Journal of Petroleum Science and Technology 10 (2020) 53-66
DOI:10.22078/jpst.2020.4030.1641

Journal of Petroleum Science and Technology

https://jpst.ripi.ir/

Using Hybrid Artificial Neural Network-Particle Swarm Optimization for Prediction of HIPS Mechanical Properties

Mehdi Pakdel[1] and Alireza Behroozsarand[2*]

[1] *Chemical Engineering Department, Islamic Azad University, Ilkhchi Branch, Ilkhchi, Iran*

[2] *Faculty of Chemical Engineering, Urmia University of Technology, Urmia, IranIhiciisitat aut, Iran*

Abstract

Artificial neural networks (ANN) have emerged as a useful artificial intelligence concept in various engineering applications. Also, ANN only recently has been used in modeling the mechanical behavior of polymers. This study aims to show the applicability of ANNs, to predict and determine the mechanical properties of High Impact Polystyrene (HIPS). Moreover, Izod, Vicat, and MFI of pure HIPS were considered, and the effect of 25 different parameters on them investigated. By using ANN, a black-box model is considered as a calculator of mechanical properties. It is not easy to predict the accurate value of these properties without experimental works for two reasons: (1) the nonlinear behavior of the polymerization process and (2) the inaccuracy of experimental results of measurement of each of the properties. To overcome these problems, an alternative prediction model was proposed for calculating properties using a hybrid ANN-PSO model. All parameters in various cases have been gathered from the industrial DCS system and laboratory for the training of the ANN. First, by using the ANN model, the sensitivity analysis of parameters has been performed. It is then filtered using the effective ANN-PSO hybrid parameters. Out of 25 proposed parameters, 14, 10, 11 of them were selected in MFI, Izod, Vicat, respectively, and used to predict new parameters in the modified ANN. Ultimately, according to the obtained results, it was found that the hybrid ANN-PSO model was powerful in predicting properties with an average relative error of 6, 5, and 1% for predicting considered properties between industrial and computed ANN-PSO hybrid model data.

Key words: High impact polystyrene (HIPS), Izod, Vicat, MFI, Artificial neural network (ANN), Particle swarm optimization (PSO), Hybrid ANN-PSO.

Introduction

Polymers have been widely used in industrial applications due to their suitable thermal and electrical insulation properties, low density, and high resistance to chemicals, but they are mechanically weaker and exhibit lower strength and stiffness than metals [1]. High Impact Polystyrene (HIPS) is one of the oldest styrenic polymers [2]. It is a critical commodity resin because of its improved tenacity when comparison has been made between it and General Purpose Polystyrene (GPPS), competing with Acrylonitrile Butadiene Styrene (ABS), and other impact-resistant plastics in application fields that require good impact properties. This polymer has unique features such as an outstanding balance between rigidity and elasticity that is not found in the unmodified GPPS. Besides, HIPS also present fine optical properties. For this reason, HIPS is used for the manufacture of a large variety of objects, ranging from plastic cups to refrigerator chambers. The main difference between HIPS and GPPS is the fact that GPPS is constituted of polystyrene molecules, while HIPS is produced through grafting of polystyrene chains onto previously prepared elastomeric chains (almost always polybutadiene, PB), using suspension or bulk polymerization processes [3]. Because HIPS is a blending of various materials, accurate estimation of mechanical behavior through experimental testing is essential in blend characterizations and structural design [1]. The ability to predict the physicochemical properties of polymeric materials from the repeating units of their molecular structure is of great value in designing polymers before synthesis [4].

**Corresponding author:* Alireza Behroozsarand, *Renewable Energies Department, Faculty of Chemical Engineering, Urmia University of Technology, Urmia, Iran*
E-mail addresses: a.behroozsarand@uut.ac.ir
Received 2019-12-27, Received in revised form2020-09-01, Accepted 2020-09-19, Available online 2020-11-22

The design of structures and components using newly developed composite materials usually requires extensive (and expensive) testing programs. Ideally, the designer should accurately assess the performance of new material or an existing material under untested conditions using a relatively small database of test results. For these situations, when it is difficult to find an accurate mathematical-based solution and the existing data are incomplete, noisy or complicated, the biologically motivated computing paradigm of artificial neural networks (ANN) has emerged as a superior modeling tool [5].

ANNs are mathematical systems that mimic how the human brain works. A neural network is a collection of interconnecting computational elements simulated like neurons in biological systems. The development of ANN is based on essential computational elements. The first work on neural networks was done by Frank Rosenblatt in the late 1950s and early 1960s. At the same time, by using simple neural models, the first adaptive systems studied by Bernard Widrow and Ted Hoff, and thereby the learning mechanism has been developed by them. ANNs improved by scientists based on ability to apprehend difficult and intricate samples of the brain. ANNs learn from the data, which are related to the problem under study. In other words, the system is trained by experience using appropriate learning examples and without programming. Furthermore, neural networks gather their knowledge by detecting the patterns and relationships in data [6]. Since the process of experimentally investigating a blend's properties can be costly and time-consuming in producing the HIPS unit, this paper explores the potential use of hybrid ANN-PSO methodology in the field of this polymer characterization. It addresses the use of hybrid-ANN in predicting the three main mechanical properties of HIPS. Several useful industrial parameters have been considered. The experimentally acquired data were used to train and test the neural network's performance. The key system inputs for the modeler are 25 effective industrial parameters. The modified multilayered ANN predicted outputs were compared and verified against the available experimental data. In this study, it is indicated that a modified multilayered ANN can simulate the effect of the various effective parameters on the mechanical behavior and properties to a high degree of accuracy. It also demonstrates that the ANN approach is an effective analytical tool which is time-consuming and cost-effective, and will broaden the range of potential applications of polymers in diverse fields.

Materials and Methods

Process Description of Hips Plant

In several petrochemical plants with various licensors, PS PROCESS covers all of the styrenic resins, i.e. 1) GPPS, an amorphous, colorless polymer of styrene as the sole monomer, 2) HIPS, a graft polymer in which synthetic rubber is chemically bonded to GPPS resulting in having impact strength, 3) Styrene Acrylonitrile copolymer (SAN), a copolymer of styrene and acrylonitrile which results in having chemical resistance, and 4) Acrylonitrile Butyl Styrene (ABS) resin that has both impact strength derived from polybutadiene rubber and chemical resistance derived from acrylonitrile. The BFD of this process for producing these products has been shown in Figure 1.

PS PROCESS, a continuous bulk polymerization process, which has a specially designed reactor and devolatilizer using thermal initiation polymerization and precise control of the degree of polymerization as essential technologies, has the following features:

(1) simple process scheme and compact plant layout, (2) the simple and easy operation with fewer grade change times, (3) environmentally friendly, (4) fewer wastes, (5) stable operation and appropriate countermeasures for an emergency, and (6) low raw materials/utility consumption.

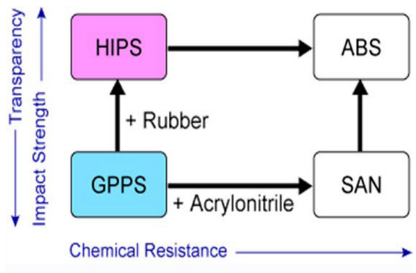

Fig. 1 BFD of styrenic product comparison from the perspective of impact strength, transparency, and chemical resistance.

Especially, the ABS process is an environment-friendly process in comparison with competent technology in terms of the negligible amount of acrylonitrile in the wastewater. There are two significant differences in the production process of these two group products:

1- The number of reactors:

Two series reactors in GPPS and SAN and three of them in HIPS and ABS

2- Feedstocks:

Rubber in HIPS and ABS production processes

Styrene

The manufactured styrene monomer is fed to the polystyrene plant by feeding the line coming from storage facilities for the HIPS unit. The physicochemical specifications of used styrene (at 25 °C) is tabulated in various studies. The specifications are tabulated in appendix#1 of this paper.

