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Investigating the Influence of Mixing Speed in Mechanical Physical Properties of Acrylonitrile Butadiene Styrene/Polycarbonate Alloy and Simulating Laboratory Data by Artificial Neural Networks

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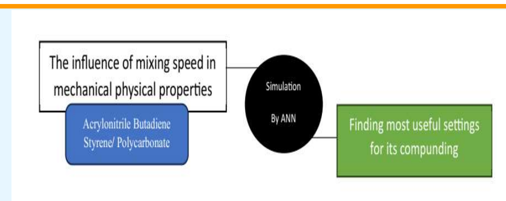
Abstract: The rapid growth of science and technology has created a demand for polymers with unique and specialized properties that cannot be met by existing polymers alone. As a solution, the process of alloying, in which involves two or more polymers are combined, has gained significant attention. Alloying offers several advantages, including the flexibility in the choice of materials, the ability to design the final product, unique properties and characterizations, and cost efficiency. Among the various commercially available alloys, polycarbonate (PC) and acrylonitrile butadiene styrene (ABS) alloys hold great importance due to their wide range of applications. In particular, the PC/ABS alloy, which is made from a blend of PC and ABS polymers, is widely used worldwide. This article deals with the production of PC/ABS alloys by mixing different ABS percentages with different PC proportions (20, 30 and 40%) at different stirring speeds (30, 40, and 50 rpm). The prepared alloys are subjected to various tests, including evaluations of polymer softness, impact strength, melt flow index, tensile strength at yield point, and polymer hardness. The laboratory data collected during these tests are then subjected to simulations with artificial neural networks (ANN). The simulation results agree remarkably well with the laboratory data and show a high degree of accuracy. These simulation results can also be used to predict properties of untested alloy compositions. The results demonstrate that increasing the stirring speed improved the quality of the product, while increasing the PC content in the alloy leads to an improvement in most properties, with the exception of the melt flow index, which shows a decrease.



Keywords: Acrylonitrile butadiene styrene (ABS), Polycarbonate (PC), Alloy, Mechanical physical properties

1. Introduction

The flexibility of polycarbonate (PC) plays a crucial role in its alloying with other polymers, allowing weaknesses to be overcome and the range of applications to be extended. Through this process, a variety of products can be produced that offer a balance between affordability and efficiency that is of interest to manufacturers of various components. The alloying of PC with other polymers serves to overcome several weaknesses and limitations of PC. These include problems such as low flexibility in terms of processability and flow behavior, lower toughness at low temperatures, susceptibility to scratches and small cracks, as well as limited chemical and atmospheric resistance. The use of alloying processes can mitigate these weaknesses and improve the overall performance of polycarbonate-based materials. Among the polymers commonly used as alloy partners for polycarbonates, warm polyesters such as polyethylene terephthalate (PET) and polybutylene terephthalate (PBT), as well as the acrylonitrile butadiene styrene (ABS) copolymer are often used. These alloy combinations provide improved properties and offer a wider range of applications for polycarbonate-based materials. By taking advantage of alloys, manufacturers can improve the properties of PCs and expand their application, resulting in the production of cost-effective and efficient products that meet the various needs of the industry.[1-9] In addition, some polymers such as polyetherimide, the copolymer acrylonitrile styrene acrylonitrile (ASA), the copolymer acrylonitrile ethylene styrene (AES), and copolymer styrene maleic anhydride (SMA)[10-14] are used in small quantities in PC blends for special applications. One of the markets for this alloy is its use in the construction computer equipment and official machinery. Properties such as high mechanical resistance, very good thermal resistance, electrical insulation, and flame resistance mean that this alloy is frequently used in this industry. This alloy is used for the construction of monitor, computer, printer, and even in mouse and keyboard. It is also used in the manufacture other office equipment such as telephones.[15-18]

The conventional method for the producing this alloy is to melt-mix the components together. as with other alloys, melt mixing can be carried out in continuous and discontinuous mixers.[19] Discontinuous mixers offer several advantages in the connection with mixing processes. These include better dispersing and distributing mixing quality, easy material feeding with different aggregate states, the ability to apply and control a uniform stress curve, and the option to take samples and study the mixing process at different stages and time intervals. These mixers usually consist of a chamber with two spinners of different sizes and geometric shapes. Heat transfer to the materials is facilitated by thermal systems using electricity or oil, and various stresses, such as tension and shear, are generated in the chamber to promote mixing. By utilizing these mixers and collecting data on a laboratory scale, it is possible to estimate the optimum time required for diffusion and distribution mixing. It is also possible to determine the order and timing of addition of the components during alloy production. Other advantages offered by these mixers further aid in the study and refinement of the alloy manufacturing process on the laboratory scale. However, it is worth noting that discontinuous mixers are generally not used on an industrial scale. Despite their advantages and capabilities, alternative mixing methods are often used in industrial for reasons of scale, efficiency, and economic considerations.[20,21] Researchers have reported that the appropriate temperature and spin speed to produce PC/ABS alloys in these mixers are 220-240 °C and 50-60 rpm.[15,17] Among the other mixers used to produce these alloys, continuous mixers such as single-screw and double-screw extruders equipped with special areas should be mentioned. These mixers have advantages such as the distribution of residence time, uniform heat, the fewest dead zones, and the ability to release gases. These mixers are also used on an industrial scale in the production of alloys.

