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Investigating the Influence of Nanoclosite Particles on the Mechanical Properties of Polystyrene Using Artificial Neural Networks

S. Ghazanchaie, F. Derakhshanfard*, L. Amirkhani

Department of Chemical Engineering, Ahar Branch, Islamic Azad University, Ahar, Iran

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ABSTRACT

The synthesized polystyrene has weaknesses in terms of mechanical, physical and thermal properties which limit the use of this polymer. Therefore, the use of the mixtures of polymers can improve these properties. Different parameters like the mixing speed can affect the quality of the properties of the polymer being prepared from the mixture of several polymers. In this study, different percentages of nanocomposites in different stirring speeds have been added to polystyrene. Different tests have been performed on the prepared polymer and investigating the tests shows that in different stirring speeds the values of the tensile strength and impact resistance of the prepared polymer can be increased while the values of the Vicat Softening Temperature (vicat) and Melt Flow Index (MFI) test numbers remain constant. The obtained results from the laboratory data have been simulated by Artificial Neural Networks (ANNs) in order to predict the results for the points which have not been tested and the simulated results show that the laboratory data covered the simulated data perfectly. The results of tests show that by increasing nanoparticles, the resistance of the polymer against impacts will be increased and in addition, increasing the rate of the stirrer causes all other values of tests to increase.

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1. Introduction

Although the polystyrene is one of the highly used plastics having practically helpful properties like water and humidity insulation properties, clarity and optical properties, it has some undesirable properties like low impact resistance and high flammability. Therefore, many researches have been done in this field. In a research, the preparation of polystyrene composites with the modified

*Corresponding author: f.dfard@gmail.com (F. Derakhshanfard)

nano clay has been investigated. By using fillers in nano scales such as types of clay and polystyrene / clay nano composites have been prepared. It has infrastructural, mechanical and thermal properties and improved flammability compared to the pure polystyrene [1].

In a study starch has been mixed with the polystyrene which has impact resistance and the mechanical, thermal, electrical and physical properties of the alloy and of which the bio and optical degradations have also been investigated. Also, the effect of starch on the tensile strength and the hardness of the samples before and after staying on UV exposure has been evaluated. Polystyrene is resistant against impacts, because of having a non-saturated butadiene dual bond which breaks when being exposed to UV waves and suffers from thermal oxide degradation, and is considered as an optically destructible material. Therefore, long chains have been converted to molecules with light weights and after this elimination, the samples have been separated and placed under the tension of lower than 5 percent of breaking tension. Finally, after 5 or 6 months being outside under the sunlight, the impact resistant polystyrene becomes a material with the molecular weight between 1000 to 3000. After 200 hours staying under the optically destructive condition, the biodegradation level has been evaluated. Unlike the resistant polystyrene, starch is a material which is highly biodegradable. Shortly, the alloys, after being under UV waves or in the outdoor environment under the sun, become the materials with lower molecular weights and these polymeric pieces are easily attacked by micro-organisms and suffer from biodegradation, which means these alloys not only suffer from the optical degradation but also suffers from biodegradation. So, after being outdoors for 5 or 6 months, there would not be so much of wastes left from these materials. In general, according to the experiments, the resistance, tensile and flexibility modulus, impact resistance, surface and volumetric resistance, flotation, density, and melt flow index have been reduced by adding starch to the resistant polystyrene. In return, the water hardness, softening temperature and vicat have been increased. On the other hand, it has been proven that the prepared alloy has suffered from both optical degradation and biodegradation. These properties are remarkable and can be used in food packaging industries and the packaging of other products, like disposable tableware, pen, bung and etc., which have short life time and after that time they will be considered as waste. [2-4].

In a study, the preparation of the HIPS nanocomposite and clay nanoparticles and the improvement of their properties have been investigated. The impact resistant polystyrene composites with two types of commercial nano clays, Closite10A and Closite30B, in 3 different percentages of weight at 200 °C and in a time period of 10 minutes, inside an internal mixer have been prepared. Also, in order to compare the results of the samples prepared in the mixer and extruder, 3 samples in extruder with 2 companion spirals with a speed of 70 rpm have been prepared. In order to investigate the morphology, mechanical properties and flowability of mixtures, the small angle UV waves scattering test, optical electron microscopy stress-strain test, impact test and rheology-dynamic test have been done. In the small angle scattering of UV waves test, peaks for the samples prepared from the internal mixer are observed at 2H > 4/6° and 2H > 4/78°. These peaks represent the collapse of the general construction because of the thermal degradation; and these peaks are not observed for processed mixtures in extruder because they were not high [5-8].

