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Manufacturing and Modeling of Polypropylene-based Hybrid Composites by Using Multiple-Nonlinear Regression Analysis

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Abstract

In this research, artichoke stem particles and wollastonite were used as organic and inorganic fillers in order to improve the mechanical properties of polypropylene. In this regard, PP-matrix composites containing AS and W were produced as non-hybrid and hybrid using a high-speed thermo-kinetic mixer. Mechanical properties of polymer composites were investigated by the tensile test. Experimental results reveal that the highest elastic modulus was obtained in PP-W, and the highest tensile strength was obtained in raw PP while the lowest ultimate strain value was obtained in PP-W-AS. Then, multiple-nonlinear regression analysis was employed to determine the effect of weight ratios of W and AS in PP on elastic modulus, tensile strength, and ultimate strain. Experimental results were expressed with polynomial, rational, and trigonometric models. The results show that the proposed models fit well with the experimental results. The coefficient of determination (R^2) values were found between 0.95 and 1 in all models. Also, boundedness check control of the proposed models, which gives information about whether models are realistic or not, was carried out by calculating the maximum and minimum values produced by the relevant model.

Keywords: hybrid polymer composites, multiple-nonlinear regression, boundedness check, modeling

1. Introduction

In recent decades, synthetic fibers have been replaced by lignocellulosic fibers in many industrial and daily applications. Automotive interior parts and non-structural building applications that do not require high strength and high thermal stability come to the forefront among these application areas. Researchers working on the development of polymer matrix composite materials demand to design and manufacture recyclable materials in order to minimize the effects of damage to the environment. In the production of thermoplastic matrix composite materials, lignocellulose based fibers such as kenaf, cotton, sisal, jute, ramie, sugar cane, coconut fiber are used together with thermoplastics in order to reduce the production cost and to minimize the damage to the environment (Rong et al., 2001; Saba et al., 2015; Sever et al., 2012; Verma & Gope, 2015; Xu et al., 2010). In addition, agricultural wastes such as vine stem, olive pomace, corn, wheat, rice, almond shell, and lignocellulose-rich corn cob were used as filling/reinforcement material (Essabir et al., 2013; Guimarães et al., 2009; Kaya et al., 2018; Kılınc et al., 2016; Mengeloglu & Karakus, 2008; Nourbakhsh & Ashori, 2010; Yao et al., 2008). Although such non-hybrid studies are widespread in the literature, the number of studies on agricultural waste and mineral-filled hybrid composites is limited. The use of hybrid structures aims to provide many essential features in engineering design, such as reducing material weight, increasing strength, reducing production costs, improving thermal properties, and ensuring easy recycling of materials (Mattos et al., 2014).

In the manufacturing of composites, lignocellulosic materials are used as filling/reinforcement materials, and thermoplastics such as polypropylene (PP), polyethylene (PE) and polylactic acid (PLA) are used as matrix materials. In scientific studies, it has been observed that the use of lignocellulosic materials using as filler/reinforcement with different matrix materials in the production of composites has increased significantly. Thermoplastic matrix material PP is one of the most important commercial polyolefins, and it has a wide range of uses from the automotive and aerospace industries to household plastic products. Various filling materials can be added to the matrix to provide the desired physical and mechanical properties and low cost. Lignocellulosic fillers and mineral fillers can be mixed into the thermoplastic polymer matrix as a hybrid form and can directly affect the composite materials' physical, mechanical, and thermal properties. Although the experiment is an important process to determine mechanical and physical properties of lignocellulose-based hybrid composites, it is worth noting that putting forward mathematical models that can correctly explain and verify the experimental results is a necessity that cannot be ignored. In this regard, Response Surface Method and ANOVA are frequently used together in the literature (Ashenai Ghasemi et al., 2016; Ayaz et al., 2018; Nor et al., 2021; Ragunath et al., 2021; Srivabut et al., 2021; Syed et al., 2020; Yiga et al., 2021). Supporting the experimental results with mathematical models makes it possible to create alternative designs, determine the effects of the design parameters correctly, and depending on these can be improved the obtained values of the response variables. In this respect, Syed et al. (2020) considered optimization of talc filled polypropylene material. In the study, a Taguchi-based multi-objective approach was used to maximize tensile strength and minimize shrinkage simultaneously. It was seen that selected as design parameters: injection pressure, injection speed, mold temperature, and melt temperature had a significant effect on tensile strength and shrinkage. As a result of the optimization process, the tensile strength was found as 24.40 MPa with 10% increment, and the shrinkage was found as 2.28% with a 30% reduction. Ghasemi et al. (2016) optimized tensile strength, tensile modulus, and impact resistance of polypropylene-based hybrid composites. In order to examine the effects of three design parameters loading ratios of talc, maleic anhydride grafted polypropylene (MAPP), and talc and exfoliated graphene nanoplatelets (xGnPs) fillers on mechanical properties, fifteen experiments were designed utilizing Box Behnken method. Researchers proposed second-order polynomial models with response surface methodology to determine the effects of design parameters on mechanical properties. It was shown that the talc and xGnP fillers ratios considerably affect the mechanical properties. They found that the desirable values of the design parameters to maximize mechanical properties simultaneously were 30 wt% for talc, 4 wt% for MAPP, and 0.69 wt% for xGnP. Yiga et al. (2021) conducted a study to enhance the tensile strength of fiber-reinforced PLA composites. Rice husk fiber and clay filler were employed as additive materials. The effects of five design factors, clay filler loading, rice husk variety, rice husk fiber loading, alkali type, and alkali concentration on tensile strength, were determined by variance analysis (ANOVA). Filler loading and fiber loading factors were found as the most significant model terms. In another study in which the response surface method came to the fore, the mechanical and physical properties of wood-plastic composites were mathematically modeled using linear and quadratic functions. The coefficient of determination (R^2) parameter was considered as a success criterion to evaluate the prediction performance of proposed models. It was found that the R^2 gets changing values between 0.86 and 0.99 for all models (Srivabut et al., 2021). The experimental investigation and mathematical modeling were carried out regarding the mechanical properties of sisal and glass fiber reinforced hybrid composite (Ragunath et al., 2021). Tensile and flexural strength results of material were modeled with second-order polynomial while impact strength results were predicted well fit by a linear model. Sisal and epoxy volume fraction was considered as design variables, and the effects of those parameters on mechanical properties were investigated. It was understood that while the sisal has the more important effect on tensile and impact strength results of hybrid composite, it hasn't a noticeable effect on flexural strength results. In the literature, it is seen that there are many studies regarding design, modeling, and optimization to improve the mechanical properties of recyclable hybrid composites. However, to evaluate the success of the models proposed in these studies, criteria such as R^2, R^2 adjusted, and R^2 predicted, which show the relationship between observed and predicted values, are taken into consideration. These criteria alone may not be sufficient to test the success of a model. In this context, Polatoğlu et al. (2020) came up with boundedness check as an additional success criterion to evaluate whether the proposed mathematical model is appropriate or not.