In research work on PET reuse and reducing environmental problems, PET waste was mixed with ABS under different conditions such as temperature, time, and extruder speed; the laboratory data were simulated by artificial neural networks (ANN). The results of the simulation covered the laboratory data well.[22] In another research study, the effects of the general performances of ANN with laboratory data on nanoparticles in various states of viscosity of crude oil were studied. The results showed a good performance for RBF networks due to their strong academic foundation and ability to filter the noise.[23] In another study, ANN simulated EPS polymerization using conventional and MID methods. Multilayer perceptron (MLP) networks were trained using an algorithm. The simulation results showed good and acceptable results.[24]

Another study investigated a blend of GPPS and ABS polymers. The laboratory data were simulated using ANNs and the results of the simulated data covered the laboratory data well.[25] A study of the thermal and mechanical properties of ABS/PC shows that by adding PC to butadiene and PC particles dispersed in acrylonitrile styrene (SAN) matrix, respectively, ABS becomes more brittle.[26] The penetration resistance of ABS/PC alloy was investigated and the reinforcement against burning was studied.[27] Capture of ABS/PC alloy with new yarns was investigated. Results of melt viscoelastic properties indicated that the rheological behavior in these alloy samples is generally controlled by ABS.[28]

Previous studies have investigated the effect of different polymer percentages, but the effect of mixing speed has not been examined. Additionally, previous studies did not use ANN to analyze the data. One unique aspect of this study is the use of ANN to analyze the data. ANN can be used to predict polymer properties within any desired range or even beyond specified data. This flexibility allows for more accurate predictions and a deeper understanding of the relationship between mixing rate and polymer properties. Furthermore, this research project is the first to apply the MLP method of ANN to analyze commercial desired percentages. This method improves the accuracy and reliability of the predictions. ABS containing different percentages of PC was prepared at different mixing rates. Various experiments were performed with the prepared polymer. The collected laboratory data are simulated using ANNs and the results of simulation were acceptable. By increasing the percentage of PC in ABS at a constant stirring speed, the numerical value of the impact test, softening point index, polymer hardness, and yield stress increase and the melt flow index is decreases. It is better to add PC to ABS with high conversion, because studies declare that this material has the highest value in all tests.

2. Materials and Equipment

Materials and specifications

ABS and PC were purchased respectively from Tabriz Petrochemical Company and Khuzestan complex. The ABS polymer contains 53 percent SAN and 27 percent G-ABS (SD-0150 Grade) (Table 1). The poly carbonate's Grade is PC1100 (Table 2).

Table 1. Properties of ABS

ABS-SD0150D **Density** = 1.04 gr/cm^3

Property	Test Method	Test Condition	Unit	Typical Value
Melt Flow Index (MFI)	ASTM D 1238	(200 ºC/5 kg)	g/10 min	1.7
Izod Impact Strength (notched)	ISO 180	1/8 inch	kJ/m^2	25
Tensile Strength at yield	ASTM D 638	5 mm/min	kgf /cm^2	440
Elongation at Break	ASTM D 638	5 mm/min	%	40
Flexural Strength at Yield	ASTM D 790	2.8 mm/min	kgf/cm^2	640
Flexural Modulus	ASTM D 790	2.8 mm/min	kgf/cm^2	20500
Vicat Softening Temperature (unannealed)	ASTM D 1525	5 Kg	ºC	99
Rockwell Hardness	ASTM D 785	-	R-sCALE	104
Flammability	UL 94	1.5 mm Specimen	Recognized	HB

Equipment and tools

Extruder (twin screw) from SM plate having a screw diameter of 20 mm and a length-to-diameter ratio of 32 for mixing

Table 2. Properties of PC

Properties	Test Method	Test Condition	Unit	Accepted Value
Melt Flow Index	ASTM D1238	300 °C/1.2 kg	g/10 min	9~ 11
Vicat Softening Temperature (Un annealed)	ASTM D1525	5 kg/50 °C/hr	°C	Min 145
Flexural Modulus	ASTM D790	23 °C	MPa	Min 2300
Appearance		Granular or plate powder		

polymeric materials and injector device having extruder temperature of 190 °C, 160 bar of injection pressure, 3116 cm^3 of injection volume, and 253 cm^3 template volume from Billion, France was used for preparing needed molds for elongation at break and impact tests. ASTM D-638 SHIMADZU autograph AG-X was used for investigating the elongation at break of the samples. Coded 6967.00 from Ceast, Italy with ASTM D-256 was used for the impact test. Coded 7026.00 from Ceast, Italy with ASTM D-1238 was used to investigate the processability of the prepared mixture and index of the flow of mixtures. HD-PC from Yasuda, Japan with ASTM D-1525 was used to declare the softening point of materials without a specified melting point. The spectral radiation device SF450 model with declaration of the yellow index with ASTM E-313 was used for the measurement of the color coordinates of CIELAB and declaring the yellow index of the mixtures. To find the concentration of the residual monomer in the samples Varian 3800CP Gas Chromatographer was used.

