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A New Evaluation Criterion for Optimizing the Mechanical Properties of Toughened Polypropylene/Silica Nanocomposites

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Abstract This study aims to experiment with the mechanical properties of polypropylene (PP)/thermoplastic elastomer/nano-silica/compatibilizer nanocomposite using the melt mixing method. The addition of polyolefin elastomers has proved to be an approachable solution for low impact strength of PP, while it would also reduce the Young's modulus and tensile strength. That is why reinforcement would be applied to this combination to enhance the elastic modulus. The mechanical properties of the prepared composites were devised to train an artificial neural network to predict these properties of the system in 6256 unknown points. Therefore, the sensitivity analysis was performed and the share of each input parameter on the respective output values was calculated. Additionally, a novel parameter called nanocomposite evaluation criterion (NEC) is introduced to analyze the suitability of the nanocomposites considering the mechanical properties. Accordingly, the formulation with optimal mechanical properties of toughness, elongation at break, tensile strength, Young's modulus, and impact strength was obtained.

Keywords Nanocomposite; Polypropylene (PP); Silica; Artificial neural networks; Nanocomposite evaluation criterion (NEC); Sensitivity analysis

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INTRODUCTION

Nowadays, the usage of polypropylene (PP), which is a cost-effective polymer, is widespread due to its easy reactivity, recycling, and appropriate mechanical properties and thermal stability.^[1] PP has been used as the base material to make lightweight automotive parts, in addition to its large application in civil structures as industrial plastics.^[2] Although this thermoplastic enjoys large applications in different industries, it suffers from low toughness and impact resistance.^[3]

Therefore, concentrated efforts are made to improve the toughness and impact resistance of PP. Previous investigations have tried to ameliorate the mechanical properties using different reinforcing materials.^[4,5] Generally, the composition of PP with different kinds of elastomers such as thermoplastic styrenic block copolymers (TPS),^[6] thermoplastic polyolefin (TPO),^[7] and thermoplastic polyurethane (TPU)^[8] has proved to be practical by enhancing the impact resistance considerably. Herein, although TPOs have shown promising results in combination with PP, their nanocomposites have not been widely investigated in the literature.

Previous studies have shown that the addition of elastomers leads to a corresponding reduction in the elastic modulus and tensile stress.^[9] Bajsić *et al.*^[10] showed that the addi-

tion of 20% TPU to PP would increase the strain of failure up to 100% while decreasing the elastic modulus of the composite up to 70%. Fasihi *et al.*^[11] also investigated the effects of two different kinds of thermoplastic elastomer (TPE) on impact resistance and tensile properties of PP. The results indicated that the addition of 20% TPE to PP would enhance the impact resistance 12 times higher than PP, although reducing the modulus about 40%. It is noteworthy to mention that different types of TPE are able to reduce the modulus and tensile strength even more than 50%.^[12]

To enhance the elastic modulus of the composition, addition of nanoparticles is among the most efficient methods for improving the mechanical properties.^[13] Sahraeian *et al.*^[14] and Davachi *et al.*^[15] both showed the positive effect of nanoparticles of perlite on the thermomechanical properties of nanocomposites. Herein, nano-silica, which has widespread biomedical and industrial applications, is proved to be an appropriate candidate to improve the mechanical properties of PP.^[16,17] The addition of 5% nano-silica nanoparticles to PP would increase the Young's modulus of PP up to 40%.^[18] However, these nanoparticles would also decrease the strain of failure and the impact strength.^[19] Overall, although the addition of nano-silica would increase the Young's modulus and sometimes the tensile strength, it reduces the toughness and the impact strength. The rigid nature of nanoparticles and the poor compatibility between nano-silica and PP are the reasons for this reduction in impact strength.^[20] Therefore, many researchers have benefited from the positive ef-

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fects of compatibilizers to improve the coarse and unstable phase morphologies of the nano-silica and PP composites.

Compatibilizers can improve the compatibility of immiscible blends by the creation of interactions between them.^[21] A common method for improving the dispersion of nanoparticles in the nanocomposites is to use compatibilizing agents.^[22] Among the existing compatibilizers, polypropylene-grafted-maleic anhydride (PP-g-MA) has shown promising results in different applications.^[23] Bikiaris *et al.*^[24] investigated the usage of PP-g-MA in the propylene/nano-silica nanocomposites. Results indicated that the addition of 6% nano-silica in the presence of PP-g-MA has a minor positive effect on the tensile strength of nanocomposite. However, higher amounts of these nanoparticles would act negatively on the tensile strength and lead to the reduction of this parameter. In these nanocomposites, maleic anhydride (MA) can react with the hydroxyl groups of nano-silica to create covalent bonds.^[25] In other words, these copolymers can decrease the interfacial tension, and reduce the size of the phase-separated particles in the blend to enhance the stability. In most of the nanocomposites, the lack of compatibilizer creates agglomerations of nanoparticles. To the best knowledge of the authors, there is not any investigation evaluating the mechanical properties of the PP/TPO/nano-silica/PP-g-MA nanocomposite, and this can be a proper subject to be analyzed.

Artificial neural networks (ANN) are known as a powerful tool to model complicated and non-linear systems.^[26,27] These networks can simply create a logical relation between the input and output parameters to be used instead of simulations or experiments. In this regard, researchers can easily reduce their efforts to run multiple experiments or simulations, although some data would be needed to train ANN. For instance, Pourrahmani *et al.*^[28–30] used these networks to predict the thermal characteristics of a fuel cell. Nazari and Riahi^[31] also used ANN to predict the split tensile strength and water permeability of concrete with eight input parameters, while Camara *et al.*^[32] utilized the same procedure to model the elasticity modulus. The integration of the ANN models with optimization algorithms such as genetic algorithm (GA)^[33,34] would also calculate the optimum values of the system. However, sensitivity analysis can be used instead of optimization algorithms to calculate optimum values. In this manner, a new parameter would be defined, using the sensitivity analysis, to evaluate the appropriateness of nanocomposites.

In the training of ANN, weight vectors establish a relation between the input and output parameters. The utilization of the sensitivity analysis would determine the values of those weight vectors. Herein, Saleeb *et al.*^[35] also utilized this analysis to estimate the corresponding parameters of an anisotropic composite.

In this work, the positive effects of adding elastomers and nanoparticles to improve the toughness and impact strength of PP are investigated. The compatibilizer is also added to improve the compatibility between nano-silica and PP while preventing the agglomeration of nanoparticles. The experiments on the mechanical properties of PP/TPO/nano-silica/PP-g-MA nanocomposite, which is made by melt mixing method, are performed in 15 different cases in addition to measuring the characteristics of neat PP. After that, the mech-

anical properties of these 16 cases were utilized to train an ANN model to predict the system in 6256 points with different input parameters (the percentages of PP, TPO, nano-silica, and PP-g-MA). Then, sensitivity analysis was performed to obtain the impacts of each input parameter on the respective output value. Additionally, this analysis was used to calculate a novel parameter to predict the suitability of the nanocomposite based on mechanical properties. This parameter is not dedicated to a special problem and it can be used for different nanocomposites having mechanical properties such as toughness, elongation at break, tensile strength, Young's modulus, and impact strength.