The present paper examined the production of AS and W-filled PP hybrid and non-hybrid composite materials. The elastic modulus, ultimate tensile strength, and strain of the composite materials were obtained by experimentally. Multiple-nonlinear regression analysis was used in the modeling of the experimental results. In this regard, polynomial, rational, trigonometric models and their performance in estimating observed values were compared with each other. It was shown that the R^2 success criterion was insufficient to describe experimental results accurately. As an additional criterion, the importance of boundedness check in model selection was emphasized.

2. Materials and Methods

In this work, lignocellulose-based artichoke stem particles (AS), mineral-based wollastonite (W), and AS-W as hybrid were used to improve the mechanical properties of polypropylene (Table 1). The PP-copolymer (PP, LG Chem M 1500, Korea) used in this study has a melt flow index of 16 g/10 min. (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 fruit plant field in Çiğli, İzmir. To make artichoke stems suitable for milling, stems were broken into small pieces then mill with a laboratory-type grinder. Later on, 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 (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 carried out to a laboratory-scale high-speed thermo-kinetic mixer and a laboratory-type heated-cooled hydraulic press (Gülnar Makina, Turkey). The mechanical properties (ultimate tensile strength, ultimate strain, and elastic modulus) of these materials were obtained using a tensile testing machine (Shimadzu AGS-X, 5 kN, Japan). Tests were carried out according to "ASTM D638-14 Standard Test Method for Tensile Properties of Plastics" (D20 Committee, n.d.). The cross-head speed was determined as 50 mm/min during the tensile test. The tests were repeated at least five times for each type of material produced to increase the sensitivity of the tests. Test results were determined according to the average values, taking into account the standard deviations. Table 1 shows the mixing ratios of the materials. The results signed with a star in Table 1 are taken from the literature (Sever & Yılmaz, 2020).

Table 1. The mixing ratios of the materials

Trial	Material	Wollastonite (wt %)	Artichoke stem (wt %)
1	PP*	0	0
2	PP-10AS*	0	10
3	PP-20AS*	0	20
4	PP-30AS*	0	30
5	PP-10W	10	0
6	PP-20W	20	0
7	PP-30W	30	0
8	PP-3W-7AS*	3	7
9	PP-7W-3AS*	7	3
10	PP-5W-5AS*	5	5
11	PP-10W-10AS	10	10
12	PP-14W-6AS	14	16
13	PP-6W-14AS	6	14
14	PP-15W-15AS	15	15
15	PP-21W-9AS	21	9
16	PP-9W-21AS	9	21

3. Regression Analysis

The researchers try to find the most appropriate models which correctly estimate the results obtained using experimental or numerical methods. Regression analysis is one of the statistical methods used for this purpose. There are distinct type of mathematical models to estimate relationship between independent and dependent parameters. Among these, models including only linear functional terms are appropriate for problems whose non-complex and having few independent variables. In case the relationship between parameters is nonlinear, a regression model consisting of advanced mathematical functions would be more suitable to many engineering processes (Aktaş

& Aydın, 2021). In the literature, the most commonly used criteria for evaluating model success is coefficient of determination. R^2 consists of two parameters that show the relationship between predicted-observed and observed-mean values and are named as the sum of square error and the total sum of square, respectively (Equation 1). The fact that the R^2 value is close to 1 indicates that the proposed mathematical model very well defines the phenomena.

$$SSE = \sum_{i=1}^{n}(x_i - \hat{x}_i)^2 \qquad SST = \sum_{i=1}^{n}(x_i - x_{mean})^2 \qquad R^2 = 1 - \frac{SSE}{SST} \tag{1}$$

where $x_i, , x_{mean,}\ \hat{x}_i\ and$ n show observed, mean, predicted values and the number of rows, respectively.

4. Results and Discussions

In this section, various regression models have been proposed for PP-based hybrid materials design. In the modeling phase, experimental data were produced within the scope of this study, and some (signed with star in Table 1) were obtained from the study conducted by Sever and Yılmaz (2020) were used. Considered PP-based hybrid composite includes artichoke stem and wollastonite as filler. First, the effect of the weight ratio of AS and W fillers regarding elastic modulus, ultimate tensile strength, and ultimate strain is investigated experimentally. After that, 12 distinct regression models with two parameters were tested in terms of fitting performance.