Methods and techniques

Different amounts of PC ranging from 0% to 40% were mixed with the main material, ABS, using an extruder device. The mixing process was carried out at various speeds, including 30, 40, 50, and 60 rpm, and a constant mixing temperature of 240 °C. The total mixing time was set to 6 hours. The resulting product, ABS-PC alloy, was exited from the extruder in a molten state. To facilitate the cooling process, the alloy was subjected to two cold baths with temperatures ranging from 60 °C to 75 °C and 40 °C to 45 °C, respectively. Subsequently, the water from the alloy was removed using a dedicated drying device, and the material was transformed into polymer granules through a cutting and shaping process utilizing a cutter and templating and pressing device. Polymeric templates and sheets were then created from the granules. The specifications and properties of these templates and sheets were measured using various devices and techniques to assess their quality and performance.

MLP method of ANNs

The MLP is an ANN method that carries out mathematical operations on input data. The MLP consists of layers of neurons, with the number of neurons customizable to meet the requirements of the task at hand. However, it is important to note that using many hidden neurons in the MLP can lead to unnecessary degrees of freedom. To train the MLP network, a technique called backpropagation, or any other optimization procedure, is employed to adjust the synaptic weights. During the training phase, the network output is compared with the desired output. In this article, the technique of steepest-descent optimization with a constant step length parameter (η) is utilized. The steepest-descent optimization technique involves iteratively updating the synaptic weights in the direction of steepest descent of the error surface. By using a constant step length parameter, the weights are adjusted in a consistent manner throughout the training process. This approach allows the MLP network to learn and improve its performance by iteratively adjusting its synaptic weights based on the error between the network's output and the desired output.

Quadratic methods, like Newton-like techniques, are commonly used to compute the optimum performance of MLP networks. These methods converge faster near the optimal point compared to other methods and may not necessarily be far from it. To predict the optimum learning rate, the "line search" technique is often employed, in contrast to the Newton step length method. This technique helps determining the appropriate learning rate for the model. Quasi-Newton techniques, such as Levenberg-Marquadt or Gauss-Newton, are frequently used in MLP networks because they also converge quickly near the optimal point. These methods are favored due to their efficiency in finding optimal solutions.[29]

Steepest-descent methods, such as backpropagation, are commonly used for training neural networks due to their robustness and ability to avoid trapping into suboptimal solutions. These methods control the step length to improve the efficiency of optimization. In contrast, Newton like optimization methods, such as the quadratic techniques, are seldom used in practice for neural network training as they are more prone to getting trapped in sub-optimal solutions. The algorithm of the MLP network is shown in Figure 1.

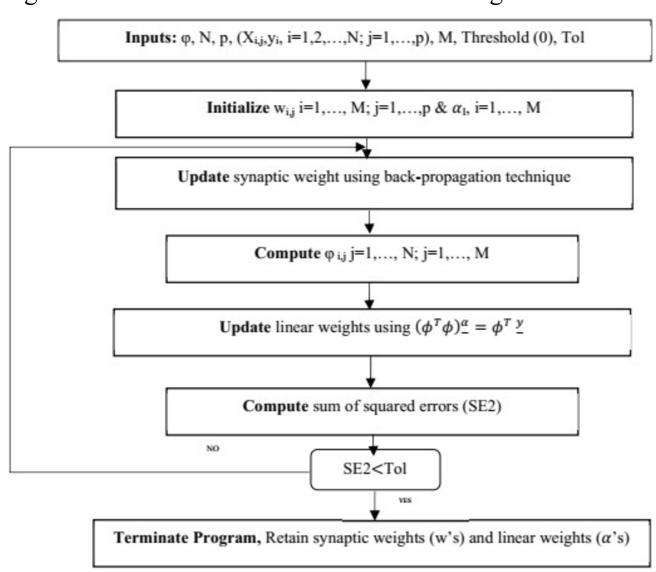


Figure 1. Learning algorithm for MLP Networks.

3. Results and Discussion

Laboratory data and results

PPC with different percentages (0, 20, 30, and 40%) was mixed with ABS, and different tests like the toughness of the polymer, the tension in the yield point, melt flow index, and impact test were performed in different rates of mixing (30, 40, 50 and 60 rpm) on prepared polymer. The results are shown in Figures 2-6.[30-32]

It is known that PC is from thermoplastic families, which means the toughness of the polymer increases by increasing its amount. Figure 2 shows the toughness of ABS polymer by increasing the amount of PC. In Figure 2, it is evident that increasing the mixing rate of PC leads to an increase in the amount of PC, resulting in an improvement in polymer toughness. This trend is observed even when the percentage of PC remains constant. Greater mixing rates facilitate a more thorough blending of the polymers, resulting in a higher quality alloy with enhanced toughness. The data from Figure 2 provides evidence that the mixing rate plays a crucial role in achieving optimal polymer toughness in ABS/PC alloys. By increasing the mixing rate, the alloy composition becomes more homogeneous, leading to improved mechanical properties. These findings highlight the importance of carefully controlling the mixing rate during the preparation of ABS/PC alloys to achieve the desired level of toughness. The results suggest that fast mixing rates can contribute to the production of high-quality alloys with enhanced toughness characteristics.