METHODOLOGY

Materials

In the current study, the polymer matrix was polypropylene (PP) with the commercial name of RG 1102G, a product of Rejal Petrochemical Company. The utilized compatibilizer was polypropylene-grafted-maleic anhydride (PP-g-MA) produced by Kara Negin Co., with the industrial name of KARABOND A-100. The powder nano-silica (AEROSIL® 200) with the specific area of $200 \pm 25 \text{ m}^2/\text{g}$ was also provided by Degussa Co. in Germany, while the polyolefin elastomer was produced by ExxonMobil company with the commercial name of Vistamaxx 6102. It is noteworthy to mention that the utilized elastomer is a kind of thermoplastic elastomer and it is mentioned as TPE throughout the text.

Method of Experiment

In this study, 15 different cases of PP, nano-silica, elastomer, and compatibilizer in addition to neat PP were selected to perform the experiments. In this regard, the respective shares of input parameters became mixed together in the Brabender melt mixing device to produce the nanocomposite. The mixing temperature was 190 °C in the rotor speed of 80 r/min considering 15 min for the mixing time. Then, the samples were molded in the hot press device by the temperature of 220 °C and pressure of 15 MPa. The neat PP was also provided to run the test in a similar manner.

Characterizations

SANTAM STM-150 UNIVERSAL measured tensile properties of the samples with a crosshead speed of 50 mm/min based on ASTM D638. For each formulation, at least three replicates were subjected to test. The notched-Izod impact test was also performed according to ADST D256 with a notch depth of 2.5-mm on the specimens. For morphology studies, the samples were frozen in liquid nitrogen to make it brittle and quickly broken. Then SEM images were taken from the surface after surface coating of samples with gold using a scanning electron microscope (TESCAN, VEGA II) made in the Czech Republic.

Problem Description

In the first step of this research, 15 different shares of polypropylene, polyolefin elastomer, nano-silica nanoparticles, and polypropylene grafted maleic anhydride were considered to obtain the mechanical properties of the created nanocomposite. Additionally, neat PP was also experimented to evaluate the positive effects of the mentioned additives. The experiments became evaluated through a scanning electron microscope (SEM). Then, the calculated mechanical properties of the crea-

ted nanocomposite were utilized to train an artificial neural network (ANN). This ANN model can predict the mechanical properties of the system in the cases, which they have not experimented. Therefore, a large amount of data was produced to perform sensitivity analysis and optimization. The sensitivity analysis revealed the impact of each input parameter on the respective mechanical property. Additionally, it contributed to the determination of a new parameter called nanocomposite evaluation criterion (NEC), which can analyse the appropriateness of the nanocomposite. This parameter does not belong to a specific problem and it can be used for different nanocomposites with different base materials (PP in the current study). Using this parameter, there would be a single objective to optimize the system. Therefore, the optimum shares of input parameters to reach the highest NEC were determined and presented.

ANN Modeling Procedure

Artificial neural networks (ANN) are renowned to model complicated systems. Usually, these networks can predict the behavior of the system when simulation or experiment is not possible. In the current investigation, training, validation, and testing of the ANN achieved using 16 different cases of experimental data. It is noteworthy to mention that each case has five different outputs (toughness (TO), elongation at break (EB), tensile strength (TS), Young's modulus (YM), and impact strength (IS)), while the input parameters are the percentages of PP, TPE, nano-silica, and PP-g-MA. Herein, training (using the Levenberg-Marquardt algorithm) becomes possible by the usage of twelve cases, while two cases are dedicated to each of the validation and testing. In the current analysis, as the number of data samples is not high enough, the main aim is to provide the enough input data samples to train the model. However, both validation and testing are necessary and it cannot be done by only one data for each of them. Therefore, it was decided to dedicate two data samples for each of them and use the remaining data (12 data samples) for training of the model. It is noteworthy to mention that the numbers of utilized neurons and the hidden layers are both equal to nine. Typically, the numbers of neurons and hidden layers are different in every problem with different numbers of data samples. The determination of number of hidden layers is the most critical part in the ANN modeling since the low values of them would not be able to fit the right model, while the high number of them would result in overfitting. In the current analysis, the suitable number of hidden layers is determined using the mean squared error (MSE) as follows:

$$MSE = \frac{1}{N} \sum_{i=1}^N (Y_{ANN} - Y_{Experiment})^2 \quad (1)$$

where, N is the total number of samples and Y is the response of the system. This error parameter is used to evaluate 400 neural networks with different initial weights and biases, which were trained for different numbers of hidden layers from 5 to 14. Fig. 1 illustrates the minimum MSE for each number of hidden layers, which shows a neural network with 9 hidden layers as the best option for the ANN modeling of the current data samples.

In each ANN model, weight vectors provide a logical relationship between the input and output parameters. The aim

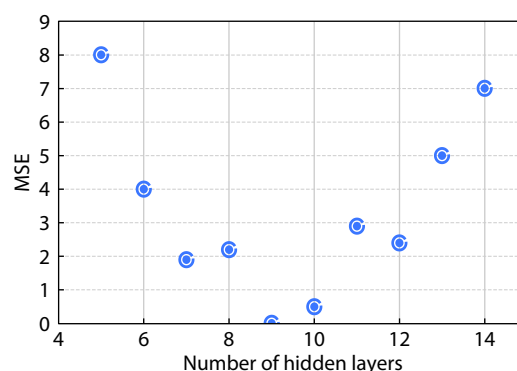


Fig. 1 The minimum values of MSE for different numbers of hidden layers.

of utilizing sensitivity analysis is to calculate these weight vectors. Therefore, the regression diagram would validate both ANN model and sensitivity analysis. To prevent repetition, the needed equations and concepts of ANN model and sensitivity analysis are referred to the previous publications of the same author.^[28–30] The application of sensitivity analysis in the current investigation has two major outputs. First, finding the impact of four input parameters of PP, TPE, nano-silica, and PP-g-MA on the corresponding values of TO, EB, TS, YM, and IS of the created nanocomposite. Second, finding the suitable exponents of the new parameter called nanocomposite evaluation criterion (NEC). Additionally, Fig. 2 shows the flowchart of ANN modeling and sensitivity analysis. In the current work, the sensitivity analysis becomes possible through the calculation of ANN model's weight vectors. The required algorithm to calculate these vectors is also published in the previous article of the author.^[28]

Fig. 3 shows the regression values of the trained ANN model. Based on this figure, the trained ANN model can predict the system with high accuracy, as the regression values are near to unity. It is noteworthy to mention that the mentioned 16 cases of experimental cases are the target values, while the predicted data by the ANN are the output values.

