

Applications of Multi-Layer Perceptron Artificial Neural Networks for Polymerization of Expandable Polystyrene by Multi-Stage Dosing Initiator

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ABSTRACT: *In this research, Expandable Polystyrene (EPS) polymerization with conventional and Multi-stage Initiator Dosing (MID) methods is simulated by Multi-Layer Perceptron (MLP) Artificial Neural Networks (ANN). In order to optimize MID method, an efficient algorithm was employed for optimal training of the neural network. An algorithm was used to train the MLP networks more rapidly and efficiently than the conventional procedures. The main objective of MID method implementation is to reduce the time of the polymerization and because of that, by having different tests (first stage polymerization at 4, 3.5, 3, 2.5 hours and different amounts of used initiator at common state 100, 80, 75, 70 percent and the different number of dosings 12, 10, 8, 6) it was found that in an optimal state, the first stage polymerization time can be 3 hours and amount of the used initiator can be reduced to 70% in comparison to common state and number of dosings can be 6 times. The results of the simulation showed that the time of the first step of the polymerization has been reduced, the amount of the used initiator has been optimized and the count of the dosing times reduced to half, and therefore the time of the EPS polymerization is reduced to 60% of the conventional method.*

KEYWORDS: *Artificial neural network; MLP; Expandable Polystyrene; Initiator dosing polymerization.*

INTRODUCTION

Expandable polystyrene is produced from the polymerization of polymeric monomers by the suspension polymerization method. Polymer foams have a wide range of industrial uses, like thermal insulation, excellent shock absorption, moisture resistance, and many other applications. Polystyrene foam is produced by expanding the expandable polystyrene beads. Expandable polystyrene is formed

from styrene polymeric network including pentane and in a suspension polymerization process, styrene gained polymeric structure [1-4] Flame-retardant and smoke-suppressant expanded polystyrene (EPS) foams were prepared [5]. An efficient method has been used to synthesize micro-sized EPS foams which can assist future investigations into the environmental effects of EPS

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foams [6]. The behavior of PS foams and microplastics adhered to PS foams were investigated [7]. Polystyrene foams are produced in three steps: pre-expansion, middle storage, and final expansion. In the first step, beads are heated up and polystyrene has been softened. With the evaporation of expansion factor, bubbles of polystyrene grow rapidly as much as heat and expansion factor exists. It is possible for the bubbles to expand nearly 30 times their original size. In the second step, which is between the first and last step, it is needed to let the air infiltrate into cells. In the final step, the air is needed as completing the expansion factor. Air softened cell structures become resistant in front of atmospheric pressure when they separate from the template. Usually, the final expansion occurs automatically. Templates of the pre-expanding beads have been filled and exposed to steam [8].

Suspension polymerization is an important heterogeneous polymerization technology that has been used in order to produce special polymeric granules. The production process of EPS by suspension polymerization of styrene with the addition of blowing agents (as pentane gas) is well known. Polystyrene is a long-chain hydrocarbon in which carbon centers are attached to phenyl groups [9-11]. Many researchers declared that data-based modeling methods such as neural networks in an industrial process have major importance. ANN is a computational method for prediction. In ANN method, which is a nonlinear mapping structure, the method takes different units in the input and output layers. ANN has several units interconnected with each other in order to discover the relationship between them and to estimate outputs. ANNs can be used in order to extract patterns and detect trends [12-14]. Neural networks generally consist of several interconnected neurons in one or more hidden layers. These neurons can be grouped from different aspects such as the type of the input transformation, their structural architecture, and the type of learning algorithm [15]. Neural networks can work either as projection or kernel-based transformations to calculate the relationship between the inputs. In the first change, the inputs are machinated on a single axis, the projection can be linear or non-linear. The MacCulloch-Pitt neuron, Perceptron, and Adaline are examples of linear projections. In the second change, the input vector norm with respect to a fixed point is used. Radial basis function networks are a very popular kernel-based input change method. The obtained parameters are capable of study

in ANN, therefore, RBF and MLP methods of the ANN can be used in order to reduce the number of experiments [16,17].