Also, the existence of benzene rings in the corrector Closite10A caused a high thermal stability compared to the corrector Closite30B and the observed peaks for Closite10A / HIPS nanocomposites at 2H > 4/6° and 2H > 4/78° had less intensity. By adding only 2 percent of the overall weight, the modulus showed intense increases while the tensile strength did not differ much. By increasing the density of nanoparticles to higher than 5 percent by weight, and because of the aggregation of silicate particles and the strain focus which has been obtained, the modulus and tensile strength will be reduced. Generally, also by adding clay, the length increases until rest and the impact strength decreases intensely. HIPS / Cloistie10A nano composite, because of the strong interaction between silicate sheets and chains, has shown better mechanical properties compared to the similar mixtures of HIPS / Closite30B. Adding only 2 percent by weight of the nano clay, caused an increment in the heat stability of the pure polymer and the temperature of the start of degradation increased to 30 °C. By increasing the overall density (< 5), because of filer-filer interactions and nanoparticles having been cloned, the thermal stability of nanocomposites decreased intensely. By an increase in the density of the clay in lower frequencies, the shear viscosity became zero, storage modulus increased, the Newtonian range decreased and the samples in lower frequencies behaved like plastics. Also, by increasing the frequency, the shear viscosity and nanocomposites storage modulus, because of staying on silicate sheets in flow path to shear viscosity, approaches to pure polymer storage modulus. Because of stronger interactions with polymer matrix instead of HIPS / Closite10A nanocomposites itself, higher shear viscosity and storage modulus have been shown. By studying comfort spectrum curves, it has been observed that by increasing the density of the clay, the comfort time shifts to higher values which is because of the physical and chemical interactions between silicate sheets and polymeric chains that prevents the abandonment of chains [9].

Clay sheets, because of having higher ratio and also having nanometer sized thickness compared to polymeric chains structures, were introduced as ideal fillers. After almost two decades, in year 1993, an investigation group called Toyota caused a great transformation in the nanocomposite technology by successfully building nano composites of the polyamide-nano-clay by the polymerization method. By adding a very small percent of nano clay particles; almost 4 percent, compare to that of the respective polymer, they caused 70 % increase in the stretching modulus and 40 % increase in the tensile strength [10-13]. After that, the researchers can prepare nanocomposites of polyamide in the presence of the clay. Adding a low percent of the nano clay could improve the tensile strength of polymeric materials. However, this could decrease the fragility of polymeric materials in proportion to the impact; but in some cases, the increased elasticity of modulus by multiple times has been reported [14].

In a research, the preparation of HIPS / TiO_2 nanocomposites and their anti-bacterial properties have been investigated. In this research, in order to have HIPS polystyrene (impact resistant) with anti-bacterial properties, the composite and nanocomposite samples of the impact resistant polystyrene and Titanium dioxide have been prepared in 134 micro and p25 nano scales respectively. And their properties have been investigated by each other. Titanium dioxide plays the rule of strengthening the combination and 1 wt % of titanium dioxide in every combination creates the maximum impact resistance and tensile strength. Also, by adding titanium dioxide to the impact resistant polystyrene, the softening temperature and vicat and the MFI number have been improved. Because of better compatibility, ther polymeric matrix "Cristal132" has higher influence on the improvement of thermodynamical properties. In the results of the tensile test and natural weathering test, it has been shown that titanium dioxide plays a major role in reducing the optical destruction of the polymeric matrix. Also, the combinations prepared in this research, have good anti-bacterial effect on the microorganisms of *E. coli* and *staphylococcus aureus* (*S. aureus*) with the title of indicator samples of warm negative bacteria's and warm positive bacteria's. The influence of p25 on bactericidal antibiotics is better than that of crystal 134 due to having a smaller size and more available surface [15-18].