RESULTS AND DISCUSSION

In the first step of the investigation, 15 different cases of input parameters in addition to the base case of PP should be determined to perform the experiments. The focus of the current article is to consider the necessary data to train the artificial neural network and to perform the optimization and sensitivity analysis. Table 1 presents the nanocomposite's input parameters, from which their mechanical properties would be calculated. Afterward, Table 2 demonstrates the output results of the experiments in the mentioned cases. The results are compatible with previous assumptions, and approve the suitability of the elastomer to enhance the toughness and impact strength, while nano-silica would increase Young's modulus.

Additionally, scanning electron microscopy (SEM) is utilized to evaluate the distribution quality of the elastomer and nano-silica particles (Fig. 4). The images indicate the acceptable quality of distribution by the presence of compatibilizer, and in this condition, the size of nanoparticles is approximately 40 nm to 90 nm. Fig. 4 also illustrates that the diameter

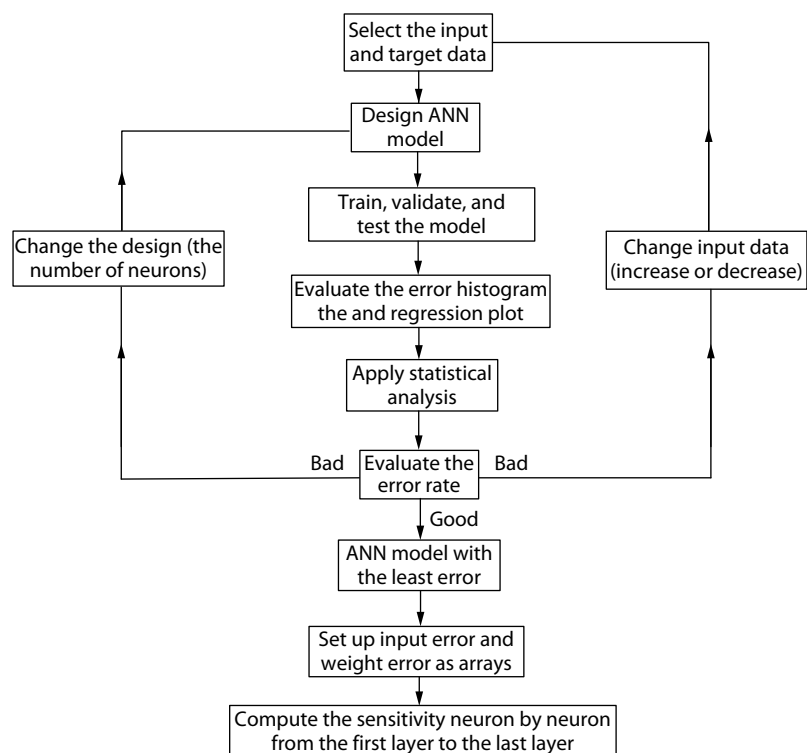


Fig. 2 The flowchart of ANN modeling and sensitivity analysis.

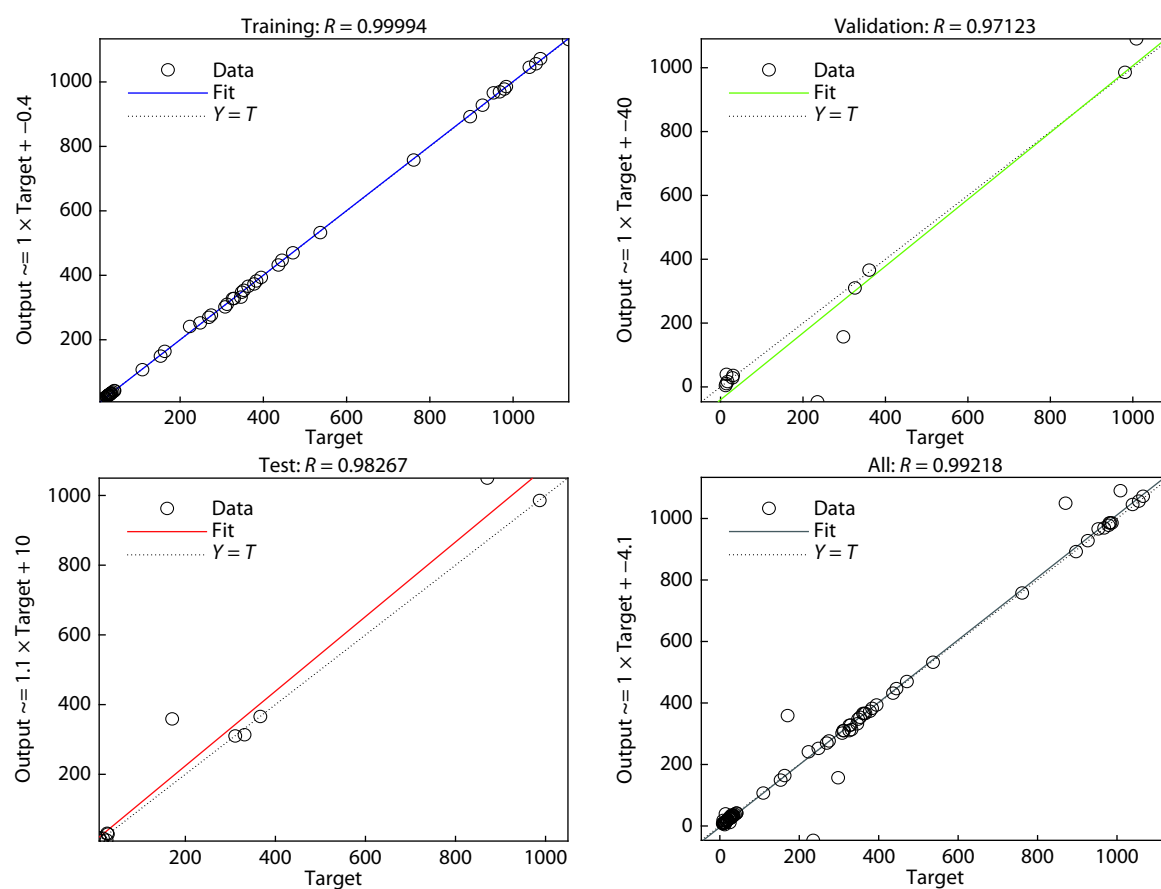


Fig. 3 The regression diagram of the trained ANN model.

Table 1 Different cases of nanocomposite's input parameters to perform experiments.

Case	PP (%)	TPE (%)	Nano-silica (%)	PP-g-MA (%)
PP	100	0	0	0
P1	76	15	6	3
P2	76	15	6	3
P3	78	10	6	6
P4	75.5	20	3	1.5
P5	79	15	3	3
P6	82	15	3	0
P7	66.5	20	9	4.5
P8	76	15	6	3
P9	74	20	6	0
P10	76	15	9	0
P11	84	10	6	0
P12	76.5	10	9	4.5
P13	68	20	6	6
P14	85.5	10	3	1.5
P15	67	15	9	9

of the elastomer phase would be enhanced by increasing its concentration. The reason stems from the higher possibility of particles' collision and their coalescence during the mixing. Table 2 also reports the average size of TPO inclusions in different samples, which was measured by ImageJ software.

