully meet all the evaluation criteria and the observed values with the experiments. Here, the values predicted by both SFN and PTN models are very close to the observed values, and the error rates of the predicted values are within acceptable limits. The graphical results, given in Figure 6, support the coefficient of determination ($R^2$) results given in Table 6.

The loss modulus optimization results obtained by using the Modified Differential Evolution Algorithm (MDEA) are given in Table 7. Within the scope of the problem, two different objective functions and two different scenarios are considered. Here, the maximum value of the loss modulus is investigated in case design parameters get values in discrete and continuous intervals.

When SFN was chosen as the objective function, the maximum loss modulus value and corresponding input parameters were 123.58 MPa, $x_1$=29%, and $x_2$=1%, respectively. In the case where PTN was the objective function, the maximum loss modulus value and corresponding input

**Table 6.** Fitting performance and boundedness of neuro-regression models for loss modulus

| Model | $R^2_{training}$ | $R^2_{adjusted}$ | $R^2_{testing}$ | Max.Value (MPa) | Min.Value (MPa) |
|---|---|---|---|---|---|
| ML | 0.62 | 0.54 | -2.29 | 90.26 | 54.64 |
| FON | 1 | 1 | -111.15 | 121.48 | -57.67 |
| SOTN | 0.82 | 0.78 | 0.90 | 165.39 | -1.76 |
| SFN | 0.97 | 0.96 | 0.95 | 123.58 | 51.52 |
| PTN | 0.91 | 0.90 | 0.93 | 129.20 | 20.63 |




**(a) SFN** **(b) PTN**

**Figure 5.** 3D plot representation of comparison between experimental and proposed models (a. SFN, b. PTN) results on loss modulus.