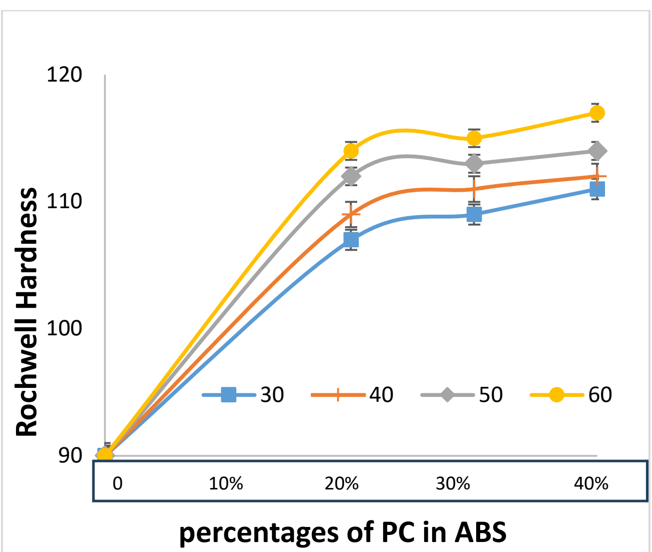


Figure 2. Results of Rockwell hardness for variant percentages of PC in ABS of the mixture in different conditions.

Figure 3 illustrates the impact test results for different percentages of PC and ABS. The data reveal that increasing the PC content leads to an increase in the rubber phase and enhances the scattering of absorbed energy during high-speed impacts. Consequently, this results in improved strength against impact. The figure clearly demonstrates that more percentages of PC correspond to increased impact resistance. Additionally, when the PC percentage remains constant, the impact resistance also increases with faster mixing rates. This indicates that the mixing rate has a positive influence on enhancing the impact resistance of the material. Overall, the findings presented in Figure 3 highlight the significant impact of PC content and mixing rate on the material's ability to withstand impacts. These insights can be valuable in optimizing the composition and processing parameters for achieving desired impact resistance properties in PC-ABS alloys.

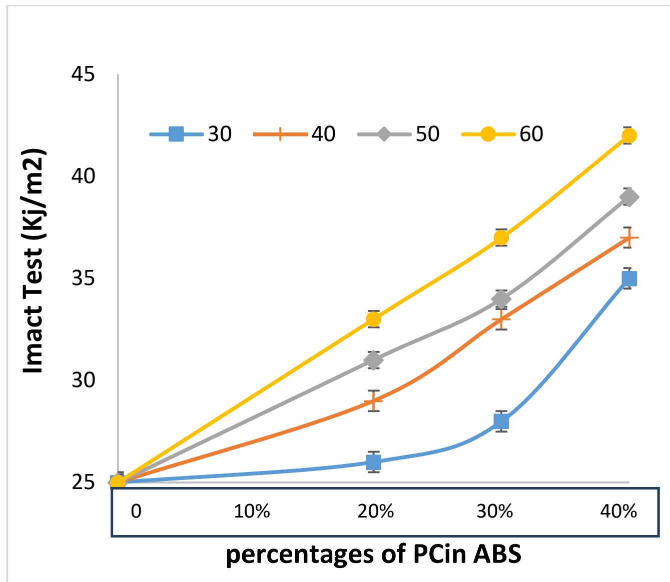


Figure 3. Results of impact test for variant percentages of PC in ABS of the mixture in different conditions.

Figure 3 presents the results for the MFI at different mixing rates and various percentages of PC/ABS. The data make known that when the mixing rate is constant, increasing the weight percentage of PC/ABS leads to a decrease in MFI. This can be attributed to the spread of the rubber phase within the matrix and the formation of lateral links between particles, which contribute to a decrease in the MFI. Furthermore, the findings indicate that increasing the mixing rate, while keeping the weight percentages of PC/ABS constant, results in a decrease in MFI. This suggests that higher mixing rates promote better blending and dispersion of the polymer components, leading to a reduction in MFI. In summary, the results presented in Figure 4 demonstrate the effect of both the weight percentage of PC/ABS and the mixing rate on the MFI of the alloy. Greater weight percentages of PC/ABS and increased mixing rates contribute to a decrease in MFI. These observations are valuable in optimizing the alloy composition and processing parameters to achieve the desired MFI values in PC/ABS alloys.