Figure 1 shows experimental results regarding the mechanical properties of PP-based non-hybrid and hybrid materials with different weight ratios of AS, W, and AS-W fillers. It is seen that the hybridization process negatively affected the strength performance of the PP material, where raw PP material gives the best results (22.34 MPa) in terms of ultimate strength. When the elastic modulus and strain results are evaluated, it can be said that while filling of PP with 30% W (PP-30W) provides the highest elastic modulus, hybridization of PP with 15% W and 15% AS (PP-15W-15AS) gives the lowest strain value.

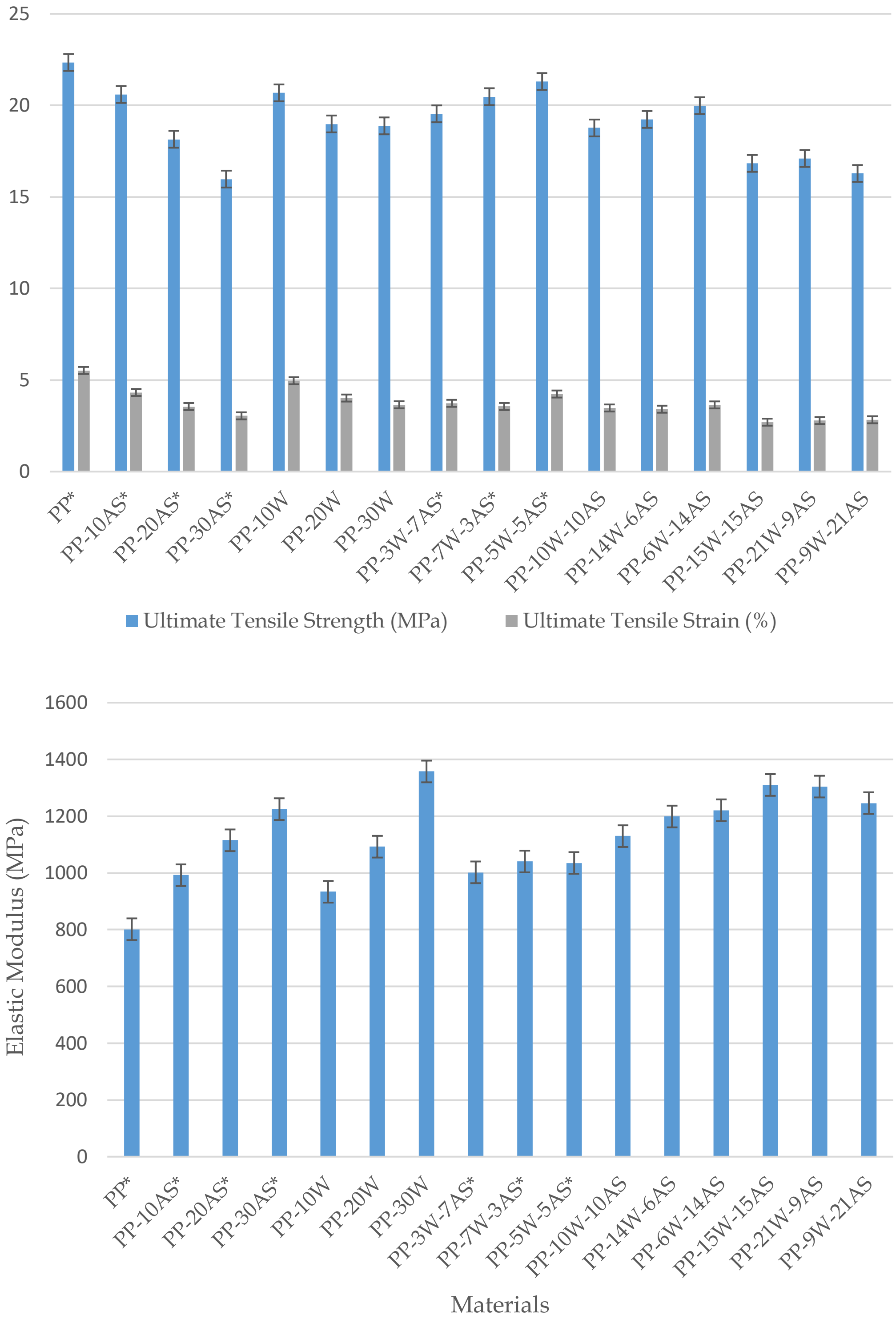

Figure 1. Mechanical properties of PP-based composite materials

In the modeling phase, multiple nonlinear regression analysis was used to describe phenomena mathematically regarding elastic behavior of PP-based hybrid composites given in Figure 1. Proposed four distinct models and their fitting performance was given in Tables 2 and 3.