Expandable polystyrene: Conventional method

In an invention, in order to have a process for making gray expanded polystyrene, it has been prepared *via* suspension polymerization by using an additive (carbon black and/or graphite) only after approximately 20 to 60 wt. % of the conversion of the styrene monomer into the polystyrene. In one non-limiting embodiment, the styrene polymerization rate has about 35 wt. % to about 60 wt. % styrene monomers remaining after 3 hours from the beginning of the polymerizing [18]. In an invention, in order to have a process for controlling the particle size of the preparation of expandable styrene polymers by suspension polymerization, the EPS is prepared by polymerizing styrene and optionally polymerizable comonomers in stirred aqueous suspension in the presence of monomer-soluble free radical initiator and dispersant to the extent that at least 70% of the monomers are polymerized (based on the total monomer) in the aqueous suspension, initially to a conversion of at least 70% by weight and then adding the remaining monomer, initiator and optional copolymerizable monomer and additives to the polymerization medium over one to three hours [19]. In a study, in order to synthesize water expandable polystyrene-activated carbon, active carbon pre-saturated with water was introduced into the styrene monomer to form a water-in-oil inverse emulsion without emulsifiers. By suspension polymerization, Water Expandable Poly Styrene/Activated Carbon (WEPSAC) beads could subsequently obtain. Low-density PS foams were produced in the CO₂ extrusion foaming process using WEPSAC [20].

Expandable polystyrene: Multi-stage initiator dosing method

In a study, EPS has been prepared on a laboratory scale by the initiator dosing method, in which unlike the conventional method that the initiator is added as a powder at the beginning of the polymerization, in this method initiator has been added in several shares into the reactor in the polymerization process. As the first step of the polymerization of this method has occurred at a higher temperature, therefore the reactor is needed to be closed and processed at higher pressure. Thus, the benzoyl peroxide

powder initiator has been prepared in styrene monomer suspension and entered the reactor with a dosing pump in several shares. The results of the study showed that the prepared polymer from this method has higher pentane absorption, better grading, and better mechanical strength in comparison to the prepared polymer from the conventional method [9]. The kinetics of the prepared polymer in the previous research has been studied, and the EPS with MID method was prepared by free radical suspension polymerization. By using kinetic relations, conversion percentage in different steps has been obtained, and by obtained conversion percentage the experiments have been compared, and the data obtained from kinetic relations had good coverage for the laboratory data [21]. In a study, enhanced productivity, mathematical modeling, and experimental study of the continuous dosing of the fast initiator during suspension polymerization have been researched. For reducing the batch time required for the suspension polymerization of the vinyl chloride in order to improve productivity by a continuous dosage of a fast initiator during the polymerization reaction, an adopted mathematical model was developed. They used a the pilot-scale reactor in order to verify the mathematical model prediction. And the results were acceptable. The maximum time reduction compared to the conventional polymerization for the predefined conversion was 53%. Final PVC product characteristics remained relatively unchanged under an optimum initiator dosage trajectory in comparison with the conventional processes [22]. In an invention, in order to involve the dosing initiators in the polymerization process, at least one peroxide, with a half-life of between 1 hour and 0.001 hours at the polymerization temperature at the moment of dosing, is dosed to the reaction mixture at the polymerization temperature. During the dosing of the peroxide, the cooling means of the reactor are kept at maximum cooling capacity and the amount of dosed initiator is actively controlled. The desired polymerization temperature is achieved and maintained within 0.3 °C of said polymerization temperature [23]. In an invention, in order to polymerize ethylene in a high-pressure reactor with improved initiator feeding, the preparation of the ethylene homopolymers or copolymers in a high-pressure reactor with at least two spatially separated initiator injection points by polymerizing ethylene and optionally further monomers in the presence of at least two different mixtures

of free-radical polymerization initiators at 100°C-350°C and pressures in the range of from 160 MPa to 350 MPa, has been processed. The process comprises providing at least two different initiators as a solution in a suitable solvent or in a liquid state, mixing the initiator, feeding each of the mixtures to a different initiator injection point of the high-pressure reactor, and apparatus for feeding initiator mixtures to a high-pressure reactor with at least two spatially separated initiator injection points [24].