In a research, polystyrene-nanocomposites / layered-silicates were synthesized having used Montmorillon Sedimi (ClositeNa$^+$) and the modified organic clay (Closite30B, Closite15A) in the two different emulsion polymerization and bulk polymerization. In addition to the polystyrene, the copolymer of styrene-metilmetacrylat and nanocomposites of this copolymer have been synthesized too and the products prepared with different techniques have been evaluated. Mont Morilont sedimi used the modified 4-aminoAntipirin combination and approved the results of the modified mont morilont structures. The results of the evaluation of the thermal properties declared that the nanocomposites of polystyrene and nano composites of copolymer have better thermal stability compared to the pure polystyrene. By using uv-vis rays and photography, it has been shown that adding layers of nano silicates to the polymer caused an improvement in the transparency of nanocomposite films. The morphology of the prepared samples has been investigated by SEM images. SEM images have shown that the powder samples of polystyrene and the nanocomposites of Montmorillon Sedimi polystyrene are formed by the spherical particles with the uniform distribution and average size of 58 nanometer (polystyrene) and 63 nanometer (nanocomposite) and the failure level of nanocomposite has been transformed to plastic form due to the existence of clay particles [19-24].

Different studies have been performed in fields of simulating laboratory data with the MLP and RBF methods of ANNs that can predict results for the areas that have not been tested [25-29]. In another study the effects of ABS on GPPS in different percentages (0.00, 0.04, 0.08 and 0.12) and in different stirring speeds (30, 40, 50 and 60) have been investigated and different tests have been performed on the prepared polymer and laboratory data have been simulated by ANNs [28]. The effect of the addition of PET on ABS has been studied and different tests have been performed in order to investigate the prepared polymer. Laboratory data have been studied by ANNS [29].

In this study, different percentages of nanoparticles have been added to polystyrene. The quality of the prepared polymer has been investigated since there has been no study in this filed. The laboratory results have been simulated by the MLP method of ANNs which showed the perfect coverage of the data. Adding nanoparticles into the polystyrene increased the impact and tensile resistance and decreased vicat and MFI values. The reduction in vicat and MFI values is very minor in high stirring speeds and these values can be assumed constant. The more the percentage of nanoparticles, the minimum and maximum values of the tests and in all of the cases, an increase in the stirring speed increases the values of all tests.

2. Materials and equipment

2.1. Materials

The polystyrene with the density of 1.04 g/cc and the residual monomer amount of less than 500 ppm which was supplied by Tabriz petrochemical and the natural clay type of nanocomposite with the density of 1.66 g/cc which was supplied by the Sufiran company and has been compatibilized by Ammonium salt, have been used in this research. The Closit A15 has been compatibilized by four components of the Ammonium salt.

2.2. Methods

In this research in order to prepare polymer nano composites, the penetration in the molten state method has been used. In this method, the mixture of the polymer and nano phase has been heated until Tg (the conversion temperature) or Tm (the melting point of the polymer). Mixing in the molten state is the fastest method for preparing polymeric nanocomposites and includes an extruder or injection device. By using the penetration method, nanocomposites with weight percentages of 0.005, 0.01 and 0.015 have been added to polystyrene and mixed in extruder spins with mixing speed of 30, 40, 50 and 60 rpm and different tests (Vicat, MFI, Tensile strength and impact tests) have been performed on the prepared nanocomposites and the properties of prepared nanocomposites have been investigated.

2.3. Equipment

For mixing the polymer, two spirals and round alignment extruder devices with the screw diameter of 20 mm and the length to diameter ratio of 32, which were supplied by SM Platek company, have been used. An injection device, from Bilion of France, with the extruder temperature 190 °C has been used. The pressure of the injection is 160 bar, the injection area is 3116 cm^2, the template volume is 253 cm^3 and this device is used for the preparation of the parts needed for the tensile and impact tests. The MFI test (coded 702600 from Ceast, Italy) matching the ASTM D1238 standard is performed for measuring the level of easiness of the flow for a molten thermoplastic polymer. For this purpose, in this research, samples in the form of granolas with the weights of 50 g have been used. For the impact test, the polymer coded 6967.00 with ASTM D-256 supplied by Ceast, Italy was used. In order to know the ability of the energy absorption of polymers in different temperatures, the impact test is performed. The greater the needed energy for breaking the polymers, the softer polymers; and contrawise, the lesser the needed energy, the more fragile the polymer. The Vicat softening temperature test, supplied by HD-PC from Yosudo, Japan with ASTM D1525 has been performed. This test is for determining the softening points of materials which have not certain melting points. The vicat softening point, is a temperature at which, and under a certain force, a needle with smooth end penetrates a 1 mm^2 cross section in form of a circle or a square of the test sample in the depth of 1mm. In order to investigate the tensile strength and elongation at break and module submission, a tensional test device has been used. SHIMADZU Autograph AG.X with ASTM D638 was used in order to investigate the elongation at break of the samples.