Table 2. Multiple nonlinear mathematical models for elastic modulus

Name	Models
Third order multiple nonlinear (TON)	$Y = 801.6 + 24.73x_1 - 0.6392x_1^2 + 0.009467x_1^3 + 22.17x_2 + 1.198x_1x_2 - 0.04765x_1^2x_2 - 0.9281x_2^2 - 0.02881x_1x_2^2 + 0.02688x_2^3$
Fifth order multiple nonlinear (FION)	$Y = 801.6 + 23.04x_1 - 0.7127x_1^2 + 0.05279x_1^3 - 0.002737x_1^4 + 0.00004797x_1^5 + 16.36x_2 + 4.502x_1x_2 - 1.326x_1^2x_2 + 0.1346x_1^3x_2 - 0.003301x_1^4x_2 - 0.361x_2^2 + 0.8592x_1x_2^2 - 0.1052x_1^2x_2^2 + 0.0008965x_1^3x_2^2 - 0.01527x_2^3 - 0.04608x_1x_2^3 + 0.00385x_1^2x_2^3 + 0.002335x_2^4 + 0.0004718x_1x_2^4 - 0.00004482x_2^5$
Third order multiple nonlinear rational (TONR)	$Y = (17.83 + 783.4x_1 + 10036.\,x_1^2 - 196.1x_1^3 - 1283.\,x_2 - 14918.\,x_1x_2 + 171.3x_1^2x_2 - 1553.\,x_2^2 + 63.24x_1x_2^2 + 159.1x_2^3)/(0.02224 + 17.87x_1 + 8.242x_1^2 - 0.1809x_1^3 - 18.64x_2 - 15.91x_1x_2 + 0.2274x_1^2x_2 + 1.17x_2^2 + 0.1519x_1x_2^2 + 0.05974x_2^3)$
Third order trigonometric multiple nonlinear (TOTN)	$279.3 + 8.723\mathrm{Cos}(\mathrm{x}_1) + 298.9\mathrm{Cos}(\mathrm{x}_1)^2 - 2.066\mathrm{Cos}(\mathrm{x}_1)^3 + 13.81\mathrm{Cos}(\mathrm{x}_2) + 122.1\mathrm{Cos}(\mathrm{x}_1)\mathrm{Cos}(\mathrm{x}_2) - 88.45\mathrm{Cos}(\mathrm{x}_1)^2\mathrm{Cos}(\mathrm{x}_2) + 273.8\mathrm{Cos}(\mathrm{x}_2)^2 - 111.2\mathrm{Cos}(\mathrm{x}_1)\mathrm{Cos}(\mathrm{x}_2)^2 + 6.739\mathrm{Cos}(\mathrm{x}_2)^3 + 29.41\mathrm{Sin}(\mathrm{x}_1) + 169.9\mathrm{Cos}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_1) - 78.91\mathrm{Cos}(\mathrm{x}_1)^2\mathrm{Sin}(\mathrm{x}_1) - 187.3\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_1) - 49.58\mathrm{Cos}(\mathrm{x}_1)\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_1) + 26.5\mathrm{Cos}(\mathrm{x}_2)^2\mathrm{Sin}(\mathrm{x}_1) + 441.3\mathrm{Sin}(\mathrm{x}_1)^2 + 138.2\mathrm{Cos}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_1)^2 + 145.\,\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_1)^2 + 65.66\mathrm{Sin}(\mathrm{x}_1)^3 + 24.02\mathrm{Sin}(\mathrm{x}_2) - 218.3\mathrm{Cos}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2) + 25.03\mathrm{Cos}(\mathrm{x}_1)^2\mathrm{Sin}(\mathrm{x}_2) + 76.52\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_2) - 59.11\mathrm{Cos}(\mathrm{x}_1)\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_2) - 65.56\mathrm{Cos}(\mathrm{x}_2)^2\mathrm{Sin}(\mathrm{x}_2) + 72.17\mathrm{Sin}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2) - 355.3\mathrm{Cos}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2) - 322.2\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2) + 40.49\mathrm{Sin}(\mathrm{x}_1)^2\mathrm{Sin}(\mathrm{x}_2) + 487.3\mathrm{Sin}(\mathrm{x}_2)^2 + 157.6\mathrm{Cos}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2)^2 + 117.8\mathrm{Cos}(\mathrm{x}_2)\mathrm{Sin}(\mathrm{x}_2)^2 + 65.69\mathrm{Sin}(\mathrm{x}_1)\mathrm{Sin}(\mathrm{x}_2)^2 + 53.88\mathrm{Sin}(\mathrm{x}_2)^3$

Table 3 denotes the fitting and boundedness performance of mathematical models used to estimate the elastic behavior of PP-based hybrid composites. The most crucial parameter showing the usability of a mathematical model in the literature is the value of R^2. When the results are examined, it will be seen that except that “TON” R^2 values of all models are 1. If we made a model selection considering only the R^2 value, we could think that all the models explain the process well. However, R^2 alone does not correctly define the phenomena of the process. Further, boundedness check control of the proposed models, which gives information about whether models are realistic or not should be carried out. We can see if there is a functional limitation (bounded) by calculating the maximum and minimum values produced by the relevant model.

Table 3. Fitting performance and boundedness of models for elastic modulus

Model	R^2	Max.	Min.
TON	0.97	1357.23	801.6
FION	1	1399.29	801.6
TONR	1	2194.14	-31020
TOTN	1	1653.29	377.42

In this context, it has been accepted that the results of polynomial models "FION" and "TON" are suitable for the nature of the problem by expert researchers in production and material selection. However, the view that models "TONR" and "TOTN" give results that cannot be obtained experimentally came to the fore.

Figure 2 represents the 3D plot of polynomial, rational and trigonometric models that best fit the experimental results. When the graphics are examined, it is seen that the models accurately predict all the experimental data. However, as stated when evaluating the results of Table 3, a high R^2 value does not always give accurate information about the usability of the proposed model. Whether the mathematical model gives correct information should be checked with criteria other than R^2. In problems where the number of design variables is one or two, an evaluation can be made by graphically examining the model's results. Since the weight ratios of artichoke stem particles and wollastonite filler are selected as two design variables in this study, it is possible to evaluate the mathematical models graphically. Here, rational and trigonometric models ("TONR" and "TOTN") have many local maximum and minimum points, which insignificant changes in design parameters lead to a non-negligible difference in results. On the contrary, polynomial models ("FION" and "TON") show a stable and consistent distribution within the specified range of design parameters. Therefore, these models are appropriate to estimate mathematical phenomena regarding the elastic modulus of PP-based hybrid composite.