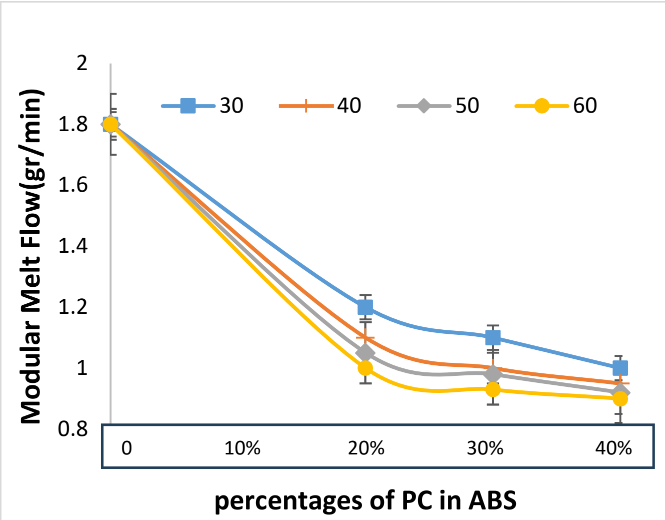


Figure 4. Results of modular melt flow test for variant percentages of PC in ABS of the mixture in different conditions.

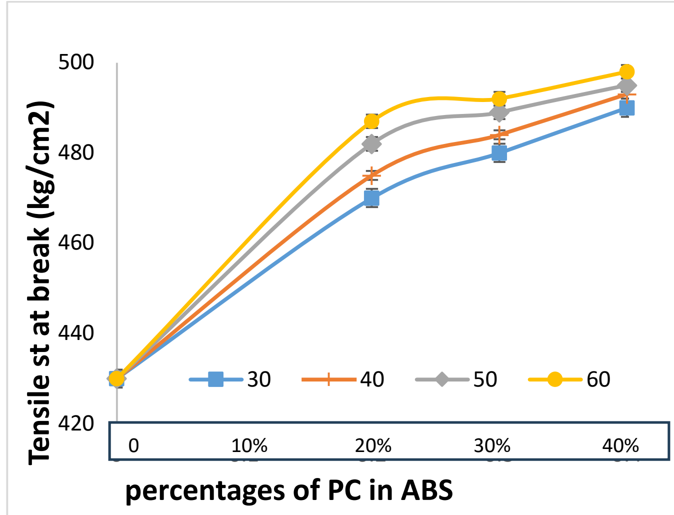


Figure 5. Results of tensile strength at break test for variant percentages of PC in ABS of the mixture in different conditions.

Figure 5 illustrates the investigation of tensile strength at the yield point for different percentages of PC/ABS in the mixture. The data reveal that as the percentage of PC increases, its rigid state transforms into a more flexible rubber-like state. Consequently, when the percentage of PC/ABS enhances while keeping the mixing rates constant, the tension at the yield point also increases compared to the state without PC. Additionally, increasing the mixing rate while maintaining constant percentages of PC/ABS leads to an increase in the tension at the yield point. This can be attributed to the improved tensile strength resulting from better mixing and dispersion of the polymer components at higher mixing rates. It is worth noting that an excess monomer percentage in the polymer composition leads to a decrease in the tension at the yield point. This suggests that the specific composition and ratio of PC/ABS have a significant impact on the mechanical properties, including tensile strength at the yield point. The findings presented in Figure 5 highlight the complex relationship between PC/ABS percentages, mixing rates, and the tensile strength at the yield point. These insights can aid in optimizing the composition and processing parameters to achieve the desired mechanical properties in PC/ABS alloys.

The results for Vicat test in various percentages of PC/ABS and different mixing rates are shown in Figure 6. By increasing the weight percentage of PC/ABS at constant mixing rate the flexibility of the polymer increases due to increasing of rubber component percentage. As PC/ABS is a rubber modified polymer, the rubber phase provides enhanced flexibility and impact resistance. Not only the weight percentage of PC/ABS increase but also the rubber component percentage lead to improved flexibility in the overall blend. This relationship can be observed by comparing the results of the Vicat test at different percentages of PC/ABS.

The mixing rate has a significant impact on the rheology (flow behavior) of polymers, which in turn affects their mechanical properties. The mixing rate determines the distribution and homogeneity of the material within the polymer structure. With an increase in mixing rate, the density and hardness of the polymer also increase. This is because greater mixing rates promote dispersion and material uniformity of the polymer structure. The density and hardness of the polymer can directly affect its mechanical properties. Furthermore, the mixing rate can also influence the mechanical properties of the polymer. With an increase in mixing rate, mechanical properties such as tensile strength, impact resistance, and hardness improve. This is again due to the enhanced homogeneity and improved distribution of the material within the polymer structure. In general, the mixing rate in the polymer production process has a direct impact on the rheology and mechanical properties of polymers. An appropriate mixing rate should be selected to ensure improved rheology and mechanical properties of the polymer.