2.4. Artificial Neural Network (ANN)

Generally, Artificial Neural Networks (ANNs) include several neuronal connections in one or more middle (hidden) layer(s). They are classified from different points of view including: the input conversion type, the structural architecture of the network and the learning algorithm type.

2.4.1. Multi-Layer Perceptron (MLP) network

As explained in previous researches, the MLP networks are made of a number of neurons which are in regular layers. The neurons of the middle layer are doing the real processes, while the input and output layers are just responsible for distributing and collecting the signals. Although several middle layers can be used in MLP networks but the networks with one middle layer are more useful for minor applications because of their simple structure [25-29].

3. Results and discussion

3.1. Laboratory results

Particles of the nanocomposite with different percentages (0.005,0.01 and 0.015) are mixed with polystyrene in different speeds (30, 40, 50 and 60 rpm). Different tests (Vicat Softening temperature, Modular Melt Flow, Tensile, Impact Test) have been performed on the synthesized polymer. The results have been shown in figures 1 to 4. The results of impacts in different mixing speeds and different percentages of nanocomposites in polystyrene have been shown in Figure 1. The impact resistance value for the pure polystyrene is 95 kJ/m^2, that according to the figure, with increasing nanoparticle percentage, this number is increased. So, it can be concluded that increasing nanocomposites in polystyrene will cause an increase in the impact resistance in a way that the higher the percentage, the higher the resistance. Increasing the stirring speed also increases the impact resistance. By increasing the stirring speed from 30 rpm to 60 rpm, the impact resistance increases with an almost constant slope. The more the rate of the mixing, the more the tension which has been entered to the matrix, and as a result, a better distribution of the nano clay and increased impact resistance will accur. In addition, increasing the percentage of the nano clay has a direct effect on the resistance properties against impacts.

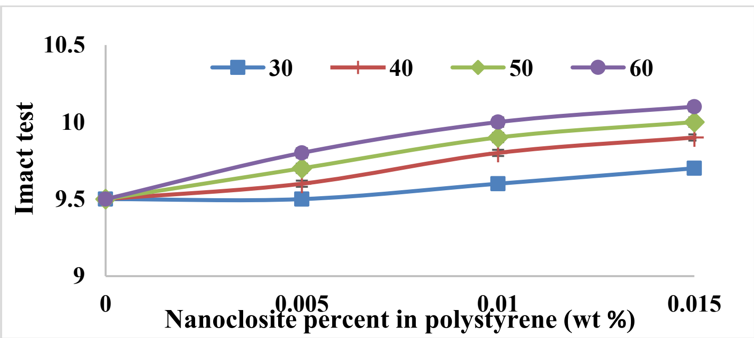


Figure 1. The amount of the impact test for different percentages of nanoclosite in polystyrene in different mixing speeds.

As shown in Figure 2, the value of the MFI number decreases with a slow slope by increasing the percentage of nanocomposites for an stirrer with 60 rpm and with a fast slope for an stirrer with 30 rpm. The result that can be obtained is the fact that in order to prevent the decrease of the MFI number for higher stirring speeds, investigations are needed.

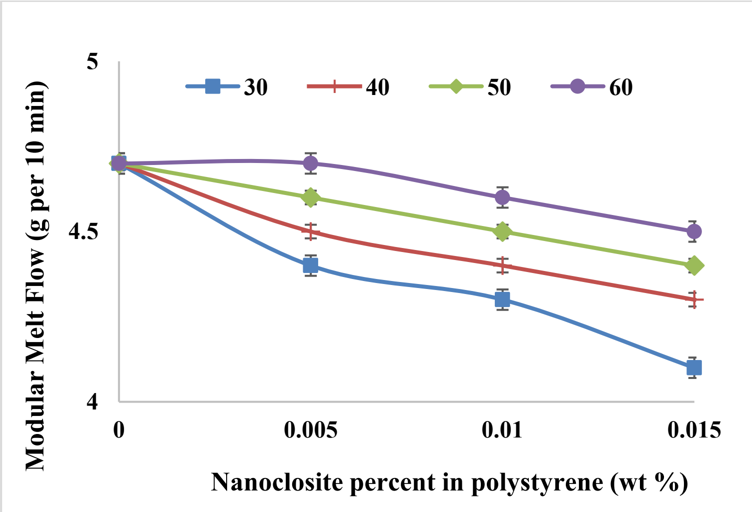


Figure 2. The Melt Flow Index test for the different percentages of nanoclosite in polystyrene in different mixing speeds.