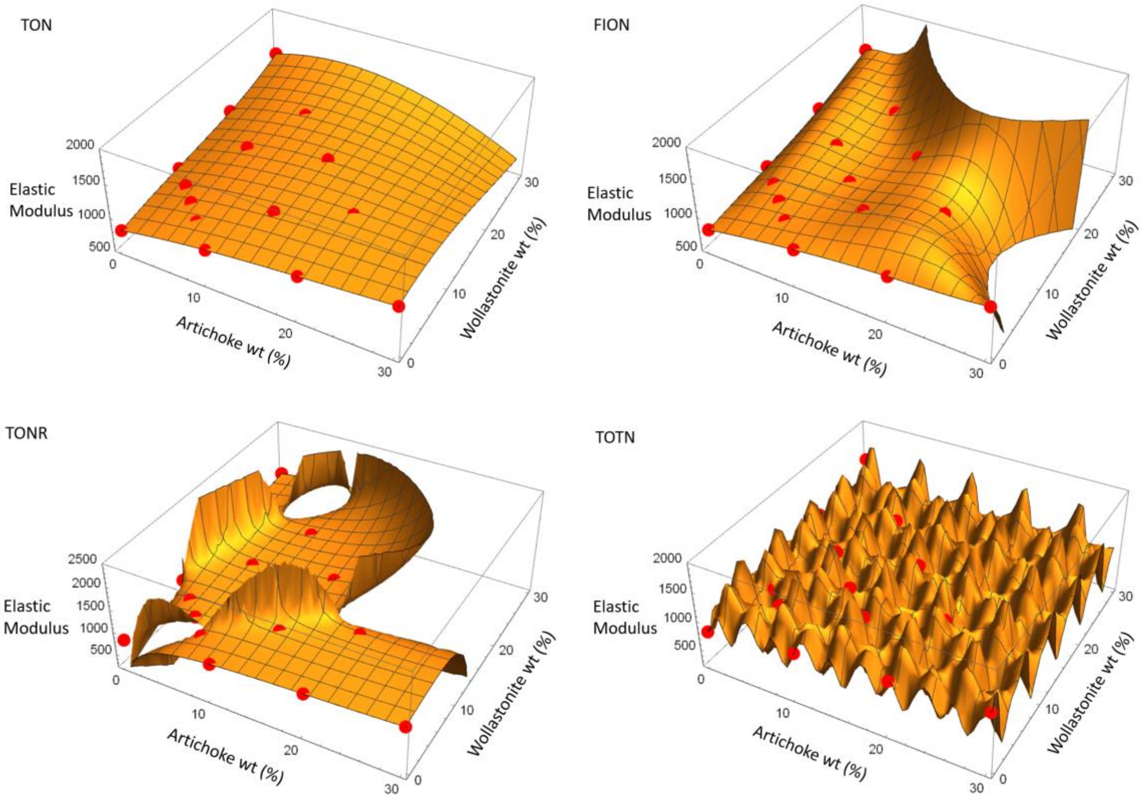

Figure 2. 3D plot representations of experimental data and recommended mathematical model for elastic modulus

Another mechanical parameter modeling with regression analysis was ultimate tensile strength. Four distinct mathematical models and their fitting performance were given in Tables 4 and 5.

Table 4. Mathematical models for ultimate tensile strength

Name	Models
Third order multiple nonlinear (TON)	$Y = 22.34 - 0.2984x_1 + 0.01022x_1^2 - 0.0002481x_1^3 - 0.1546x_2 + 0.02779x_1x_2 - 0.001013x_1^2x_2 - 0.004468x_2^2 - 0.0008286x_1x_2^2 + 0.0001926x_2^3$
Sixth order multiple nonlinear (SON)	$Y = 22.34 - 0.1237x_1 - 0.01134x_1^2 + 0.00002776x_1^3 + 0.0001375x_1^4 - (9.586 \times 10^{-6})x_1^5 + (1.76 \times 10^{-7})x_1^6 - 0.09966x_2 + 0.02216x_1x_2 - 0.01042x_1^2x_2 - 0.01065x_1^3x_2 + 0.0009603x_1^4x_2 - 0.00002011x_1^5x_2 - 0.008408x_2^2 + 0.01434x_1x_2^2 + 0.0215x_1^2x_2^2 - 0.0009108x_1^3x_2^2 - (1.304 \times 10^{-7})x_1^4x_2^2 - 0.0007965x_2^3 - 0.01181x_1x_2^3 - 0.0009454x_1^2x_2^3 + 0.00003689x_1^3x_2^3 + 0.0001704x_2^4 + 0.000916x_1x_2^4 + (2.702 \times 10^{-6})x_1^2x_2^4 - (8.699 \times 10^{-6})x_2^5 - 0.00001807x_1x_2^5 + (1.399 \times 10^{-7})x_2^6$
Second order multiple nonlinear rational (SONR)	$Y = (3141.8 - 51.011x_1 - 0.94323x_1^2 - 118.64x_2 - 2.0546x_1x_2 + 0.1594x_2^2)/(140.62 - 0.81531x_1 - 0.076061x_1^2 - 4.1694x_2 - 0.19421x_1x_2 - 0.033376x_2^2)$
Third order trigonometric multiple nonlinear (TOTN)	$Y = 4.622 + 0.7108\mathrm{Cos}(x_1) + 6.661\mathrm{Cos}(x_1)^2 + 1.155\mathrm{Cos}(x_1)^3 + 0.7972\mathrm{Cos}(x_2) - 1.973\mathrm{Cos}(x_1)\mathrm{Cos}(x_2) + 1.73\mathrm{Cos}(x_1)^2\mathrm{Cos}(x_2) + 6.162\mathrm{Cos}(x_2)^2 + 1.341\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)^2 + 1.134\mathrm{Cos}(x_2)^3 + 0.2348\mathrm{Sin}(x_1) + 2.5\mathrm{Cos}(x_1)\mathrm{Sin}(x_1) - 1.035\mathrm{Cos}(x_1)^2\mathrm{Sin}(x_1) - 1.444\mathrm{Cos}(x_2)\mathrm{Sin}(x_1) - 1.021\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)\mathrm{Sin}(x_1) + 1.34\mathrm{Cos}(x_2)^2\mathrm{Sin}(x_1) + 4.167\mathrm{Sin}(x_1)^2 - 2.086\mathrm{Cos}(x_1)\mathrm{Sin}(x_1)^2 + 0.2159\mathrm{Cos}(x_2)\mathrm{Sin}(x_1)^2 + 0.6172\mathrm{Sin}(x_1)^3 + 0.001065\mathrm{Sin}(x_2) - 2.13\mathrm{Cos}(x_1)\mathrm{Sin}(x_2) + 1.414\mathrm{Cos}(x_1)^2\mathrm{Sin}(x_2) + 1.698\mathrm{Cos}(x_2)\mathrm{Sin}(x_2) - 0.2111\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)\mathrm{Sin}(x_2) - 1.467\mathrm{Cos}(x_2)^2\mathrm{Sin}(x_2) + 5.109\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 8.071\mathrm{Cos}(x_1)\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 9.091\mathrm{Cos}(x_2)\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 5.494\mathrm{Sin}(x_1)^2\mathrm{Sin}(x_2) + 5.08\mathrm{Sin}(x_2)^2 + 0.4327\mathrm{Cos}(x_1)\mathrm{Sin}(x_2)^2 - 0.7113\mathrm{Cos}(x_2)\mathrm{Sin}(x_2)^2 - 3.866\mathrm{Sin}(x_1)\mathrm{Sin}(x_2)^2 + 0.3384\mathrm{Sin}(x_2)^3$