Rubber

Stereospecific polybutadiene made by the butyl lithium process (low cis content) is used:

Microstructure types which are as follows:

Trans 1- 4, which is approximately 51%, Cis 1-4, which is approximately 35%, and Vinyl 1-2, which is approximately 11%.

Physical and chemical characteristics:

Uncolored food grade products which are as follows:

Volatiles which their maximum value is 0.7 Wt.%,

Ash which its maximum value is 0.2 Wt.%,

Wet gels which its maximum value is 4 ppm,

Dry gels which its maximum value is 300 ppm,

Viscosity (5 % in styrene), which its value is between 150 to 190 cP,

Color (5 % in styrene) which its maximum value is 15 Alpha,

Antioxidant, with a maximum value in the ranges of 0.25 to 0.5 Wt.%.

The specific grade for HIPS production
A styrene-butadiene block copolymer, polymerized in solution with a lithium catalyst system is used.

Stabilizer System

BHT	%	0.2-0.4	PJ 283
Irganox 1076	%	0.35-0.45	PJ 115
Bound styrene	%	38-42	PJ 272
Toluene insoluble ppm	%	300	PJ 267
Volatiles	.max %	0.2	ASTM D 1416
Ash	.max %	0.2	ASTM D 1416
Soap	%	0	ASTM D 1416
Organic acid	%	0	ASTM D 1416
Viscosity number		210-230	PJ 274

Process Description
The HIPS unit feed is made from polybutadiene rubber in the styrene monomer and adds additives to it. The amount of rubber in the feed varies depending on the type of product that has the lowest value of 3.2% for the 3630 grade, and its maximum value is 14% for the grade 1235. The rubber type for the production of 1235 grade is Styrene-Butadiene Rubber (SBR). Moreover, the SBR used in this process is low cis type, and its high cis type, which is a product of the Arak Petrochemical Complex, has been used up to 50%. The feed preparation process is discontinuous, and the feed supply tank is about 170 m3, which has an agitator. Styrene monomer is recovered in it, and the rubber is crushed and sent to a masonry machine to be dissolved by mixing in the specified time in the styrene monomer and prepare the solution. The solution is also added to the amount of mineral and antioxidant oil and the internal lubricant of zinc stearates. After providing the feed conditions and finishing the mixing time, the solution is sent to two storage tanks to be supplied continuously with the feed unit. In the solution path to the polymerization section, there is a two-stage filtration unit that removes the dissolved particles up to 50 microns, and there is also a filtering step before being sent to storage tanks. The polymerization process is a solvent mass type that is continuously carried out. The start of the reaction in this process is thermal in which up to 5% of the ethylbenzene solvent is used. The reaction section of the HIPS unit consists of three reactors, and the arrangement of these reactors is in series. The reaction feed passage into the reaction section passes through the three reactors above, and the polymerization process is performed. Finally, at the outlet of the third reactor, the percentage of polymer materials is about 75-80%.
The reactor in the first flow path has different types from other reactors. This reactor is of the CSTR type. The operation of this reactor is controlled by the temperature of the feed, reactor temperature, reactor pressure, and fluid height. The amount of polymer formed at the outlet of this reactor is between 25% and 32%, which is a function of the production-grade. In this reactor, the phenomenon of fuzzy phase change occurs. Thus, by converting styrene monomers into polystyrenes and increasing the polystyrene content in the system, the solid polystyrene is transformed into a continuous phase, and the other is converted into a spreadable phase into it. The size of the rubber particles in the continuous phase is very effective on the properties of the polystyrene resistance.
The particle size of the rubber can be adjusted with the mixing rpm of the first reactor.
The flow of the pre-polymer reactor passes through two other Static Mixer Reactor (SMR) type reactors, and eventually, it leaves the reaction portion at about 75% to 80%. Inside these reactors, some coils transfer heat generated by the reaction to the oil that circulates inside these coils. In this way, reaction heat is taken from the system, and the temperature of the reactors is controlled, and the reaction is carried out in a constant temperature profile. The outflow stream contains 20-25% of the monomer that is not reacted to the ethylbenzene solvent. These materials should be separated from the flow and return to the first path of the reaction, which is done in part called the evasive.
The outflow of reactors prior to entering this section (evaporators) is heated by a heat exchanger with hot oil, and the temperature reaches 220 to 230 degrees Celsius. After that, prodduct enters a container with a shallow pressure (15 millimeters of pure mercury). The molten polymer, monomer, and solvent under this condition are showered from the top of the container. The monomer and solvent are isolated from it; product stream direct to a converter in the form of steam. Afterwards, it is converted to liquid and reacts to the first part and is mixed with the original feed. The molten polymer is transferred from the first container to the evaporative vapor of the polymer through the polymer pump, which is injected into the water between two containers of about 0.5%. Water makes the remaining monomer in the final product reach below 500 ppm.
In both containers, the temperature of the polymer is about 230 to 240 °C. The molten polymer is transferred from the second evacuation duct by the polymer transfer pumps to the grinding portion. The molten polymer was deposited based on a 40 degree of contact with the water after it exited from the DIE section of the crushing section, and then it was cooled down by the cutter portion of the plasticizer, in the form of granules, which its diameter and length are 2.5 and 3 millimeters respectively. The granules are transferred to the dry part by water. Their water was then separated and dried by airflow. The granules are then screened, and the fine and coarse grains were separated, and the rest was transferred to the analytical silos by airflow. A laboratory test has been carried out nine times a day on the product, and if there is a problem, it is realy notified to the relevant authorities.
Moreover, because the DCS control system is a control system, the deviation from the control condition is transferred to the operator in the least amount of time. If the analysis silo product is within the defined range of specifications, it is transferred to storage silos. Then it is packaged from there. In Figure 2, the block flow diagram (BFD) of the studied HIPS unit has been presented.
One of the most important issues involved in the polymerization processes and the production of polymer products is the final quality of the product.

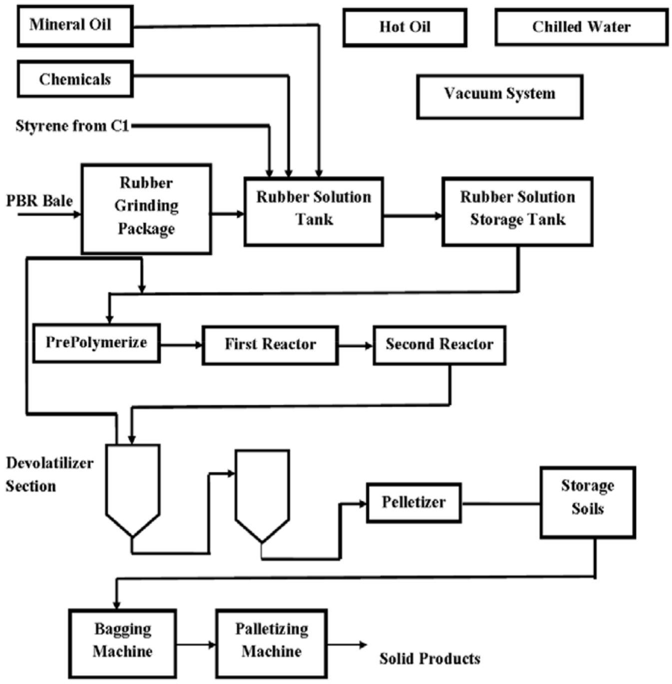

Fig. 2 Simple schematic BFD of studied HIPS unit.