The Effects of Input Variables on Mechanical Properties

As mentioned in the introduction, PP suffers from low values of toughness (TO) and impact strength (IS). The usual method

for obviating this deficiency is to add elastomer, although it may have adverse effects on Young's modulus and tensile strength. Fig. 5(a) illustrates that the utilized polyolefin elastomer in the current nanocomposite has positive effects on TO. According to this figure, the nanocomposite can reach TO of 450 MPa by 20% share of elastomer. Figs. 5(b) and 5(c) also indicate the minor effects of nano-silica and PP-g-MA on the corresponding values of TO. The figures illustrate that higher TO can be achieved by the approximate values of 4.5% and 2% for nano-silica and compatibilizer, respectively.

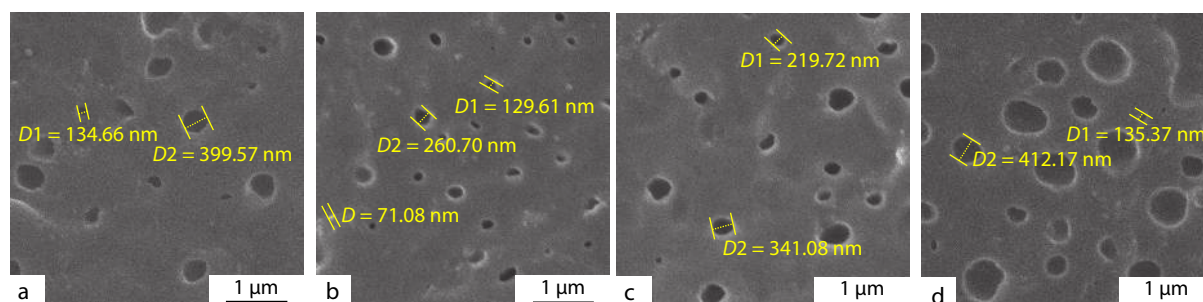
Fig. 6(a) demonstrates the similar influence of elastomer additive on the corresponding values of elongation at break (EB). The interesting part about the figure is the analogous trend of variation in EB with the toughness one (see Fig. 5a). However, this trend is not analogous to the influences of nano-silica and PP-g-MA and lower values of these parameters are needed to achieve the maximum EB (Figs. 6b and 6c).

As mentioned in the introduction, the elastomers have adverse impacts on the Young's modulus (YM) and tensile strength (TS). Fig. 7(a) completely approves the current assumption about elastomers, while Fig. 7(b) shows the suitability of the utilized approach to solve this problem. In this figure, higher values of nano-silica would increase TS up to 26 MPa, which would somehow compensate for the negative effects of elastomers in the composition of PP. Fig. 7(c) also indicates that higher amounts of PP-g-MA compatibilizer would enhance TS. The reason stems from better compatibility between nano-silica and PP in the presence of PP-g-MA.

Fig. 8 shows the changes in Young's modulus (YM) by the

Table 2 The mechanical properties of considered cases to experiment.

Case	TO (MPa)	EB (%)	TS (MPa)	YM (MPa)	IS (kJ/m ²)	Diameter (nm)
PP	374.1 ± 28.3	13.2 ± 2.5	35.2 ± 0.8	1071 ± 22	2.9 ± 0.7	–
P1	360.6 ± 17.5	16.9 ± 3.0	28.9 ± 0.5	981 ± 21	14.0 ± 1.8	325 ± 11
P2	363.5 ± 29.2	16.8 ± 1.2	28.5 ± 0.2	983 ± 12	10.3 ± 2.3	312 ± 12
P3	326.2 ± 11.3	11.7 ± 1.8	33.4 ± 0.9	1065 ± 25	32.8 ± 3.9	153 ± 15
P4	377.8 ± 25.1	19.7 ± 4.4	27.2 ± 0.5	926 ± 18	41.4 ± 5.3	348 ± 12
P5	170.6 ± 16.4	8.5 ± 1.6	26.3 ± 0.7	870 ± 8	24.9 ± 1.7	331 ± 9
P6	436.1 ± 19.7	19.3 ± 3.4	28.8 ± 0.4	978 ± 14	27.3 ± 3.4	353 ± 10
P7	444.6 ± 31.5	20.4 ± 0.5	26.1 ± 0.2	967 ± 24	34.9 ± 4.8	383 ± 13
P8	366.4 ± 23.5	16.8 ± 4.1	27.8 ± 1.3	987 ± 14	12.1 ± 2.7	310 ± 15
P9	394.6 ± 29.1	19.4 ± 1.1	24.5 ± 1.2	896 ± 6	38.0 ± 5.4	471 ± 23
P10	223.3 ± 17.2	9.9 ± 1.4	28.3 ± 1.0	952.9 ± 27	19.6 ± 5.9	346 ± 16
P11	163.0 ± 14.8	8.4 ± 2.2	32.3 ± 2.6	1054 ± 35	7.45 ± 2.2	109 ± 7
P12	297.8 ± 16.9	12.2 ± 0.5	30.4 ± 0.3	1008.6 ± 26	14.3 ± 3.7	235 ± 11
P13	536.7 ± 24.5	27.5 ± 3.4	23.6 ± 0.4	761.1 ± 28	42.2 ± 4.5	274 ± 16
P14	329.6 ± 21.4	14.7 ± 2.4	33.0 ± 0.4	1133.7 ± 14	11.9 ± 2.7	269 ± 14
P15	248.1 ± 17.6	9.3 ± 1.5	30.3 ± 0.7	1039.3 ± 18	23.1 ± 4.1	308 ± 18

**Fig. 4** SEM images of the PP/elastomer/nano-silica/PP-g-MA nanocomposite in the cases: (a) P6, (b) P14, (c) P5, and (d) P9.