Table 5 denotes the fitting and boundedness performance of mathematical models using to estimate ultimate tensile strength (UTS) of PP-based hybrid composites. According to results, sixth-order polynomial, second-order rational, and third-order trigonometric models show the best fitting performance in terms of R^2. However, rational and trigonometric models contain maximum and minimum values that cannot be encountered in practice. For this problem, ultimate tensile strength, which gives information about the material's resistance under tensile loading does not get a negative value. In addition to this, experimental results display that the minimum value of UTS is obtained as 16 MPa. Namely, the minimum strength value (7.38 MPa) obtained by model "SON" does not seem realistic. Because of all these reasons, the third-order multiple nonlinear model ("TON"), which has a more straightforward structure and produces more realistic values, is recommended in PP-based hybrid composite material design where strength is considered an important parameter.

Table 5. Fitting performance and boundedness of models for ultimate tensile strength

Model	R²	Max.	Min.
TON	0.95	22.14	15.89
SON	1	30.66	7.38
SONR	1	22.34	-15.06
TOTN	1	28.98	-0.31

Figure 3 demonstrates a 3D plot of polynomial, rational and trigonometric models that best fit the experimental results concerning ultimate tensile strength. As mentioned above, graphical demonstration gives an essential idea to us concerning mathematical model selection. The rational model, which has many discontinuities and extreme values, is not suitable for expressing strength mathematically. It is decided that although the trigonometric model shows well fit with the experimental results, it is not a suitable model taking into account expert opinions. For similar reasons, "SON" model cannot be used either. In this regard, it can be said that the third order polynomial model is the most appropriate model that gives realistic results.

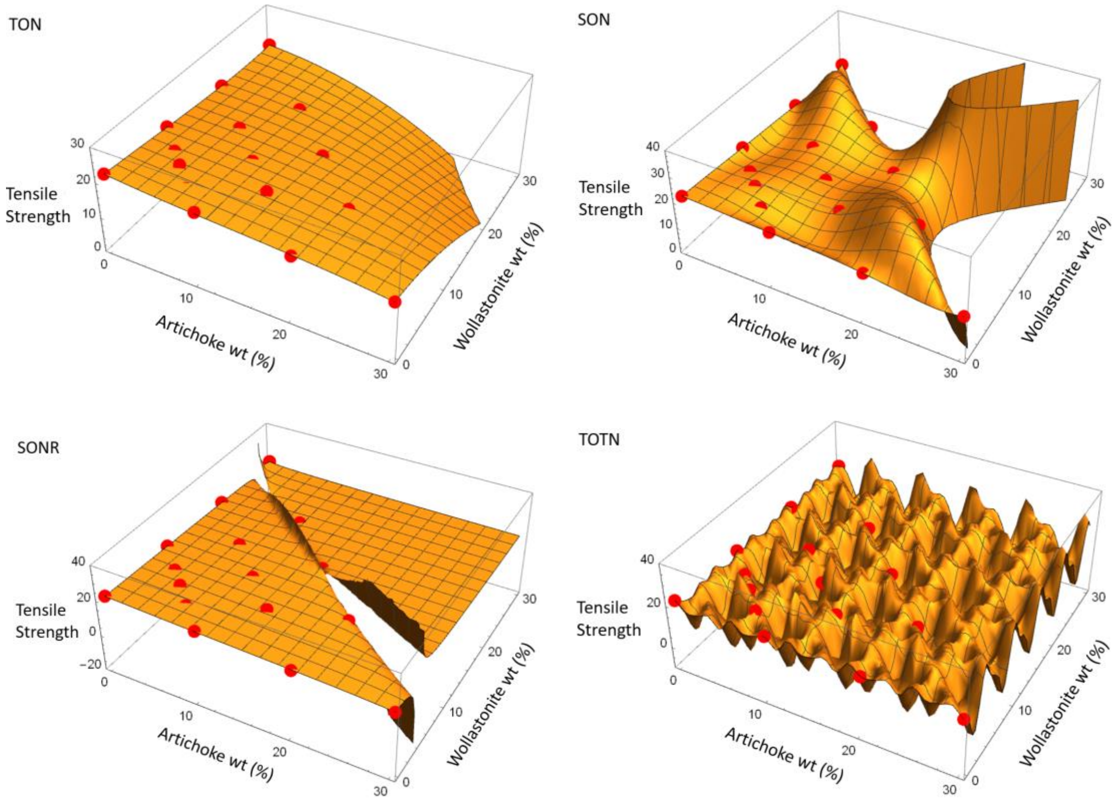

Figure 3. 3D plot representations of experimental data and recommended mathematical model for ultimate tensile strength