Many indicators have been proposed to evaluate the quality of polymer products, which are referred to below. These indices are measurable for all polymer products, but for each polymer product, some of them are very important. Among all these indicators for the polymer product, MFI, IZOD, and VICAT Indexes are very important for HIPS. Therefore, in this research, the following indexes are considered as the target indexes, which are as follows:

1) The percentage of ethylbenzene and styrene and the volume of impurities in the return flow
2) MFI (melt flow index)
3) IZOD impact strength index
4) VICAT soft Temperature Index
5) The amount of monomer remaining in the SMR product
6) FOOD grade property
7) Permissible moisture content

Applied Hybrid Algorithm

ANN Algorithm

Neural Networks (ANNs) now play an important role in the modeling, control, and optimization of polymerization processes [7]. ANN is one of the most accurate and widely used approaches in forecasting models. It has been shown that a network can approximate each continuous function to any desired accuracy. ANNs are nonlinear and non-parametric methods, unlike traditional plans. However, they may be incomplete because the basic mechanism is nonlinear. Real-world systems are often nonlinear. ANNs are known as stable competition for different polymerization models.

The use of neural networks (ANNs) has become increasingly popular for applications where the mechanistic description of the interdependence of dependent and independent variables is either unknown or very complex. They are now applied as the most popular artificial learning tool with implementation in areas such as pattern recognition, classification, process control, and optimization [7-14]. In the past decade, many weak-reviewed articles showing good results on the application of ANNs have been published in the literature. But several studies with ANNs failed due to the poor predictions outputted by the ANN. These failures resulted in some mistake for the ability of ANNs to deal with some kinds of processes. In part, the criticism is founded due to the fact that although ANNs have been known for some time, they are still in the early stages of development of their underlying theory and many improvements in their structure.

Most papers on the use of ANNs apply a multilayered, feed-forward, and fully connected network of perceptions. Reasons for this kind of ANN are the simplicity of its theory, ease of programming, and good results, and because this ANN is a universal function in the sense that if the topology of the network is allowed to vary freely, it can take the shape of any broken curves.

PSO Algorithm

Particle swarm optimization (PSO) is considered one of the most important methods in swarm intelligence; it utilizes the information of the velocity vector alongside the location of best local and global qualities to update the current values of various problem parameters of each particle in the swarm. In this way, it calculates the value of the optimization function for each swarm particle in their respective locations. Correspondingly, the associated velocity vector of each particle is updated based on the historical backdrop of each particle's problem parameters and misfit-function value. This history stores the knowledge gained by each particle and also by the swarm as a whole, conceptually representing an autobiographical memory. In this manner, the misfit-function estimation of every particle in the swarm is updated by utilizing the social behavior of the swarm, which adjusts to its surroundings by coming back to previously found promising locales of the solution space via looking for optimal misfit function values overtime.

This can be used to solve a wide range of optimization problems such as unrestricted optimization problems, limited optimization problems, nonlinear programming (such as polymerization process), multi-objective optimization, randomized scheduling, and combined optimization problems. Furthermore, PSO is presented in the literature, and it is successful in life applications. The flow diagram of the PSO algorithm is shown In Figure 3.

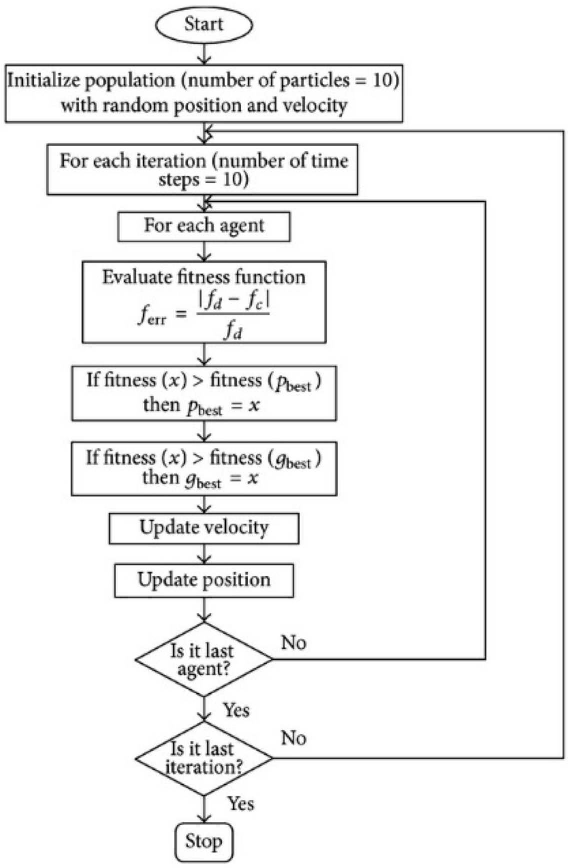

Fig. 3 Mathematical flowchart of the PSO algorithm [15].

Hybrid ANN-PSO Algorithm

The prediction of the mechanical properties of polymers plays a vital role in the planning of the production and selling a program of a petrochemical plant. The quality of the final polymerization product is strongly dependent on the accuracy of operating parameter values, and they also depend on the accuracy of forecasting methods.

It has operational parameters. Conventional methods, including time series, regression analysis, or ARMA model, bring external inputs along with several assumptions. The use of neural networks is an economical technique. But their training, usually with a backward algorithm or other slope algorithms, is shown with some defects such as very slow convergence and easy recording at the local minimum. In this paper, a combination of a neural network with a particle swarm optimization training algorithm for the development of prediction accuracy is presented. Experimental results show that the proposed approach can achieve better predictive performance.

Problem Formulation

In each process, there are process parameters for achieving the desired quality product, which can be achieved by changing them within a reasonable range. In the considered production of HIPS, these parameters have been tabulated in Table 1.

It should be noted that some of the parameters mentioned can be controlled and changed. In the modeling sections, the parameters used in this paper are mentioned.

All values of these parameters have been gathered from the DCS office of the considered industrial HIPS plant. The number of these set data is 200. The final members of these set data are MFI, Izod, and Vicat values as target values or objective functions. In Table 2 An example of the data used in the modeling of the different sections has been shown.

The modeling work of the system has been done in three steps:

1- Modeling of the system by using all data sets with the ANN tool.

2- Filtration, identification, and classification of all data sets in two categories, i.e. effective and ineffective parameters by using the PSO algorithm.

3- Modeling of the system by using new data sets with the ANN tool.

Neural Network Models

In recent years, the concept of neural networks has gained wide popularity in many fields of chemical engineering, such as dynamic modeling of chemical processes, design of catalysts, modeling of chemical reactors, and modeling of the complex chemical process [16]. In this research, to simulate the HIPS plant and predict the mechanical properties value, the arrays of appropriate 25-layer neural networks have been designed with a different number of hidden layer neurons and network training algorithm.

Table 1 List of effective parameters on MFI, Izod, and Vicat indexes.

No.	Parameter name	No.	Parameter name	No.	Parameter name
1	EB % in V201	10	Temperature of 1th loop	19	rpm of P-209
2	SM % in V201	11	Temperature of 2th loop	20	Pressure of the first devolatilizer
3	Temperature of R-202 in the middle section	12	Temperature of 3th loop	21	Pressure of the second devolatilizer
4	Temperature of R-202 at the bottom section	13	Temperature of 4th loop	22	Temperature of the cutter
5	Level of R-202	14	Temperature of R-203 outlet	23	SM content of the daily feed
6	rpm of R-202 mixer	15	Temperature of 5th loop	24	Rubber content of the daily feed
7	rpm of P-202	16	Temperature of 6th loop	25	Mineral oil content of the daily feed
8	Fresh feed	17	Temperature of R-204 outlet		
9	Recycle stream	18	Pressure of R-204 outlet		

Table 2 Sample of modeling data of HIPS plant.