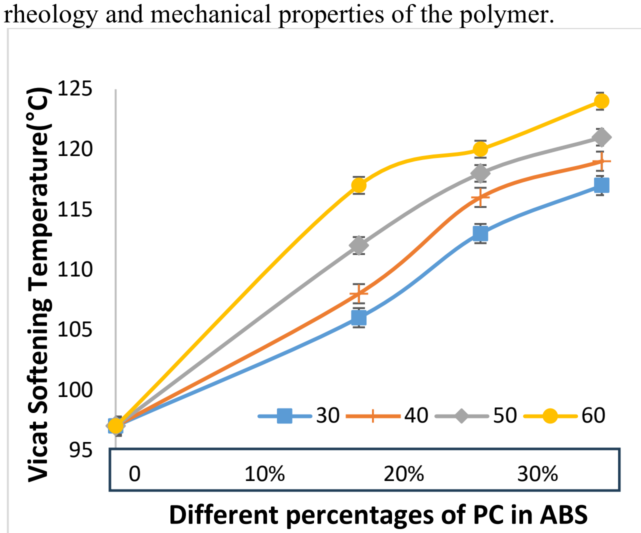


Figure 6. Results of Vicat softening temperature test for variant percentages of PC in ABS of the mixture in different conditions.

The results of simulation with MLP method of ANN

The laboratory data were simulated by the MLP method of ANN in different conditions of mixing rates and PC/ABS percentages. Then different tests including roughness measurement, impact test, melt flow index in yield point, and flexibility index were performed on PC/ABS polymer. The results of the simulation are shown in Figures 7-11.

According to Figure 7, the performance diagrams of the roughness test of the polymer are shown at top of the figure cumulatively and the generalization diagram is shown as a flat surface due to the good performance of the diagram. Therefore, this suggests that the laboratory data were taken accurately. For areas where tests were conducted, simulation diagrams can be utilized.

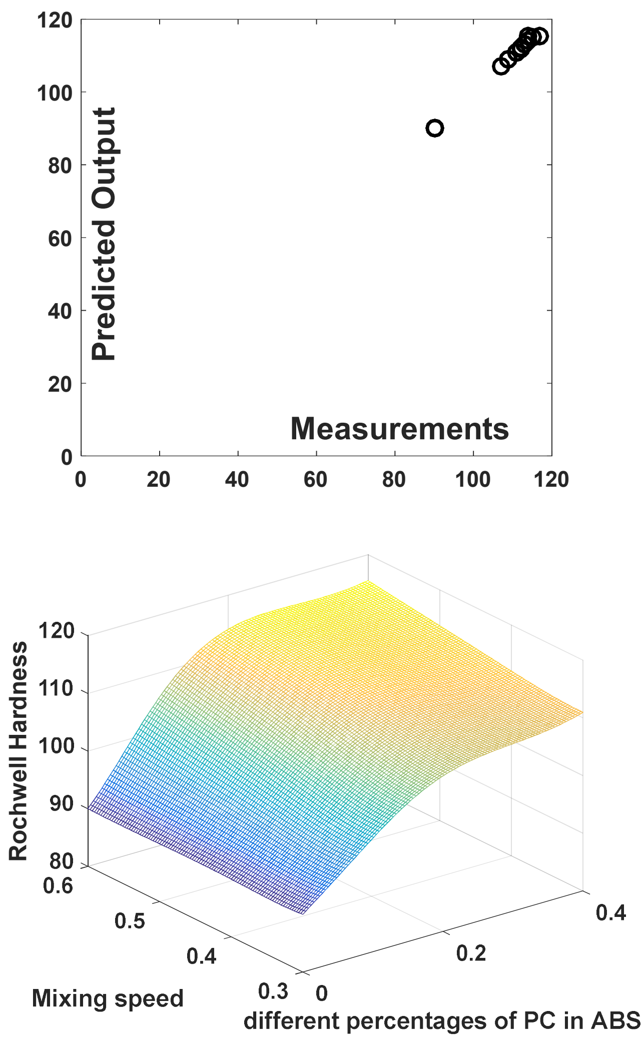


Figure 7. Recall and regeneration of ANN for Rockwell hardness test in various mixing rates and various percentages of PC/ABS.

Figure 8 shows the recall and regeneration performance of the MLP network for impact test in different rates of mixing and different percentages of PC/ABS. According to the figure, the MLP network used for the impact test demonstrates consistent recall and regeneration performance. The measured amounts and predictions align perfectly, indicating a high level of accuracy in predicting data. The resulting figure, which represents a surface, can then be used to make predictions for points where tests were not performed. This demonstrates the ability of the MLP network to generalize and predict results beyond the tested data points.