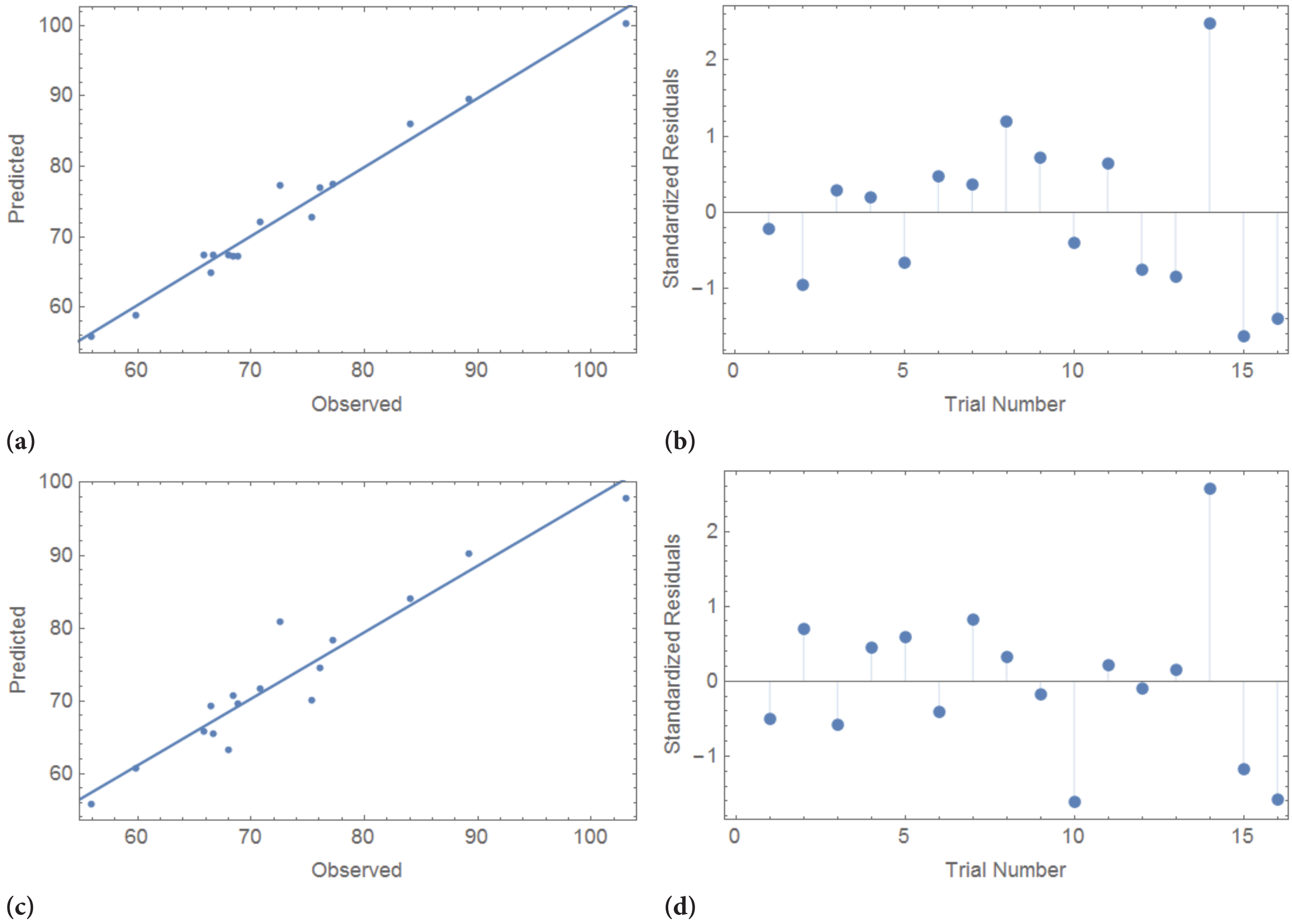



**Figure 6.** Plots of predicted versus observed values and standardized residuals for (a, b) SFN model, (c, d) PTN model.

| Objective | Objective function | Constraints | Loss Modulus (MPa) | Suggested design |
|---|---|---|---|---|
| Max. Loss Modulus | SFN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$, $\{x_1, x_2\} \in$ Integers | 123.58 | $x_1=29$, $x_2=1$ |
| | SFN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$ | 123.58 | $x_1=29$, $x_2=1$ |
| | PTN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$, $\{x_1, x_2\} \in$ Integers | 129.20 | $x_1=2$, $x_2=23$ |
| | PTN | $0 \le x_1 \le 30$, $0 \le x_2 \le 30$, $0 \le x_1+x_2 \le 30$ | 129.63 | $x_1=1.90$, $x_2=23.23$ |

parameters were 129.63 MPa, $x_1$=1.90%, and $x_2$=23.23%. Selecting input parameters from discrete or continuous intervals for both hybrid models did not significantly affect the results. It should be noted that the present paper was aimed only to improve the dynamic-mechanical properties of polypropylene. However, many other parameters affect the performance of the material during the application stage, such as raw material cost, material supply, environmental factors, and production processes. Considering these parameters, hybrid structures with different filling weight fractions can be obtained.

## CONCLUSION

Within the scope of this study, it was aimed to improve the dynamic-mechanical properties of the polypropylene filled by artichoke stem particles and wollastonite in different weight ratios. Using the data obtained as a result of the experimental study, the effect of the usage of artichoke stem particles and wollastonite in polypropylene in different weight ratios on the storage modulus and loss modulus was modeled mathematically. When the models were examined, it was seen that the models containing expressions consisting of polynomial, trigonometric and special functions (Bessel) exhibited good consistency with the experimental results, while linear or nonlinear models consisting of only polynomial expressions could not meet all success criteria.

One of the essential points to be considered here is that only the $R^2$ value was not used to evaluate model success. If only this criterion were to be considered, all models except linear models could be admitted as successful. It should be noted that $R^2$ is only a parameter that shows the consistency between the model and the experimental results. In order to obtain a model that defines the experimental process with high accuracy, all four test criteria specified in this study must be fulfilled. In this regard, SFN and PTN mathematical models, which satisfy all criteria successfully, are utilized as an objective function in optimization problems to maximize storage and loss moduli. The maximum storage modulus has been found as 2245.84 MPa, and the corresponding input parameters are $x_1$=2.80 and $x_2$=27.20, while the maximum loss modulus value has been found as 129.63 MPa and corresponding input parameters are $x_1$=1.90%, $x_2$=23.23%. Both the experimental results and the modeling-optimization results have shown that the hybrid structure consisting of polypropylene-artichoke stem particles-wollastonite minerals improves the dynamic-mechanical properties of the material by approximately 40% when it is used instead of raw polypropylene material.

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## AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

## DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

## CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

## ETHICS

There are no ethical issues with the publication of this manuscript.

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