Input Process DCS Data							
DAY PA-RAMETER	V201-EB (wt.%)	V201-SM (wt.%)	TI207 (˚C)	TIC208 (˚C)	LIC203 (m)	MX201 (rpm)	P202 (rpm)
1	5	92	131	131	72	36	72
2	4.72	91	131.06	131.26	71.67	35.63	71.8
3	4.73	91.02	130.82	130.97	72.24	36.62	71.79
4	5.62	89.4	130.89	131.02	71.97	36.73	71.71
5	5.72	90.49	130.26	130.37	72.16	35.63	71.76
6	6.38	89.15	128.24	128.73	71.71	38.55	69.9
7	6.79	89.88	129.02	130.14	71.4	38.53	69.07
8	7.16	89.3	128.67	129.57	71.7	38.53	68.39
9	7.26	89.3	128.13	129.34	71.88	38.53	69.82
10	8.21	89.9	130.38	130.83	70.13	40.57	70.91

Input Process DCS Data									
FIC201 (m^3/hr)	FI202 (m^3/hr)	TIC214 (^{0}C)	TIC224 (^{0}C)	TIC235 (^{0}C)	TIC245 (^{0}C)	TI246 (^{0}C)	TIC255 (^{0}C)	TIC265 (^{0}C)	TI267 (˚C)
7.00	5	158	157	175	167	164	165	131	207.00
6.98	4.59	158	157.99	174.58	167.99	165.66	165.07	131.96	208.12
6.98	4.65	157.94	157.98	174.63	167.96	166.81	164.53	130.97	208.54
6.50	4.76	158.02	157.96	175.55	168.91	167.41	164.9	130.99	206.47
6.34	4.94	157.3	156.98	173.47	168.02	162.32	164.35	133.47	206.47
7.70	3.67	141.71	142.77	146.90	151.11	159.23	142.01	140.05	168.20
7.98	3.53	141.97	142.88	146.81	151.00	159.59	142.03	140.02	167.96
7.98	3.55	141.83	142.98	146.94	151.09	159.41	141.02	139.91	166.5
7.84	3.72	141.8	142.91	146.91	151.06	159.17	141.94	140.01	167.22
7.48	4.3	140.94	144.88	150.88	152.96	159.80	151.51	130.45	175.06

Input Process DCS Data							
PIC265 (bar g)	P209 (rpm)	PI271 (mbar)	TI286 (^{0}C)	TIC341 (^{0}C)	Feed SM (Ton/day)	Feed PBR (Ton/day)	Feed Min. oil (Ton/day)
4	25	66	150	38	113.00	12.00	3.00
4.46	24.56	57.18	163.49	38.92	119.34	13.36	2.89
4.44	24.38	58.57	162.58	39.38	119.37	13.34	2.89
4.36	24.08	66.24	160.93	39.78	116.19	12.99	2.82
4.42	24.11	54.93	148.05	39.67	114.46	12.96	2.78
4.45	23.36	56.82	166.21	39.86	136.12	16.2	4.88
4.39	23.37	52.44	166.04	39.8	137.49	15.92	4.99
4.44	23.09	52.49	163.47	39.95	136.22	16.00	4.98
4.37	23.51	58.25	165.12	40.05	136.12	16.27	4.82
4.41	24.19	46.91	162.57	39.86	132.25	15.74	3.20

Input Process DCS Data		
Output-Experimental.		
MFI(gr/10 min)	IZOD (kJ/m^3)	VICAT(^{0}C)
5.17	8.7	97.6
5.00	8.6	97.7
4.85	8.1	98.2
5.17	8.8	98.1
4.53	9.1	96.2
4.90	8.5	98.2
4.90	8.2	98.4
4.78	9.5	97.8
4.08	9.9	97.4
4.38	8.4	96.7

The network includes 25 input layers that provide input data to the network, ten hidden layers and an output layer that represents network response, as seen in Figure 4. The number of input and output nodes is governed by functional requirements of the ANN sigmoid transfer function used for the hidden layer, and the output transfer function was a linear function. The system was trained with a backpropagation neural network (BPNN), and Levenberg-Marquart was used as a training algorithm in all modeling cases.

Training of the designed ANN was performed using DCS results of industrial HIPS plant in changes of independent variables. Since the applied transfer function of hidden layers is sigmoid, we scaled all input vectors in the interval [0, 1].

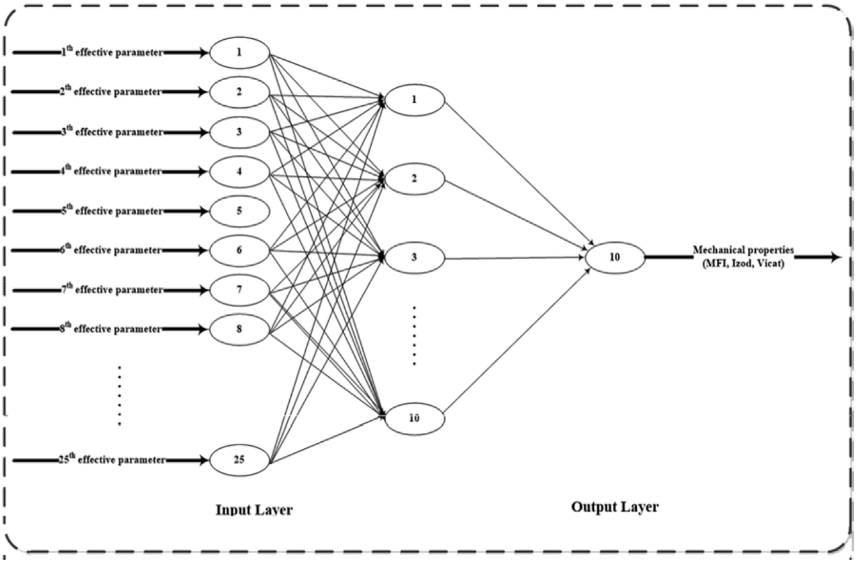

Fig. 4 Final proposed neural network scheme.

The data were split into three subsets: training, validation, and test set. Splitting of samples plays an important role in the evaluation of an ANN performance. The training set is used to estimate the model parameters and the test set is used to check the generalization ability of the model. In this work, 1594 data were gathered from the DCS system. The training, validation, and test sets include 139 data (70% of total data approximately), 30 data (15% of total data), and 30 data (15% of complete data) respectively.

Results and Discussion

In Figures 5, 6, and 7, the results of regression between network outputs and data sets of validation, and training and test targets MFI, Izod, and Vicat are shown respectively. It is observed that the Izod and Vicat track the targets well. The correlation coefficient (R) measures the correlation between outputs and objectives. The R-value of 1 means a close relationship and 0 a random link. As shown in Figures 8 to 10, the correlation coefficients between all independent variables and dependent variables (MFI, Izod, and Vicat) are about 0.498, 0.942, and 0.989 respectively. The performance curve of the 10 hidden neurons for the Izod variable is shown in Figure 8.