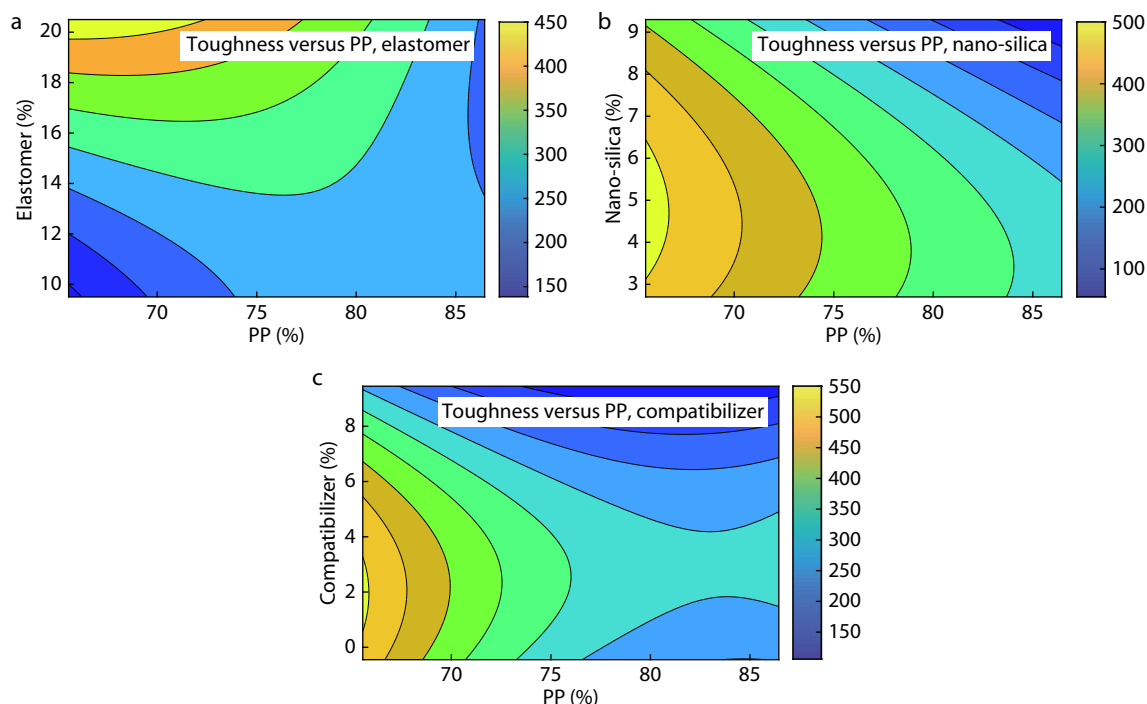


Fig. 5 The impacts of nanocomposite's input parameters on toughness (MPa): (a) the effects of elastomer, (b) the effects of nano-silica, (c) the effects of compatibilizer.

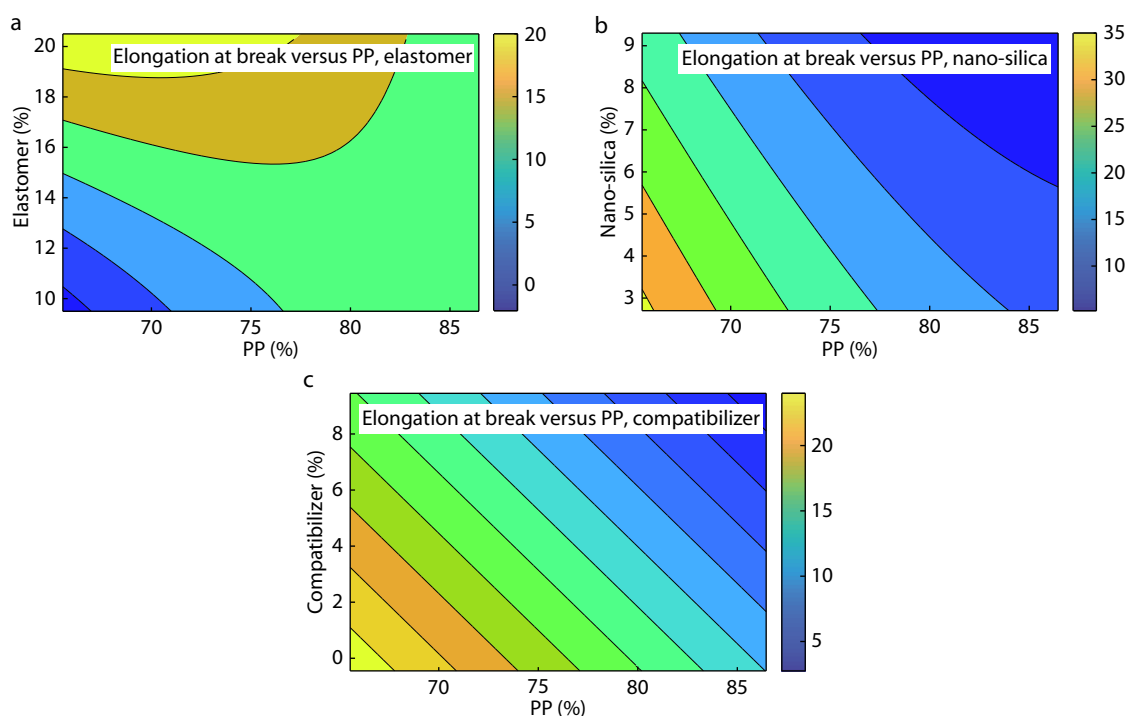


Fig. 6 The impacts of nanocomposite's input parameters on elongation at break (%): (a) the effects of elastomer, (b) the effects of nano-silica, (c) the effects of compatibilizer.

variation of PP, elastomer, nano-silica, and compatibilizer. The results (Fig. 8a) indicate that higher percentages of elastomer would considerably decrease YM, while the higher amount of PP-g-MA is preferable to increase this parameter (Fig. 8c). Fig. 8(b) also shows the variable trend of nano-silica as a func-

tion of PP percentages. When the PP share is less than 82%, higher values of nano-silica would increase YM. This trend becomes the opposite when the PP percentages experience the higher values of 82%, and in this condition, the lower values of nano-silica are suitable to enhance YM.

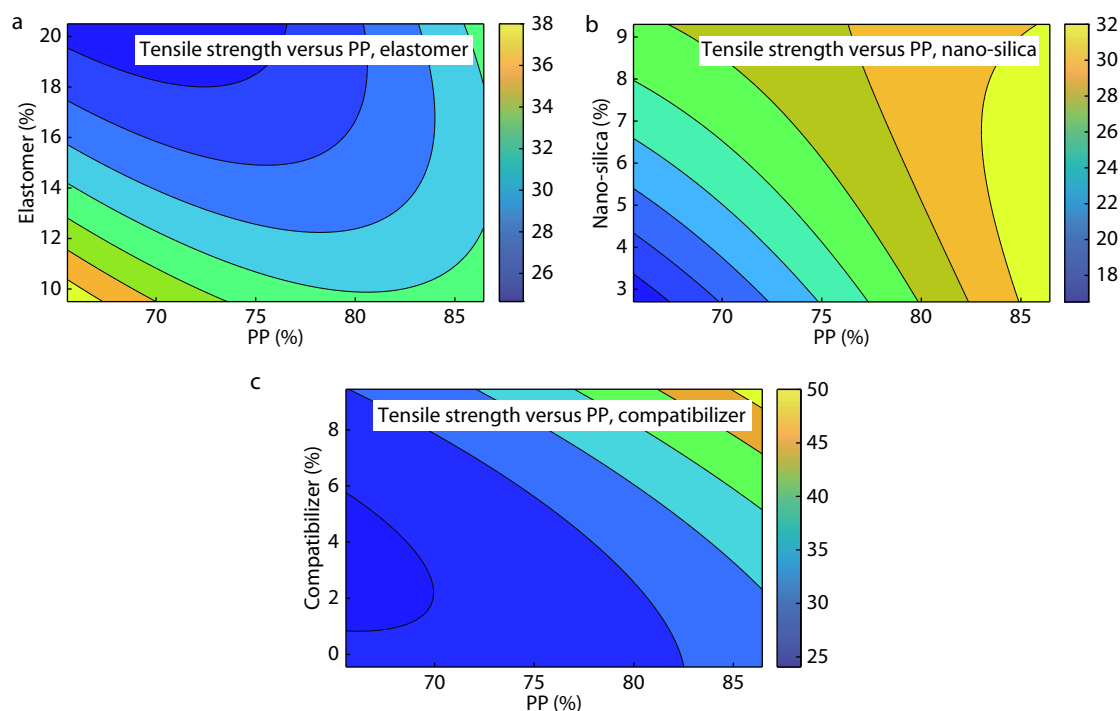


Fig. 7 The impacts of nanocomposite's input parameters on tensile strength (MPa): (a) the effects of elastomer, (b) the effects of nano-silica, (c) the effects of compatibilizer.