In order to define physical phenomena regarding the ultimate strain of PP-based hybrid composites, alternative four distinct mathematical models were given in Table 6.

Table 6. Mathematical Models for Ultimate Strain

Name	Models
Fourth order multiple nonlinear (FON)	$Y = 5.52 - 0.1943x_1 + 0.01213x_1^2 - 0.0005466x_1^3 + (8.891 \times 10^{-6})x_1^4 - 0.1006x_2 - 0.07173x_1x_2 + 0.006727x_1^2x_2 - 0.0001407x_1^3x_2 + 0.008007x_2^2 + 0.004726x_1x_2^2 - 0.0002343x_1^2x_2^2 - 0.000555x_2^3 - 0.00007394x_1x_2^3 + 0.00001102x_2^4$
Sixth order multiple nonlinear (SON)	$Y = 5.52 - 0.1422x_1 + 0.00196x_1^2 - 0.0004241x_1^3 + 0.00008384x_1^4 - (4.667 \times 10^{-6})x_1^5 + (7.816 \times 10^{-8})x_1^6 - 0.05474x_2 - 0.02993x_1x_2 + 0.007392x_1^2x_2 - 0.006162x_1^3x_2 + 0.0004825x_1^4x_2 - (9.539 \times 10^{-6})x_1^5x_2 - 0.001292x_2^2 - 0.002668x_1x_2^2 + 0.01165x_1^2x_2^2 - 0.0004904x_1^3x_2^2 + (8.529 \times 10^{-7})x_1^4x_2^2 - 0.0001888x_2^3 - 0.005781x_1x_2^3 - 0.0004778x_1^2x_2^3 + 0.00001849x_1^3x_2^3 + 0.00007167x_2^4 + 0.0004986x_1x_2^4 - (4.091 \times 10^{-8})x_1^2x_2^4 - (4.948 \times 10^{-6})x_2^5 - 0.00001018x_1x_2^5 + (9.358 \times 10^{-8})x_2^6$
Third order multiple nonlinear rational (TONR)	$Y = (-282.1 - 19300.x_1 - 51008.x_1^2 + 1498.x_1^3 - 22910.x_2 + 88659.x_1x_2 + 4026.x_1^2x_2 - 51201.x_2^2 - 839.8x_1x_2^2 + 4221.x_2^3)/(-51.15 + 40204.x_1 - 17431.x_1^2 + 463.2x_1^3 + 73167.x_2 - 3229.x_1x_2 + 2132.x_1^2x_2 - 23464.x_2^2 + 1371.x_1x_2^2 + 1388.x_2^3)$
Third order trigonometric multiple nonlinear (TOTN)	$Y = 0.921 + 0.2069\mathrm{Cos}(x_1) + 1.408\mathrm{Cos}(x_1)^2 + 0.3694\mathrm{Cos}(x_1)^3 + 0.1811\mathrm{Cos}(x_2) - 0.3544\mathrm{Cos}(x_1)\mathrm{Cos}(x_2) + 0.5762\mathrm{Cos}(x_1)^2\mathrm{Cos}(x_2) + 1.342\mathrm{Cos}(x_2)^2 + 0.5977\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)^2 + 0.2719\mathrm{Cos}(x_2)^3 + 0.03054\mathrm{Sin}(x_1) + 0.5365\mathrm{Cos}(x_1)\mathrm{Sin}(x_1) - 0.406\mathrm{Cos}(x_1)^2\mathrm{Sin}(x_1) - 0.3352\mathrm{Cos}(x_2)\mathrm{Sin}(x_1) + 0.005495\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)\mathrm{Sin}(x_1) + 0.237\mathrm{Cos}(x_2)^2\mathrm{Sin}(x_1) + 0.6831\mathrm{Sin}(x_1)^2 - 0.9424\mathrm{Cos}(x_1)\mathrm{Sin}(x_1)^2 - 0.1696\mathrm{Cos}(x_2)\mathrm{Sin}(x_1)^2 + 0.1425\mathrm{Sin}(x_1)^3 - 0.05898\mathrm{Sin}(x_2) - 0.4338\mathrm{Cos}(x_1)\mathrm{Sin}(x_2) + 0.2482\mathrm{Cos}(x_1)^2\mathrm{Sin}(x_2) + 0.6653\mathrm{Cos}(x_2)\mathrm{Sin}(x_2) + 0.4743\mathrm{Cos}(x_1)\mathrm{Cos}(x_2)\mathrm{Sin}(x_2) - 0.7262\mathrm{Cos}(x_2)^2\mathrm{Sin}(x_2) + 1.119\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 0.7263\mathrm{Cos}(x_1)\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 1.424\mathrm{Cos}(x_2)\mathrm{Sin}(x_1)\mathrm{Sin}(x_2) - 1.304\mathrm{Sin}(x_1)^2\mathrm{Sin}(x_2) + 0.803\mathrm{Sin}(x_2)^2 - 0.1215\mathrm{Cos}(x_1)\mathrm{Sin}(x_2)^2 - 0.3062\mathrm{Cos}(x_2)\mathrm{Sin}(x_2)^2 - 0.7467\mathrm{Sin}(x_1)\mathrm{Sin}(x_2)^2 + 0.07127\mathrm{Sin}(x_2)^3$

Table 7 denotes the fitting and boundedness performance of mathematical models using to estimate the ultimate strain of PP-based hybrid composites. Although it has a lower R^2 value as in models expressing elastic modulus and ultimate strength, the fourth-order polynomial model is the most appropriate model to explain the experimental results related to strain. Graphical representation in Figure 4 supports this idea.