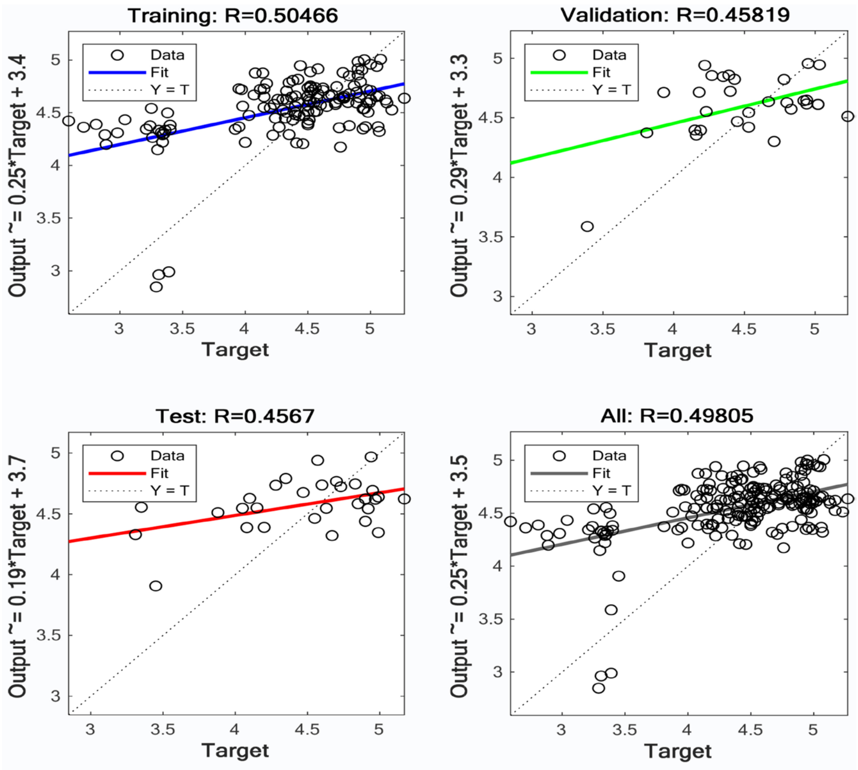

Fig. 5 Results of ANN in the modeling of MFI value.

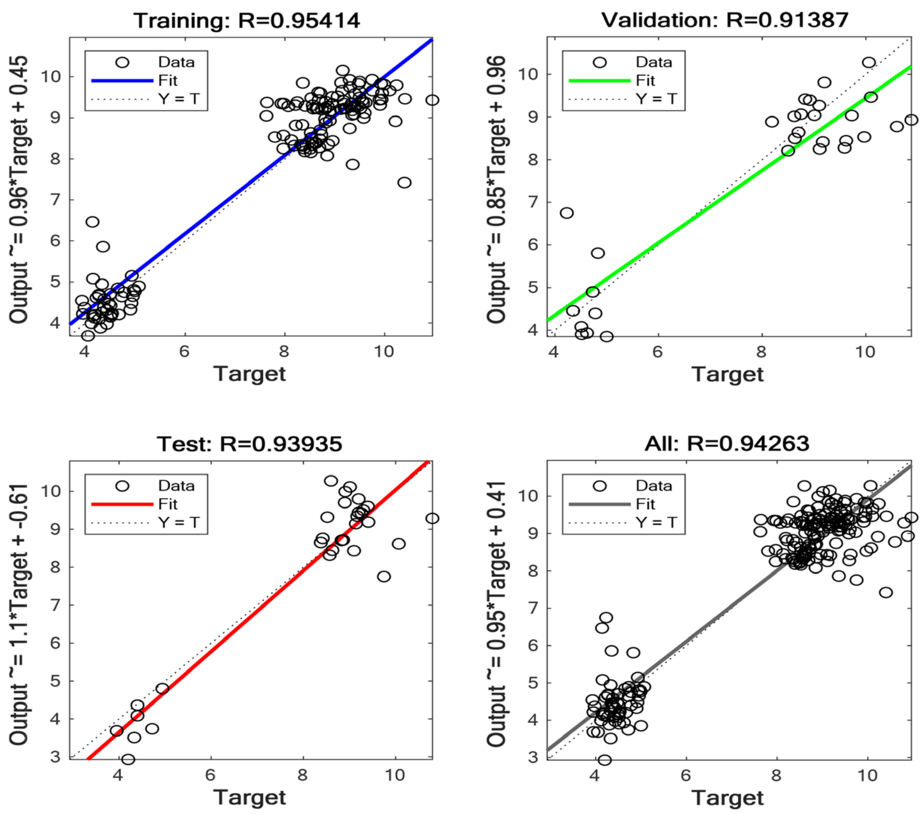

Fig. 6 Results of ANN in the modeling of Izod value.

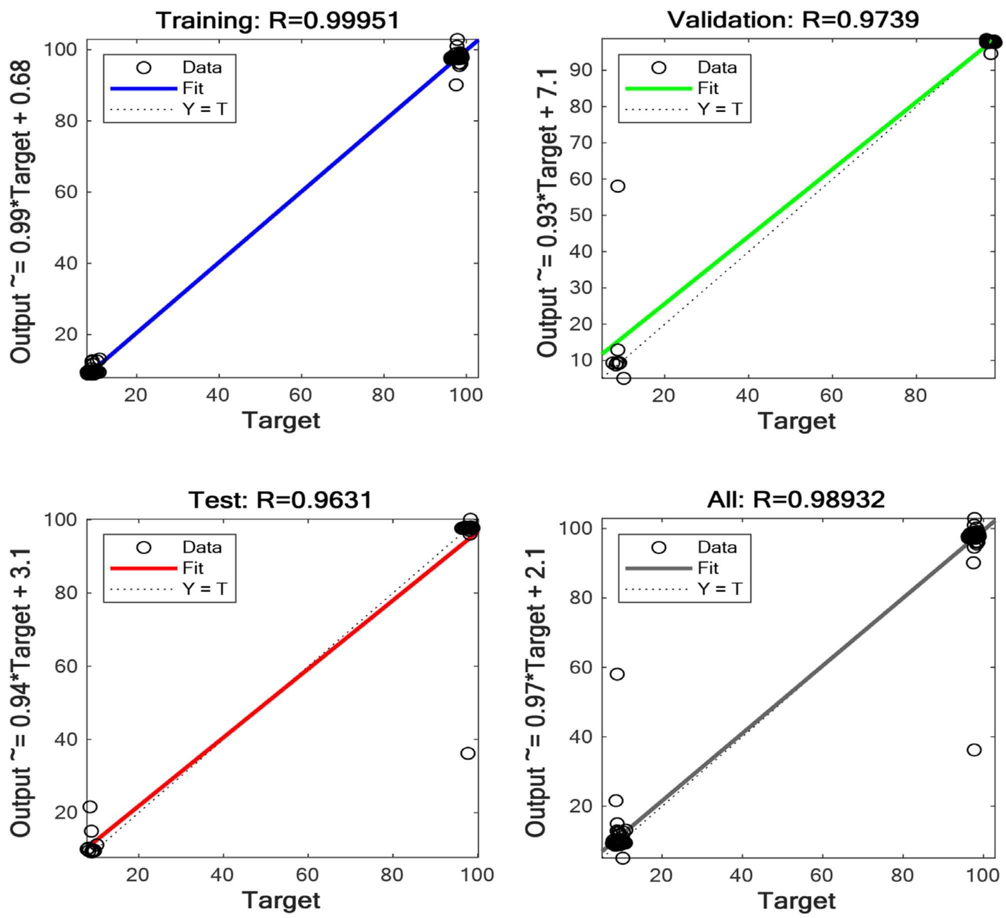

Fig. 7 Results of ANN in the modeling of Vicat value.