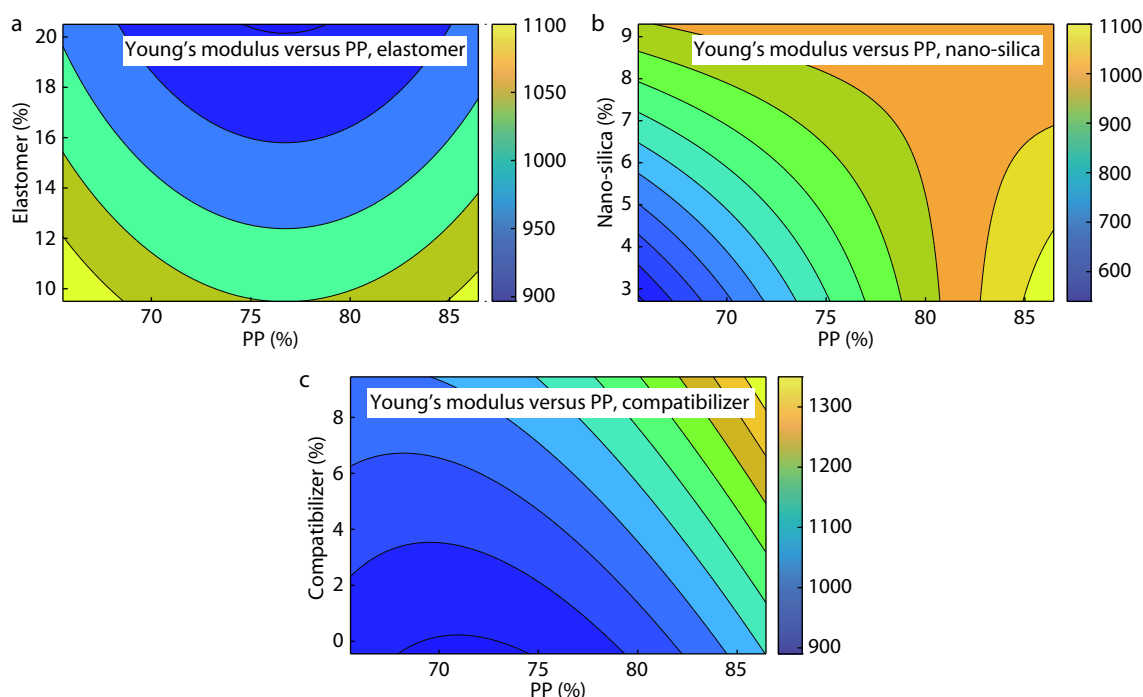


Fig. 8 The impacts of nanocomposite's input parameters on Young's modulus (MPa): (a) the effects of elastomer, (b) the effects of nano-silica, (c) the effects of compatibilizer.

Fig. 9 demonstrates the variation of impact strength (IS) changing the input parameters of the nanocomposite. Fig. 9(a) shows that higher shares of elastomer would enhance IS noticeably, while lower values of nano-silica are required to achieve higher IS. According to Fig. 9(c), although higher shares of compatibilizer would increase the IS in high amo-

unts of PP, the trend of changes is reverse in a low amount of PP, and lower values of compatibilizer are favorable.

As mentioned, the first goal of sensitivity analysis is to find the impacts of input parameters on the output parameters. Here, the input parameters are different percentages of PP, TPE, nano-silica, and PP-g-MA. The output parameters of this

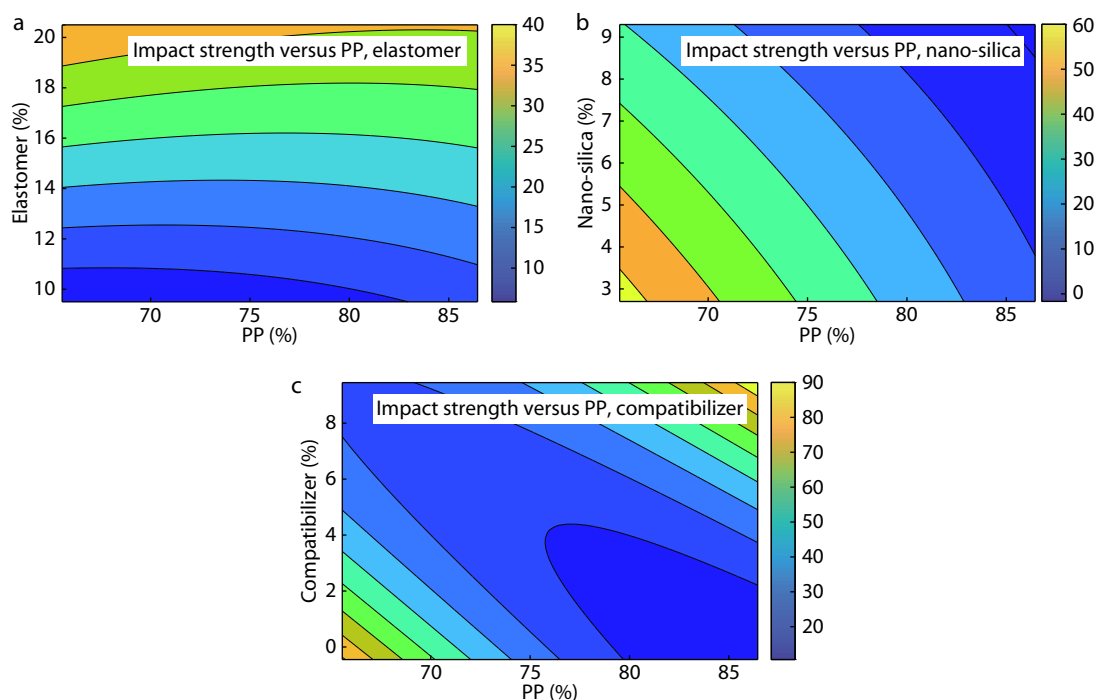


Fig. 9 The influence of nanocomposite's input parameters on impact strength (kJ/m²): (a) the effects of elastomer, (b) the effects of nano-silica, (c) the effects of compatibilizer.

section are also the respective value of the nanocomposite: TO, EB, TS, YM, IS, and elastomer's diameter. Fig. 10 illustrates that TPE has the largest influence on the respective amount of TO and EB, while PP has the least. This is compatible with the first goal of using elastomers to increase the respective values of TO (50%) and IS (24%). It is noteworthy to mention that the appropriate utilization of nano-silica would improve YM and TS. That is why the impact of these nanoparticles is high among other input parameters by 42% and 36%, respectively. Fig. 10 also demonstrates that the addition of compatibilizer would prevent the agglomeration of nanocomposite's nanoparticles with subsequent effects on some of the mechanical properties. The figure clearly shows that PP-g-MA has considerable influence on YM by 29%. The sensitivity analysis also reveals that the impact strength and the diameters are highly influenced by PP.