Table 7. Fitting performance and boundedness of models for ultimate strain

Model	R^2	Max.	Min.
FON	0.95	5.52	2.70
SON	1	9.01	-0.53
TONR	1	36.58	-16.92
TOTN	1	5.82	-0.46

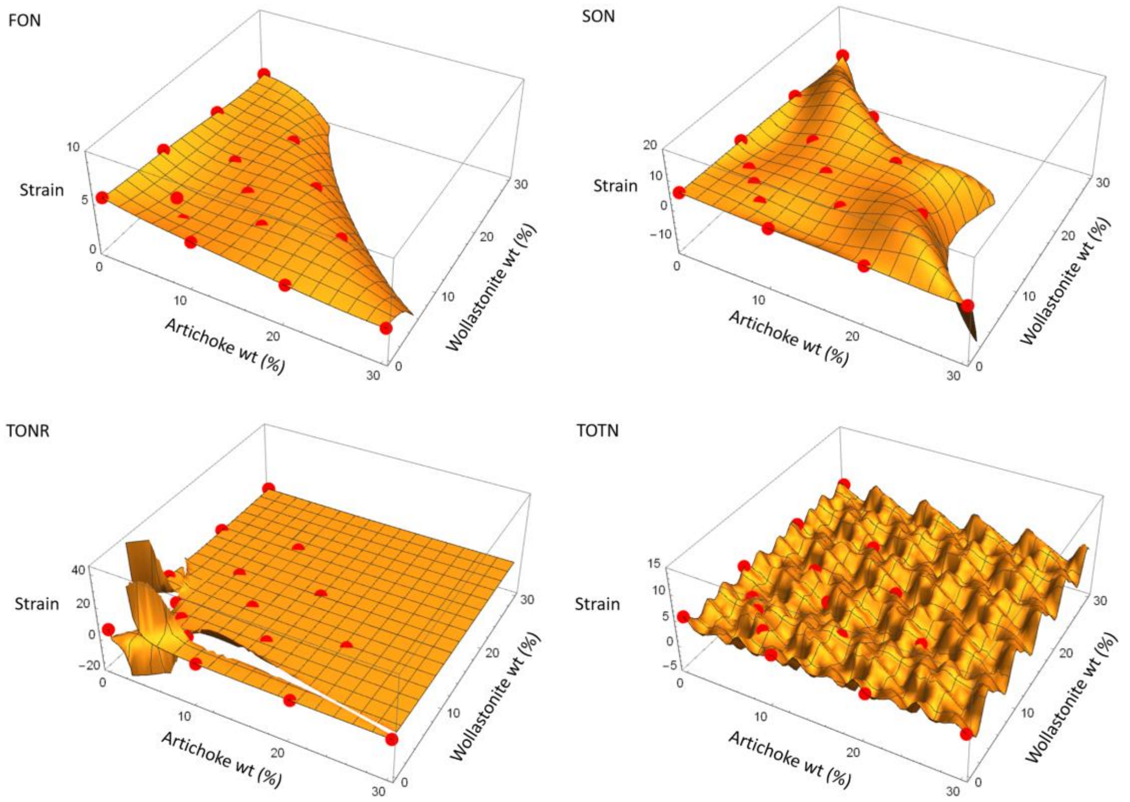

Figure 4. 3D plot representations of experimental data and recommended mathematical model for ultimate strain

5. Conclusions

In this study, artichoke stem particles and wollastonite were used as organic and inorganic fillers in order to improve the mechanical properties of polypropylene (PP). PP-based hybrid composites, including different proportions of artichoke stem particles and wollastonite, were mathematically modeled using the data regarding elastic modulus, ultimate strength, and strain obtained from the experimental study. The most critical parameter showing the usability of a mathematical model in the literature is the value of R^2. In this study, the primary purpose is to show that it is always possible to create a model with an R^2 value of 1. In this regard, 12 different polynomials, rational and trigonometric nonlinear models whose R^2 value is equal to 1 are given. However, a high value of R^2 itself does not always mean a good fit, and it does not define the entire physical phenomena of the engineering process. Graphically results given in the study denote that R^2 is not enough standalone criterion to evaluate the mathematical models. It has been specified that other criteria are needed to evaluate the models. It is impossible to obtain a realistic functional structure in cases where models are not examined in terms of stability. To overcome this drawback, by inspecting the boundedness of each candidate model the functions that produce value only within the physical limits have been admitted as successful. In the light of these evaluations, it was seen that only polynomial models fulfill the necessary success criteria.

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Author Statement

The authors confirm contribution to the paper as follows: study conception and design: Melih Savran; data collection: Mustafa Öncül, Kutlay Sever and Muhammed Yılmaz; analysis and interpretation of results: Kutlay Sever, Melih Savran, Mustafa Öncül, Muhammed Yılmaz; draft manuscript preparation: Melih Savran and Mustafa Öncül. All authors reviewed the results and approved the final version of the manuscript.

Conflict of Interest

The authors declare no conflict of interest.

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