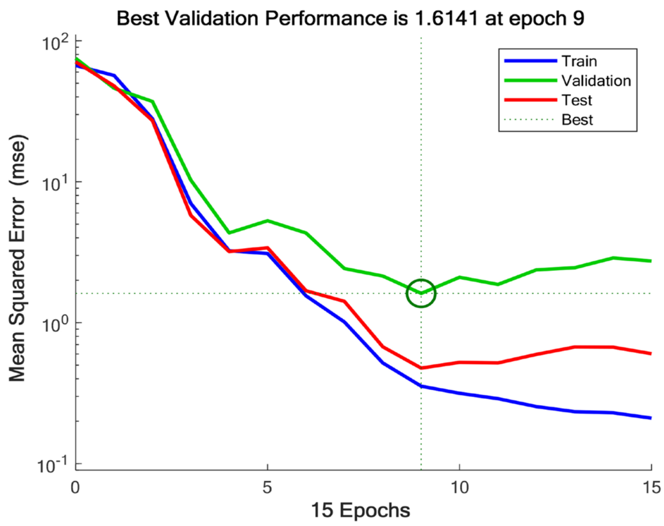

Fig. 8 The MSE performance curve of Izod modeling.

One of the most important parameters in the performance and accuracy of neural networks is the number of hidden layers in the network. Therefore, in this section, the effect of the number of neural networks hidden layers on the correlation coefficient and mean squared error has been investigated. The number of hidden layers considered in five levels (5, 10, 15, 20, and 100). Results showed that this parameter has no considerable effect on the correlation coefficient of MFI, Izod, and Vicat. The range of changes is about 0.48-0.68, 0.55-0.93, 0.48-0.68 respectively. Since the value of this coefficient is less than 0.97, it is not possible to conclude that when different parameters can be considered for the network performance, this growth factor is significant (Table 3).

Table 3 Results of several hidden layer effect on ANN performance.

MFI parameter					
Number of hidden layers	5	10	15	20	100
Training No. Sample	139	139	139	139	139
Validation No. Sample	30	30	30	30	30
Testing No. Sample	30	30	30	30	30
Training MSE	0.212	0.152	0.282	0.155	0.153
Validation MSE	0.177	0.282	0.144	0.190	0.280
Testing MSE	0.162	0.312	0.530	0.345	0.507
Training R	0.665	0.775	0.654	0.716	0.794
Validation R	0.492	0.428	0.760	0.597	0.564
Testing R	0.668	0.385	0.479	0.531	0.303
All R	0.636	0.665	0.478	0.659	0.676
Izod parameter					
Training MSE	0.521	0.48	0.717	0.431	0.478
Validation MSE	0.468	1.57	0.561	0.55	3.15
Testing MSE	1.160	0.516	1.920	0.551	1.078
Training R	0.941	0.949	0.925	0.953	0.946
Validation R	0.942	0.808	0.941	o.432	0.789
Testing R	0.894	0.949	0.779	0.550	0.855
All R	0.931	0.929	0.905	0.551	0.889
Vicat parameter					
Training MSE	0.212	0.152	0.282	0.155	0.153
Validation MSE	0.177	0.282	0.144	0.190	0.280
Testing MSE	0.162	0.312	0.530	0.345	0.507
Training R	0.665	0.775	0.654	0.716	0.794
Validation R	0.492	0.428	0.760	0.597	0.564
Testing R	0.668	0.385	0.479	0.531	0.303
All R	0.636	0.665	0.478	0.659	0.676

A Hybrid ANN and PSO Model

As seen in the previous section, the maximum correlation coefficients between the independent variables (25 variables) and the dependent variables for MFI, Izod, and Vicat were 0.68, 0.93, and 0.68. Various factors can be the reason for this weak prediction— some of the factors are mentioned as follows:

1) Inappropriate distribution of data,
2) Measurement errors in the data,
3) Severe operational changes during product production,
4) Malfunctioning of the mathematical method, and
5) The inability of some parameters.

In this study, hybrid PSO and ANN models were applied to identify the most effective variables. The model was proposed to generate an index matrix, based on a feed-forward ANN optimized by PSO. This optimization algorithm was employed for the identification of effective variables on the training performance of ANN. In this matrix (Table 4), the number 1 means that the variable affects the target function, and zero means that the variable does not affect the target function. In Table 5, all information about the hybrid PSO-ANN model is illustrated.

In the first iteration of the hybrid of PSO-ANN, index and best matrix have the same values in all elements equal 2 and 1, respectively. After ten iterations and the calculation of the correlation coefficient at each step, final results have been calculated. All output results of hybrid PSO-ANN are presented in Table 6.

As shown in Table 6, after ten iterations, the correlation coefficients gained 0.979, 0.996, and 0.999 values for MFI, Izod, and Vicat, respectively, and these values are desirable. But as previously mentioned, the goal of this algorithm is to identify variables that are effective on mechanical properties. The index matrix showed that from all 25 variables, only 14 (MFI), 10 (Izod), and 11 (Vicat) of them have considerable effects on mechanical properties.

In the next step of modeling, these effective data sets have been considered for training, validation, and testing of the modified Neural Network model.

Table 4 List of indexes value of effective parameters in three target variables.

Item Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	-
Effective parameters	EB % in V201	SM % in V201	Temp. of R-202 in the middle section	Temp. of R-202 at the bottom section	Temp. of R-202 at the top section	Level of R-202	rpm of R-202 mixer	rpm of P-202	Fresh feed	Recycle stream	Temp. of 1st loop	Pressure of the first zone	Temp. of 2nd loop	Temp. of 3rd loop	Temp. of 4th loop	Temp. of R-203 outlet	Temp. of 5th loop	Temp. of 6th loop	Temp. of R-204 outlet	Pres. Of R-204 outlet	rpm of P-209	Press. of the first devolatilizer	Press. of the second devolatilizer	Temp. of the cutter	SM content of the daily feed	Number of effective parameters
MFI	0	1	0	0	0	0	1	0	1	0	1	1	1	0	1	0	1	1	1	1	0	1	0	1	1	14
Izod	1	0	1	1	0	0	1	1	0	0	1	1	0	0	1	0	0	0	0	1	1	0	0	0	0	10
Vicat	1	1	0	0	0	1	1	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	1	0	11

Table 5 Information on hybrid PSO-ANN model.

PSO input data	
Particle size	10
Number of parameters	9
epoch	5
c1: learning factor	1.4047
c2: learning factor	1.494
ANN input data	
ANN type	generalized regression neural network
spread	0.01
Number of layers	2
Transfer function of the first layer	radial basis
Transfer function of the second layer	purelin

A Modified Neural Network Model

After filtration of all data by using a hybrid PSO-ANN algorithm, and removing ineffective data sets, the modified ANN scheme applied to a new modeling program. In addition to the change of data in the modified ANN, there is another fundamental change in the choice of the type of neural network. As mentioned previously, the generalized regression neural network method was used, while in the new state, the radial basis network was used.

Description of function in MATLAB:

net = newrb (P, T, goal, spread, MN, DF) takes two of these arguments,

P: R-by-Q matrix of Q input vectors

T: S-by-Q matrix of Q target class vectors

Goal: Mean squared error goal (default = 0.0)

Spread: Spread of radial basis functions (default = 1.0)

MN: Maximum number of neurons (default is Q)

DF: Number of neurons to add between displays (default = 25)

In this study, a new function was used with the default setting. After 170 iterations mean squared error (MSE) of the goal in all cases reached to zero value. All of the data used in this model is similar to the previous ones, and the data classifications for training and testing were similar.

In Figure 9, the performance of radial basis network models in the training step is displayed. As noted above, because of the default settings of the function used, MSE, as the main performance feature, was zero after 170 iterations, and this result shows that all training is very appropriate with the modified data.

Similar to the previous states in the study of neural networks, the best indicator in the investigation of the strength and accuracy of the method is to examine the outputs for testing data in all cases. Results showed that data predictions of new ANN were so near to actual industrial data of MFI, Izod, and Vicat properties. All results of them have been illustrated in Table 7. According to this table, maximum, minimum, and average relative error (R.E.) are 6, 5, and 1% for three properties, respectively. That is the acceptable value for an industrial styrene monomer plant as part of a nonlinear polymerization process. It is noted that, according to the calculated index matrix by hybrid PSO-ANN, sufficient value has been used for modeling and represented in Table 7.