Introducing NEC and Performance Optimization

Previously, it was discussed that the first aim of creating the mentioned nanocomposite is to improve the low TO and IS of PP. Different kinds of elastomers can improve this deficiency but they would also reduce YM and TS. The addition of nanoparticles (in this work, nano-silica) also amends the reduction of YM and TS, while high values of these nanoparticles can also reduce TO and IS. Therefore, a balance should be made to find the appropriate values of these parameters. In other words, a parameter is needed to consider all these mechanical properties with the right share of their effects on the characteristics of the nanocomposite. In this manner, the multi-objective optimization would be useful to consider all the output parameters and to calculate the optimum values. Another method is to find a suitable parameter, which considers all the output parameters to predict the appropriateness of the

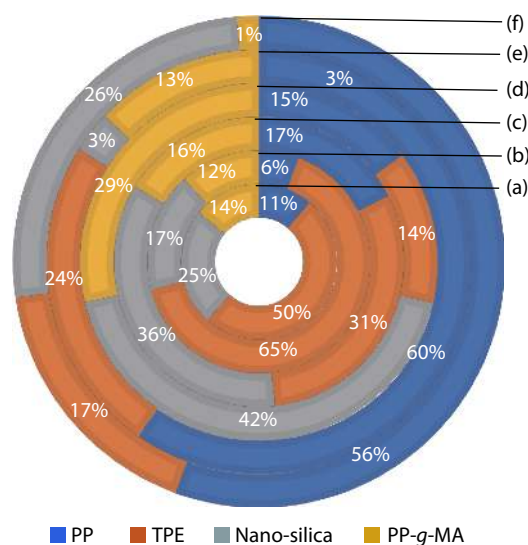


Fig. 10 The sensitivity analysis of the four input parameters of nanocomposite on the corresponding output parameters: (a) toughness, (b) elongation at break, (c) tensile strength, (d) Young's modulus, (e) impact strength, (f) elastomer's diameter.

nanocomposite. Herein, a new parameter called nanocomposite evaluation criterion (NEC) is introduced to reduce the output parameters into one. This parameter consists of the five major mechanical properties of nanocomposites and its dimensionless characteristics is appropriate for designers. The considered base case in this parameter indicates the neat polymer (in the current study, polypropylene), and the mentioned new properties are related to the manufactured nanocomposite. By the introduction of this parameter, one can easily understand the suitability

of the added additives such as elastomers, nano-particles, etc. to the neat polymer on all the mechanical properties of the nanocomposite. In other words, NEC is a new representative of all the needed mechanical properties to evaluate the right amounts of the considered additives. Additionally, this parameter can also reduce the five-objective optimization problem into a single one and mitigate the needed calculations by designers. High amounts of this parameter mention better mechanical properties of the nanocomposite, which is not necessarily a composition of the mentioned input parameters. In other words, this parameter can be used for a different composition and different materials. NECs with the higher value of one indicate enhancement in the designing of the nanocomposite and respective improvement in the mechanical properties of the neat polymer, while the lower amount of one shows the vice versa. Eq. (2) shows this new parameter:

$$NEC = \left(\frac{TO_{new}}{TO_{base}} \right)^a \left(\frac{EB_{new}}{EB_{base}} \right)^b \left(\frac{TS_{new}}{TS_{base}} \right)^c \left(\frac{YM_{new}}{YM_{base}} \right)^d \left(\frac{IS_{new}}{IS_{base}} \right)^e \quad (2)$$

In Eq. (2), the base values are the mechanical properties of case PP, which considers the output parameter of the nanocomposite in the case of 100% PP. The new values are also the calculated values in the presence of nano-silica, TPE, and PP-g-MA. Noted that the impacts of the utilized parameters in Eq. (2) are not same on the mechanical properties of the nanocomposite, and their exponents need modification. Therefore, sensitivity analysis is used to predict the suitable exponents to obtain NEC number. Table 3 shows the results of the sensitivity analysis in different exponents.

The solving method of each optimization algorithm like genetic algorithm (GA) is to find the optimum values of the input parameters without any exponent. In the first case of Table 4, all the exponents are equal to one that is equivalent to an optimization like GA. In other words, we have only considered that the output parameters should increase as much as possible to calculate the maximum NEC. However, Table 3 states that if all the exponents are considered to be one (like the GA approach), the effect of TS and YM would be only 6% and 5%, respectively, on the NEC. This means that the other parameters (like TO by 35%) are evaluating the mechanical properties of the nanocomposite. In other words, we have somehow neglected to consider the effects of TS and YM on the mechanical properties of the nanocomposite. Therefore, a suitable solution to obviate this problem is to calculate the proper values rather than one for the mentioned exponents.

In this manner, the try and error method is used to calculate the most appropriate values for a , b , c , d , and e . The procedure of this method in the current problem is to guess the presented exponents (a , b , c , d , and e) in Table 4. After that, the corresponding impact of each parameter on NEC (TO, EB, TS, YM, and IS) would be calculated using the sensitivity analysis. The final NEC would be achieved when the sensitivity of all the input parameters of NEC (TO, EB, TS, YM, and IS) becomes equal to 20%. In this case, all the effective parameters on the mechanical properties of the nanocomposite would be equal. Using the try and error method, the best case would be obtained after five iterations. In this case, the suitable values for the exponents of NEC are calculated. Therefore, Eq. (3) would be the final version of the NEC:

$$NEC = \left(\frac{TO_{new}}{TO_{base}} \right)^{0.372} \left(\frac{EB_{new}}{EB_{base}} \right)^{0.405} \left(\frac{TS_{new}}{TS_{base}} \right)^{0.836} \left(\frac{YM_{new}}{YM_{base}} \right)^1 \left(\frac{IS_{new}}{IS_{base}} \right)^{0.237} \quad (3)$$

After obtaining the suitable values of the mentioned exponents of the NEC equation, optimization can be performed. This single objective optimization, which includes all the needed parameters to evaluate the mechanical properties of the nanocomposite, would simply determine the optimum values of the PP, elastomer, nano-silica, and compatibilizer. To attain a comprehensive perspective over the changes in NEC and the optimum values of the input parameters, different objectives are selected and presented in Table 4.

Table 4 indicates that TPE has by far the highest positive impact on PP among all the additives (nanoparticles and compatibilizer) to improve the mechanical properties of the nanocomposite. According to Eq. (3), TPE becomes 24.2% while nano-silica is 9.5%, and NEC would be 2.16. However, neglecting the concerted efforts to find the suitable values of exponents in Eq. (2) and considering all of them equal to unity would result in the values of 71.2, 20, 5.1, and 3.7 for PP, TPE, nano-silica, and PP-g-MA, respectively.