The results related to the tension of prepared samples are shown in Figure 3. As it is clear, the increase in the tension happens for the samples with lower stirrer speed with gentle slope and for the samples with higher stirrer speed with faster slope. By increasing the percentage of nanoparticles, the value of the tension number also increases.

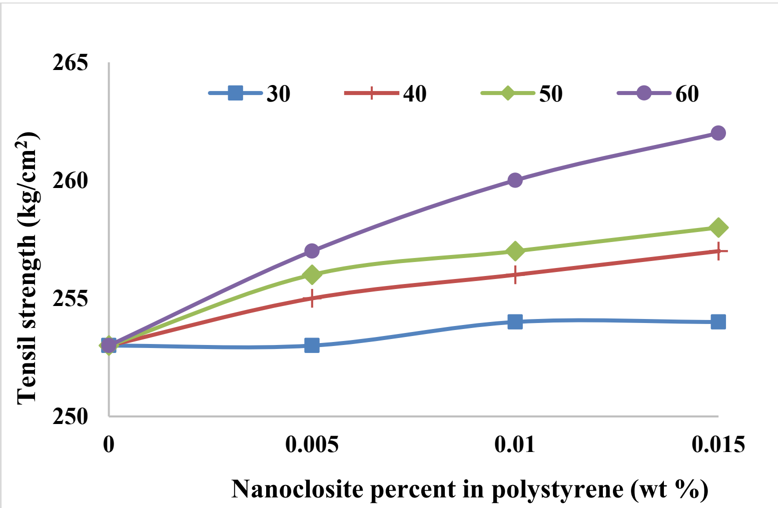


Figure 3. The tensile strength test for the different percentages of nanoclosite in polystyrene in different mixing speeds.

In Figure 4, the results of the vicat test for the prepared samples from nanocomposite in polystyrene in different stirring speeds have been shown. As shown in the figure, by increasing the nanocomposite in polystyrene the value of the vicat number decreases and this decrease is more intense in lower stirring speeds. So, it can be concluded that in higher stirring speeds the amount of the decrement of the vicat number is very minor and its value is almost constant.

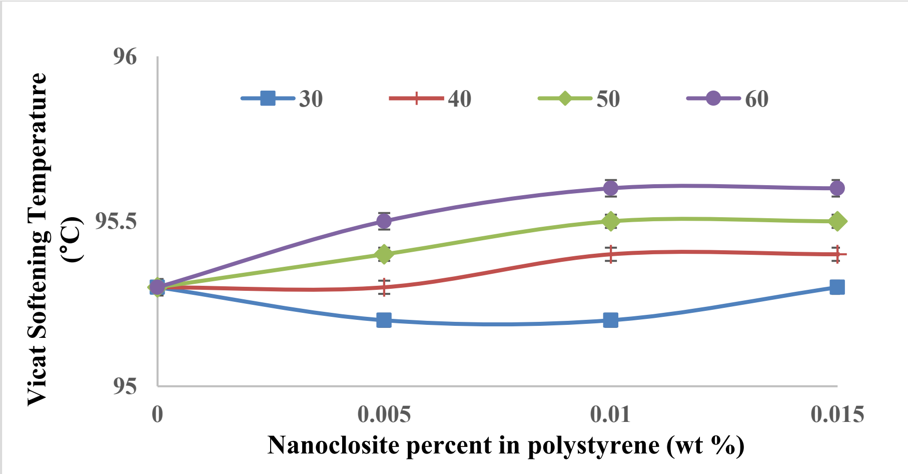
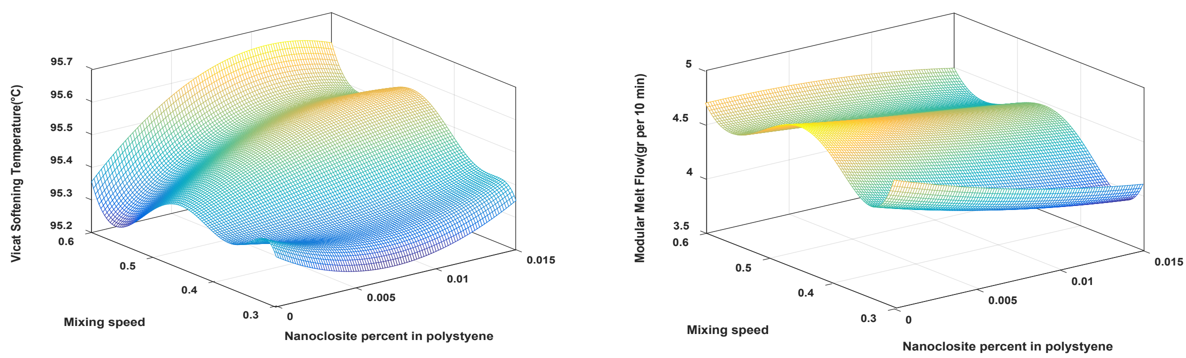