Table 6 Final results of hybrid PSO-ANN.

hybrid PSO-ANN for MFI	
Iteration = 1	Correlation=-2.165368e-16
Iteration = 2	Correlation=9.728884e-01
Iteration = 3	Correlation=9.728884e-01
Iteration = 4	Correlation=9.789867e-01
Iteration = 5	Correlation=9.789867e-01
Iteration = 6	Correlation=9.789867e-01
Iteration = 7	Correlation=9.789867e-01
Iteration = 8	Correlation=9.789867e-01
Iteration = 9	Correlation=9.789867e-01
Iteration = 10	Correlation=9.794914e-01
gbest	0.75 0.64 0.25 0.38 0.48 0.65 0.80 0.78 0.13 0.53 0.94 0.32 0.28 0.32 0.86 0.69 0.92 0.70 0.55 0.62 0.89 0.42 0.01 0.67 0.83
pbest	0.75 0.64 0.25 0.38 0.48 0.65 0.80 0.78 0.13 0.53 0.94 0.32 0.28 0.32 0.86 0.69 0.92 0.70 0.55 0.62 0.89 0.42 0.01 0.67 0.83
Index	[0 1 0 0 0 0 1 0 1 0 1 1 1 0 1 0 1 1 1 0 1 0 1 1]
hybrid PSO-ANN for Izod	
Iteration = 1	Correlation=-1.422352e-15
Iteration = 2	Correlation=9.857524e-01
Iteration = 3	Correlation=9.938434e-01
Iteration = 4	Correlation=9.959451e-01
Iteration = 5	Correlation=9.959451e-01
Iteration = 5	Correlation=9.959451e-01
Iteration = 6	Correlation=9.959451e-01
Iteration = 7	Correlation=9.959451e-01
Iteration = 8	Correlation=9.959451e-01
Iteration = 9	Correlation=9.959451e-01
Iteration = 10	Correlation=9.959451e-01
gbest	0.69 0.63 0.50 0.63 0.41 0.30 0.84 0.09 0.46 0.13 0.88 0.95 0.77 0.36 0.32 0.08 0.97 0.74 0.62 0.42 0.82 0.53 0.67 0.48 0.51
pbest	0.78 0.19 0.32 0.58 0.64 0.74 0.63 0.22 0.18 0.27 0.68 0.64 0.64 0.39 0.08 0.21 0.01 0.85 0.25 0.25 0.89 0.50 0.55 0.71 0.48
Index	[1 0 1 1 0 0 1 1 0 0 1 1 0 0 1 0 0 0 0 1 1 0 0 0 0]
hybrid PSO-ANN for Vicat	
Iteration = 1	Correlation= -1.113540e-15
Iteration = 2	Correlation=9.999688e-01
Iteration = 3	Correlation=9.999799e-01
Iteration = 4	Correlation=9.999799e-01
Iteration = 5	Correlation=9.999871e-01
Iteration = 6	Correlation=9.999871e-01
Iteration = 7	Correlation=9.999871e-01
Iteration = 8	Correlation=9.999871e-01
Iteration = 9	Correlation=9.999871e-01
Iteration = 10	Correlation=9.999871e-01
gbest	0.99 0.16 0.74 0.79 0.61 0.70 0.33 0.99 0.57 0.36 0.54 0.81 0.44 0.40 0.13 0.21 0.67 0.72 0.78 0.26 0.40 0.30 0.69 0.46 0.68
pbest	0.78 0.26 0.26 0.88 0.14 0.81 0.49 0.85 0.52 0.63 0.54 0.51 0.33 0.63 0.64 0.17 0.06 0.66 0.73 0.09 0.11 0.40 0.63 0.58 0.79
Index	[1 1 0 0 0 1 1 0 1 0 1 1 0 0 1 0 0 0 0 1 0 1 0 1 0]

Table 7 Final information and results of modified ANN.

Goal parameters	MFI	Izod	Vicat
Min. of absolute error	0%	0%	0%
Max. of absolute error	20%	16%	1%
Average of absolute error	6%	5%	1%

.Data No	SM % in V201	rpm of P-202	Recycle stream	Temp. of 2nd loop	Temp. of 3rd loop	Temp. of 4th loop	Temp. of 5th loop	Temp. of R-204 outlet	Pres. Of R-204 outlet	rpm of P-209	Press. of the first devolatilizer	Temp. of the cutter	Rubber content of the daily feed	Mineral oil content of the daily feed	MFI-Industrial	MFI-Calculated	(%) Relative Error
1	92.1	71.8	4.8	157.0	174.6	166.9	164.8	206.8	4.4	24.7	65.9	38.1	12.3	2.8	5.17	5.23	1%
2	91.0	71.8	4.6	158.0	174.6	168.0	165.1	208.1	4.5	24.6	57.2	38.9	13.4	2.9	5.00	4.83	3%
3	91.0	71.8	4.7	158.0	174.6	168.0	164.5	208.5	4.4	24.4	58.6	39.4	13.3	2.9	4.85	4.83	0%
4	89.4	71.7	4.8	158.0	175.6	168.9	164.9	206.5	4.4	24.1	66.2	39.8	13.0	2.8	5.17	4.15	20%
5	90.5	71.8	4.9	157.0	173.5	168.0	164.4	206.5	4.4	24.1	54.9	39.7	13.0	2.8	4.53	4.63	2%
6	89.2	69.9	3.7	142.8	146.9	151.1	142.0	168.2	4.5	23.4	56.8	39.9	16.2	4.9	4.90	4.95	1%
7	89.9	69.1	3.5	142.9	146.8	151.0	142.0	168.0	4.4	23.4	52.4	39.8	15.9	5.0	4.90	4.27	13%
8	89.3	68.4	3.6	143.0	146.9	151.1	141.0	166.5	4.4	23.1	52.5	40.0	16.0	5.0	4.78	4.39	8%
9	89.3	69.8	3.7	142.9	146.9	151.1	141.9	167.2	4.4	23.5	58.3	40.1	16.3	4.8	4.08	4.58	12%
10	89.9	70.9	4.3	144.9	150.9	153.0	151.5	175.1	4.4	24.2	46.9	39.9	15.7	3.2	4.38	4.70	7%

.Data No	SM % in V201	Temp. of R-202 at the bottom section	Level of R-202	Fresh feed	Recycle stream	Temp. of 3rd loop	Temp. of 4th loop	Temp. of 6th loop	Press. of the second devolatilizer	Temp. of the cutter	Izod-Industrial	Izod -Calculated	(%) Relative Error
1	4.7	131.0	131.1	71.8	6.9	157.0	174.6	164.8	65.9	149.8	8.7	8.6	2%
2	4.7	131.1	131.3	71.8	7.0	158.0	174.6	165.1	57.2	163.5	8.6	8.6	1%
3	4.7	130.8	131.0	71.8	7.0	158.0	174.6	164.5	58.6	162.6	8.1	8.6	6%
4	5.6	130.9	131.0	71.7	6.5	158.0	175.6	164.9	66.2	160.9	8.8	8.7	1%
5	5.7	130.3	130.4	71.8	6.3	157.0	173.5	164.4	54.9	148.1	9.1	8.4	8%
6	6.4	128.2	128.7	69.9	7.7	142.8	146.9	142.0	56.8	166.2	8.5	8.7	2%
7	6.8	129.0	130.1	69.1	8.0	142.9	146.8	142.0	52.4	166.0	8.2	7.6	7%
8	7.2	128.7	129.6	68.4	8.0	143.0	146.9	141.0	52.5	163.5	9.5	8.8	7%
9	7.3	128.1	129.3	69.8	7.8	142.9	146.9	141.9	58.3	165.1	9.9	9.2	7%
10	8.2	130.4	130.8	70.9	7.5	144.9	150.9	151.5	46.9	162.6	8.4	9.7	16%