Table 5 also presents the mechanical properties of nanocomposite in the optimized condition of both cases. In the current study, the first goal of creating the nanocomposite was to enhance the low TO and IS of PP. During the experimental test, however, it can be seen that the addition of elastomers and nanoparticles would decrease YM considerably. Therefore, an optimum value should be determined to enable the researchers to reach the highest TO and IS, while the reduction in the respective YM is negligible. Herein, although the values of IS and EB in the first case are lower than in the

Table 3 The impacts of different NEC exponents and the output parameters of (TO, EB, TS, YM, IS) on the sensitivity analysis of NEC.

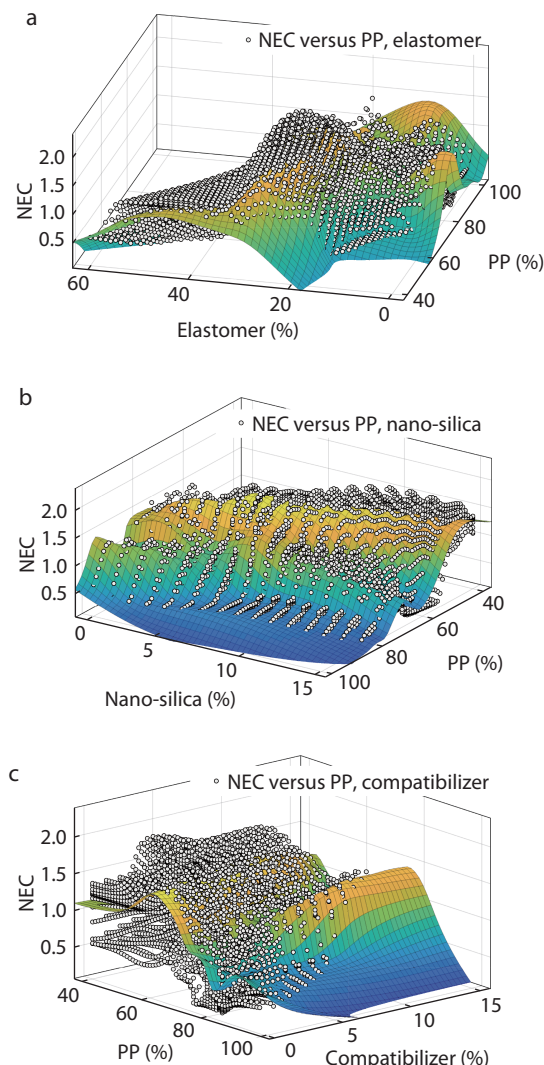
Iteration	a	b	c	d	e	TO	EB	TS	YM	IS
1	1	1	1	1	1	35%	22%	6%	5%	42%
2	0.33	0.5	1	1	0.2	15%	27%	26%	18%	14%
3	0.4	0.4	0.8	1	0.25	22%	19%	18%	20%	21%
4	0.37	0.4	0.835	1	0.23	20%	20%	20%	21%	19%
5	0.372	0.405	0.836	1	0.237	20%	20%	20%	20%	20%

Table 4 The optimum input parameters to obtain the maximum NEC.

Case	Exponents of NEC	Maximum NEC	PP	TPE	Nano-silica	PP-g-MA
1	According to Eq. (3)	2.16	64.7%	24.2%	9.5%	1.6%
2	All equal to unity	31.96	71.2%	20.0%	5.1%	3.7%

Table 5 The mechanical properties of the nanocomposite in optimized NEC.

Case	Exponents of NEC	TO (MPa)	EB (%)	TS (MPa)	YM (MPa)	IS (kJ/m ²)
1	According to Eq. (3)	577.53	31.95	24.77	989.53	33.72
2	All equal to unity	550.48	32.43	24.08	889.30	42.47

**Fig. 11** The variation of NEC (according to Eq. 3) considering the variation of the input parameters.

second one, the respective values of YM, TO, and TS are higher in the first case. It is noteworthy to mention that both mentioned cases of Table 4 are the optimized values of input parameters, one based on Eq. (3) and one based on Eq. (2) considering the values of $a = b = c = d = e = 1$. Similar procedure is also mentioned in Table 5 to show the respective values of the mechanical properties in the optimized conditions. The real mechanical properties of the nanocomposite in different input parameters have been also mentioned in Tables 1 and 2. The aim of the optimization was also to find the optimum values of input parameters (the shares of PP, TPE, nano-silica, and PP-g-MA) in a condition that all the mentioned mechanical properties have their highest values. In

this work, the introduction of NEC also enabled us to simply reduce the five-objective problem into a single-objective one. Totally, the presented values in the first case of Table 4 are the main optimum values to be considered in this specific problem to improve the mechanical properties of the mentioned nanocomposite. Fig. 11 also illustrates the variation of NEC with the changes in the input parameters. In this figure, the dots are the produced data by ANN, which are correlated by a plane to show the trend of variation. It is noteworthy to mention that the planes are not completely fitted to the data, for there are four input parameters. In other words, if there exists a five-dimensional diagram, the data would have been fitted completely to that diagram.

CONCLUSIONS

One of the goals of today's researchers is to improve the mechanical properties of polymers using different additives. In this study, the composition of PP, elastomer, nano-silica, and PP-g-MA was created and experimented in 15 different cases in addition to neat PP. In order to optimize the mechanical properties of this nanocomposite, a new parameter called nanocomposite evaluation criterion (NEC) was introduced using sensitivity analysis and artificial neural networks. The optimum values of NEC's exponents were obtained, and the corresponding diagrams of NEC's variation by the changes in PP, elastomer, nano-silica, and PP-g-MA were illustrated. The figures demonstrated that the maximum NEC would be obtained when PP is 64.7% and elastomer is 24.2%.

To achieve the precise needed values for the input parameters to reach the best mechanical properties, an optimization using the single objective (NEC) was performed. The optimization indicated that one can reach the best mechanical properties of the nanocomposite when the shares of PP, elastomer, nano-silica, and compatibilizer are equal to 64.7%, 24.2%, 9.5%, and 1.6%, respectively. In this condition, the toughness and impact strength would increase considerably, among which the former experiences 577.53 MPa in comparison to 374.08 MPa for neat PP. The latter would also enhance up to 33.72 kJ/m², while the respective value for neat PP is equal to 2.98. Although the enhancement in these two values is intriguing, the drop in Young's modulus should not be noticeable. The results indicated that the Young's modulus would only reduce 82.12 MPa and reach to 989.53 MPa (in comparison to neat PP case).

Nomenclature

ANN	Artificial neural network
EB	Elongation at break
EVA	Ethylene-vinyl acetate
IS	Impact strength
MA	Maleic anhydride
NEC	Nanocomposite evaluation criterion
PP	Polypropylene
PP-g-MA	Polypropylene grafted maleic anhydride
TO	Toughness
TPE	Thermoplastic elastomer
TPO	Thermoplastic polyolefin
TPU	Thermoplastic polyurethane
TS	Tensile strength
YM	Young's modulus

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