Figure 4. The Vicat Softening Temperature test for the different percentages of nanoclosite in polystyrene in different mixing speeds.

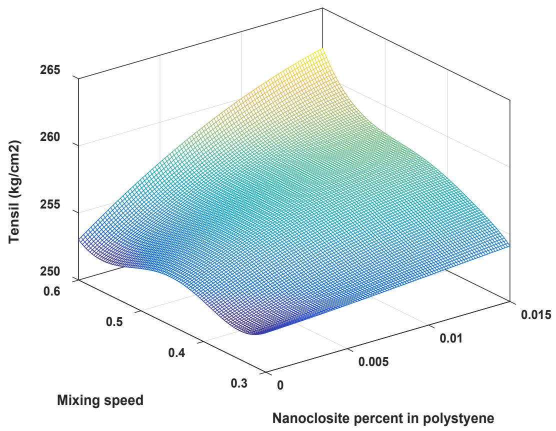
Generally, it can be concluded that with the increase in the amount of the nanocomposites added into the polymer, the values of the MFI and Vicat number decrease and the values of the Tensile strength and the impact test increase but if stirring speed of 60 rpm is to be investigated, in this speed the amount of these tests could be assumed constant by increasing the amount of nanoparticles.

3.2. Simulated results

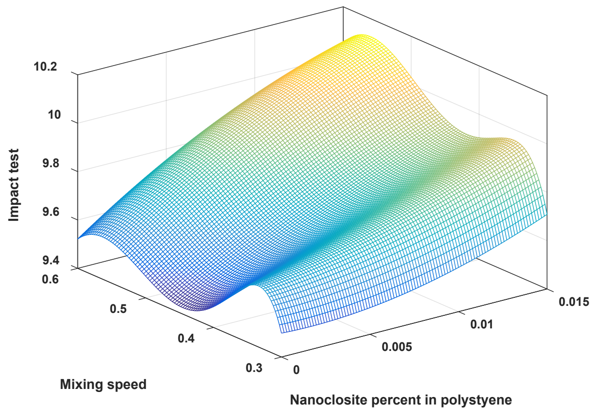
Matlab software has been used for programming artificial neural networks, (MLP) which have been used in the regression of laboratory data, and the obtained procedures show good agreement between the laboratory data and the simulated data. The results of the simulating data prepared by adding the nanocomposite with different percentages to polystyrene in different stirring speeds by ANNs are shown in Figure 5. Different tests have been performed on the prepared polystyrene and the results of the simulation have covered the laboratory data perfectly in a way that simulated results can be used to predict the numerical values of the desired points for which no test has been performed.



(a) (b)



(c)



(d)

Figure 5. The simulations of the Artificial Neural Networks for different tests: a) the Vicat Softening Temperature, b) the Melt Flow Index, c) the Tensile strength, d) the Impact test.

4. Conclusions

- The mixture of nanocomposites with polystyrene with different percentages (0.005,0.01 and 0.015) in different stirring speeds (30, 40, 50 and 60 rpm) has been prepared.
- Different tests (MFI, Vicat Softening Temperature, Tensile strength and Impact test) have been performed on the prepared polymer
- By increase in the nanocomposite added to polystyrene, the resistance of the polymer against impacts has been improved.
- In order to prevent decrease in the MFI test number, it's better to have a higher stirring speed.
- By increasing the amount of the nanoparticles, the amount of the six prepared samples of the nanocomposite and polystyrene increases. The increase ratio in the samples which have been prepared in a high stirring speed (60 rpm) is higher.
- By increasing the amount of the nanocomposite added into polystyrene, the value of the vicat decreases but in stirring speed of 60 rpm, this decrease is very minor.
- By increasing the stirring speed in a constant percentage of the nanocomposite, the numerical amount of all tests increases.
- The simulation by the MLP method of ANNs covered the laboratory data perfectly.

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