	EB % in V201	SM % in V201	rpm of R-202 mixer	rpm of P-202	Recycle stream	Temp. of 2nd loop	Temp. of 3rd loop	Temp. of 5th loop	Press. of the first devolatilizer	Temp. of the cutter	Rubber content of the daily feed	Vicat-Industrial	Vicat -Calculated
1	4.7	92.1	35.6	71.8	4.8	157.0	174.6	164.8	65.9	38.1	12.3	97.6	98.3
2	4.7	91.0	35.6	71.8	4.6	158.0	174.6	165.1	57.2	38.9	13.4	97.7	97.9
3	4.7	91.0	36.6	71.8	4.7	158.0	174.6	164.5	58.6	39.4	13.3	98.2	97.7
4	5.6	89.4	36.7	71.7	4.8	158.0	175.6	164.9	66.2	39.8	13.0	98.1	97.5
5	5.7	90.5	35.6	71.8	4.9	157.0	173.5	164.4	54.9	39.7	13.0	96.2	97.6
6	6.4	89.2	38.6	69.9	3.7	142.8	146.9	142.0	56.8	39.9	16.2	98.2	98.5
7	6.8	89.9	38.5	69.1	3.5	142.9	146.8	142.0	52.4	39.8	15.9	98.4	98.5
8	7.2	89.3	38.5	68.4	3.6	143.0	146.9	141.0	52.5	40.0	16.0	97.8	98.9
9	7.3	89.3	38.5	69.8	3.7	142.9	146.9	141.9	58.3	40.1	16.3	97.4	96.8
10	8.2	89.9	40.6	70.9	4.3	144.9	150.9	151.5	46.9	39.9	15.7	96.7	96.6

$$Relative\ errore(\%) = \frac{\left| ParameterValue(DCS) - ParameterValue(ANN) \right|}{ParameterValue(DCS)} \times 100$$

Conclusions

In this study, three scenarios were studied for predicting HIPS mechanical properties Izod, MFI, and MFI of final product; the scenarios were as follows:

1) Modeling all data by using a general neural network model, 2) modeling all data by hybrid PSO-ANN model, and 3) modeling filtered and selected data by radial basis network.

In the first model, all industrial data were used for modeling of HIPS plant. The goal of this modeling was obtaining a suitable model of the HIPS plant. Furthermore, 25 parameters were noticed as effective variables on MFI, Izod, and Vicat, respectively. These parameters have been shown in Table 4. Also, according to the obtained results, it was found that the correlation coefficients between all the independent and dependent variables were about 0.676, 0.931, and 0.676 for MFI, Izod, and Vicat, respectively. These values were inadequate to claim the defensible and trustworthy relationship between the independent and dependent variables. Various factors can be the reason for this weak prediction. One of the main causes of this behavior was recognized as the inability of some parameters. The best solution to the problem was to examine the impact of the variables on the goal parameter to remove the ineffective or ineffective variables from the dataset. For this study, a hybrid PSO-ANN methodology is applied. By using this algorithm, effective parameters were identified. Of all 25 variables, only 14, 11, and 10 of these features were identified as effective parameters on mechanical properties.

Finally, for reporting a logical relation between effective and independent variables (five variables) with a goal and dependent variable, modified ANN (newrb function used with default setting) was used. The testing step output of ANN showed that (1) maximum, (2) minimum, and (3) average relative errors between actual and calculated data were 6, 5, and 1% for MFI, Izod, and Vicat variables, respectively. Ultimately, these values were acceptable for the prediction of industrial HIPS mechanical properties by a mathematical model.

Nomenclatures

ABS: Acrylonitrile butyl styrene
BPNN: Backpropagation neural network
GPPS: General purpose polystyrene
HIPS: High Impact Polystyrene
R.E.: Relative error
SAN: Styrene acrylonitrile copolymer
SBR: Styrene butadiene rubber
SMR: Static mixer reactor

References

1. Yousef BF, Mourad A-HI, Hilal-Alnaqbi A (2011) Prediction of the mechanical properties of PE/PP blends using artificial neural networks, Procedia Engineering, 10: 2713-2718.
2. Alfarraj A, Bruce Nauman E (2004) Super HIPS: improved high impact polystyrene with two sources of rubber particles, Polymer, 45: 8435-8442.
3. Cunha FR, Costa JM, Nele M, Folly ROM, Souza Jr MB, Pinto JC (2013) Influence of reaction operation conditions on the final properties of High Impact Polystyrene (hips), Brazilian Journal of Chemical Engineering, 30: 575-587.
4. Duce C, Micheli A, Starita A, Tiné MR, Solaro R (2006) Prediction of polymer properties from their structure by recursive neural networks, Macromolecular Rapid Communications, 27: 711-715.
5. El Kadi H (2006) Modeling the mechanical behavior of fiber-reinforced polymeric composite materials using artificial neural networks—A review, Composite Structures, 73: 1-23.
6. Özcanli Y, Kosovali Çavuş F, Beken M (2016) Comparison of mechanical properties and artificial neural Networks Modeling of PP/PET Blends, ACTA PHYSICA POLONICA A, 130, 1: 444-446.
7. Fernandes FAN, Lona LMF (2005) Neural network applications in polymerization processes, Brazilian Journal of Chemical Engineering, 22: 401-18.
8. Hanai T, Ohki T, Honda H, Kobayashi T (2003) Analysis of initial conditions for polymerization reaction using fuzzy neural network and genetic algorithm, Computers and Chemical Engineering, 27: 1011-1019.
9. Krothapally M, Palanki S (1997) A neural network strategy for batch process optimization, Computers andChemical Engineering, 21:S463-S8.
10. Nascimento CAO, Giudici R, Guardani R (2000) Neural network based approach for optimization of industrial chemical processes, Computers and Chemical Engineering, 24: 2303-14.
11. Syu M-J, Tsao GT (1993) Neural network modeling of batch cell growth pattern, Biotechnology and Bioengineering, 42:376-80.
12. Tian Y, Zhang J, Morris J (2002) Optimal control of a batch emulsion copolymerisation reactor based on recurrent neural network models, Chemical Engineering and Processing: Process Intensification, 41: 531-8.
13. Tsen AY-D, Jang SS, Wong DSH, Joseph B (1996) Predictive control of quality in batch polymerization using hybrid ANN models, AIChE Journal, 42: 455-65.
14. Zhang J (1999) Inferential estimation of polymer quality using bootstrap aggregated neural networks, Neural Networks, 12: 927-38.
15. El-Shorbagy MA, Hassanien AE (2018) Particle swarm optimization from theory to applications, International Journal of Rough Sets and Data Analysis, 5, 2: 1-24.
16. Mousavi SM, Panahi P, Niaei A, Farzi A, Salari D (2012) Modeling and simulation of styrene monomer reactor: mathematical and artificial neural network model, International Journal of Scientific and Engineering Research, 3: 153-159.

Apendix#1

Physico-chemical specification of pure styrene (at 25 ^{0}C)

Property	Formula	Molecular weight	Density	Viscosity (centipoise)	Refractive index	Boiling point(^{0}C)	Latent heat of vaporization (cal./g)	Specific heat (cal./g ^{0}C)	Polymerization heat (cal./g)	Freezing point (^{0}C)	Flash point (^{0}C)	Limit of explo-siveness in the air (%vol.)
Value	C_8H_8	104	0.902	0.73	1.5439	145.2	102.65	0.416	160.2	-30.63	31	to 6.1 1.1