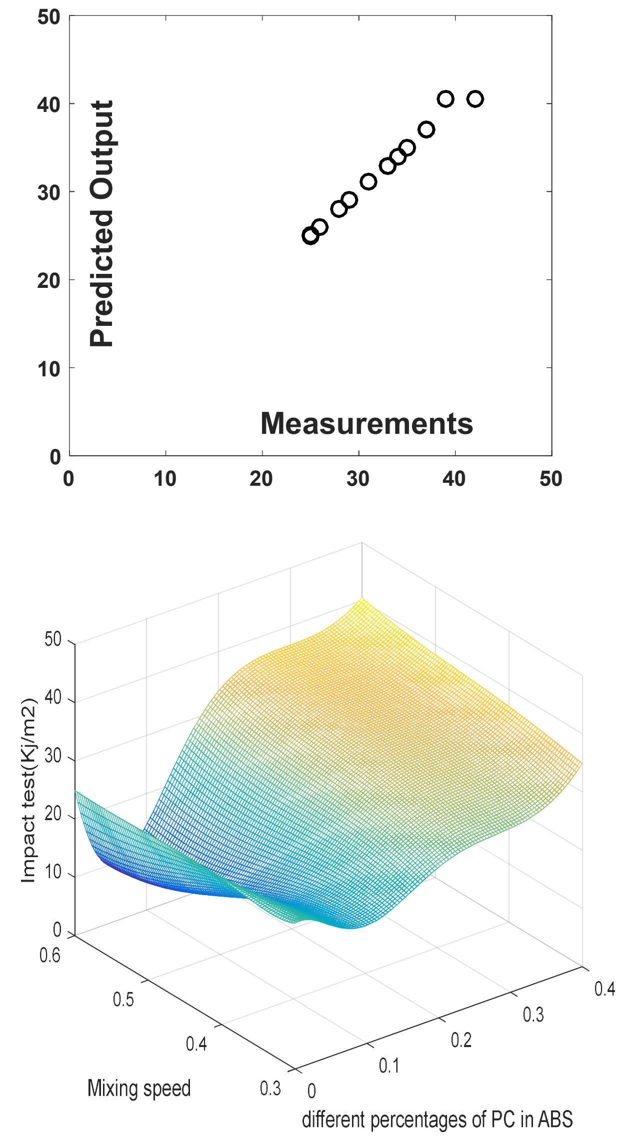


Figure 8. Recall and regeneration of ANN for impact test in various mixing rate and different percentages of PC/ABS.

The resulted data of the simulation for melt flow index test in different rates of mixing and different percentages of PC/ABS are shown in Figure 9. According to the figure, there is no overfitting, and the laboratory data cover the simulated data perfectly.

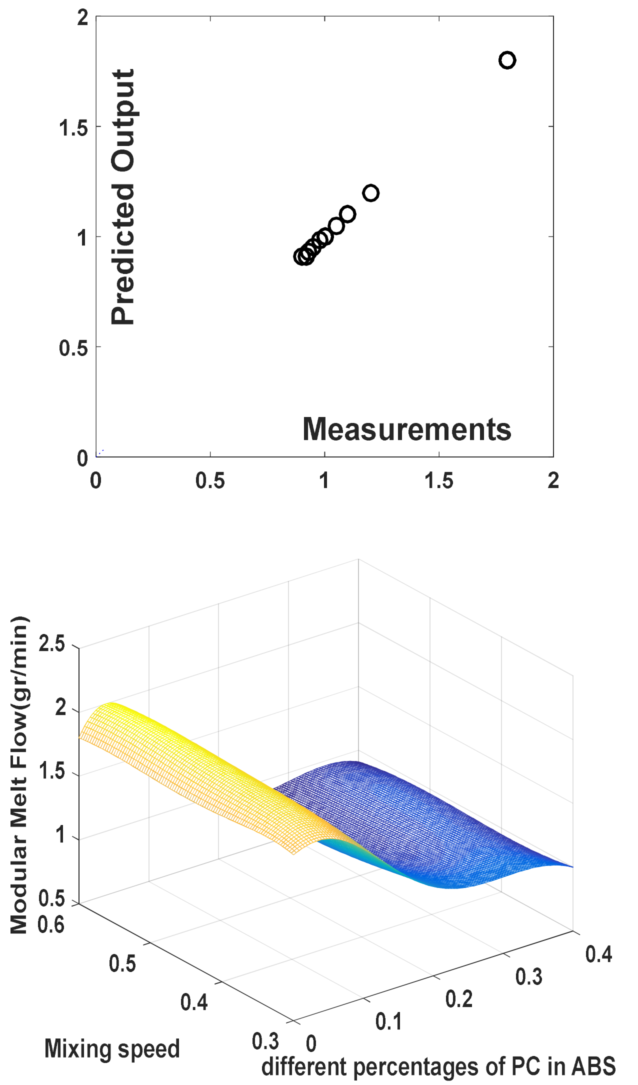


Figure 9. Recall and regeneration of ANN for modular melt flow test in various mixing rates and various percentages of PC/ABS.

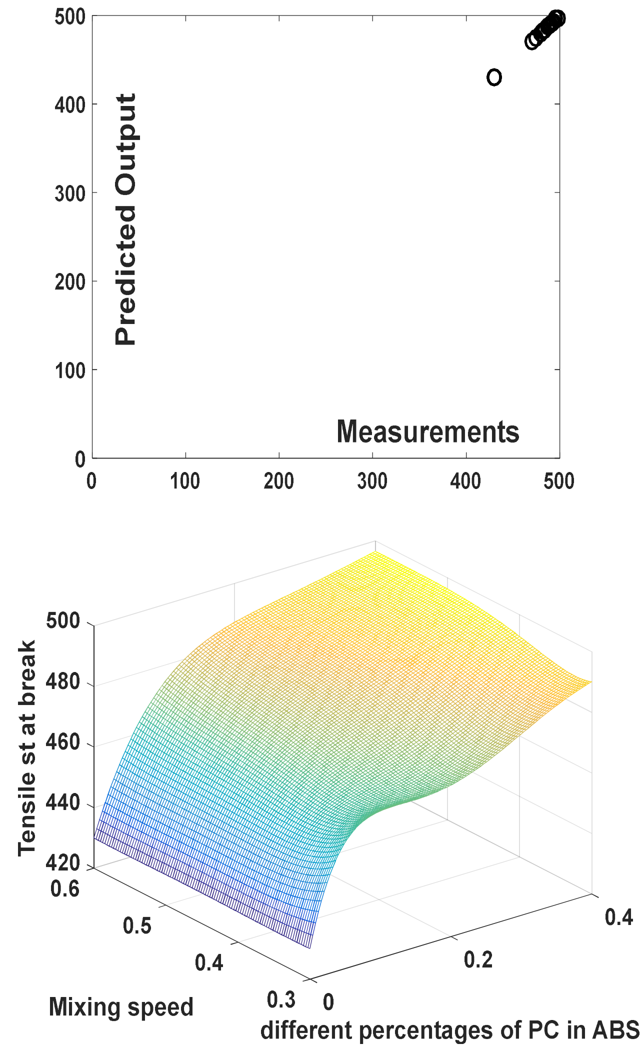


Figure 10. Recall and regeneration of ANN for Tensile at break test in various mixing rates and various percentages of PC/ABS.

The performance diagram and generalization of the results of the impact test in yield point are shown in Figure 10. The results of the simulation have perfect coverage of laboratory data.

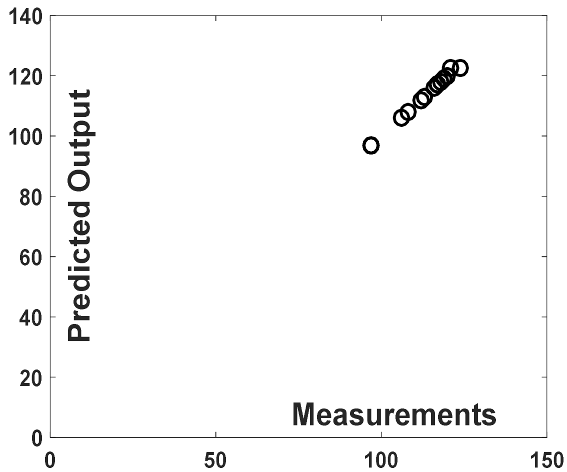
Figure 11 shows the results related to the simulation of the polymer's flexibility index that the accumulation of the points and them sitting on top of each other declares full coverage of simulation results and laboratory data. Also, the generalization performance diagram is a surface without any noise.

4. Conclusions

Collected data from simulation by MLP method of ANN cover laboratory data perfectly. By increasing the PC percentage in ABS, the value of the impact test, polymer hardness, and tension in the yield point increase and the melt flux index decreases. At constant percentages of PC in ABS, increasing the stirring rate values of all tests increase except for the MFI test. According to the high quality of produced polymer due to the high numerical value of all tests except for the melt flow index test, for reaching higher quality of this polymer, it is better to procced with higher stirring rates.

Declaration of Interests

The author declare that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.



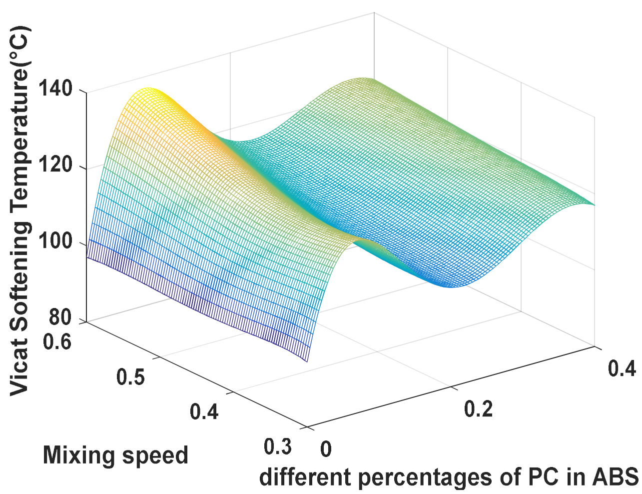


Figure 11. Recall and regeneration of ANN for Vicat softening temperature test in various mixing rates and various percentages of PC/ABS.

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