Determination of different parameters in the production of expandable polystyrene with artificial neural networks

In our previous study, the effect of general performances of RBF method of ANN with laboratory data on different nanoparticles in different temperatures and mass fractions on the viscosity of crude oil was studied. In order to learn RBF networks, the major method for calculating isotropic Gaussian basis function span for RBF networks containing special algorithm were presented. The results showed that RBF neural networks had an acceptable performance because of having strong academic basics and the ability to filter the noises. This method contains all the experimental data perfectly and provides information about the viscosity [25]. In our previous study, in order to simulate the experimental CO₂ absorption data in a packed column by application of ANN, the generalization performances of the Back Propagation Multi-Layer Perceptron (BPMLP) and RBF neural networks were compared together by resorting to several sets of experimental data collected from a pilot-scale packed absorption column. Two in-house efficient algorithms were employed for optimal training of both neural networks. The simulation results showed that the RBF networks can perform more adequately than the MLP networks for filtering the noise (measurement errors) and capturing the true underlying trend which is essential for a reliable generalization performance [26]. In a study, in order to detect the effect of different parameters on WEPS production and Thermal Behavior Prediction Using ANN, spherical Polystyrene beads containing small water droplets are applied. The effect of sodium chloride (NaCl) on water distribution into WEPS beads has been investigated. The ANN model was developed for the prediction of Differential Thermal Analysis (DTA) data in different temperatures. The results showed that there is a good agreement between predicted thermal behavior

and the actual values [11]. In a study, an ANN model has been used in order to estimate reservoir parameters from experimental data. Theoretical pressure derivative curves with Pseudo Steady State (PSS) inter porosity flow has been used to train the ANN. Coefficients of the interpolating Chebyshev polynomials have been used on the pressure derivative data in a log-log plot as input to the ANN. Different training algorithms have been used to train ANN and obtained an optimum number of neurons for each algorithm by minimizing Mean Relative Error (MRE) over the test data. The results showed that the Levenberg-Marquardt algorithm has the lowest possible MRE among other algorithms and has been used to train the ANN. The coefficients of the conventional polynomials and pressure derivative data have been normalized to train the ANN. The results of this study declared that using the coefficient of conventional polynomials makes the learning phase of the neural network worse compared to the normalization method [17]. In a study, *M. M. Al-Dousari et al.* used an ANN model for predicting the recovery performance of surfactant polymer floods. In order to estimate the recovery performance of a reservoir subjected to a Surfactant-Polymer (SP) flood, they developed a supervised feed-forward back-propagation neural network model. They designed the optimal network paradigm by conducting extensive experimentation on the proper number of hidden layers and neurons in each of these layers. They trained the network model on a data set consisting of 499 simulations, generated by using a three-dimensional compositional chemical flood simulator. Their simulation runs consisted of 90% tertiary chemical floods and 10% secondary chemical injections. Their optimal network architecture was able to estimate back the oil recovery from the training set within 1.5% average absolute error. Their ANN model predicted the oil recovery for a blind-test data set of 125 simulated field cases within approximately 3% average absolute error. Their ANN model outperformed the non-linear multivariate models available in the literature study [27]. In a study, an ANN model has been designed for dual lateral well applications. The objective was to generate ANN tools that can provide the necessary knowledge to evaluate the utilization of the dual horizontal well technique in tight gas reservoirs. Rate profile, gas recovery profile, dual horizontal well configuration, and pattern size have been predicted. Two ANN models have been developed,

forward and inverse, in order to achieve the main objective. The ANN model has been trained, validated, and tested by using training data generated by a commercial simulator. The forward tool that has been developed was tested and granted a mean square error of 7.5%, while the inverse tool which has been developed was tested yielding a mean square error of 9.8%. The developed tools can compare thousands of different input combinations in a much more rapid way as compared to commercial simulators [28]. In a study, various characterization methods have been investigated by using a generalized distribution model and ANN. In order to investigate the accuracy of various characterization methods based on the attainable input data of heptane plus fraction (C7+) using a generalized distribution model, a statistical analysis over a wide range of experimental data has been carried out. Also, a new accurate approach based on Riazi's generalized distribution model with input data of molecular weight (M7+), specific gravity (SG7+), and true boiling point distribution (Tb) has been developed. In addition, an ANN model has been trained and tested for three different sets of input data including (M7+, SG7+), (M7+, SG7+, Refractive index), and (M7+, SG7+, Tb7+). The last input data showed the most precise results in good agreement with experimental data. Ultimately, the impact of characterization methods and lumping on phase behavior for two crude oil samples has been investigated [29].

In this study, the MID method of EPS polymerization in a semi-industrial unit scale has been simulated by ANN. The mechanical strength of the synthesized EPS by MID method has been investigated in three different parameters: a) Initiator dosing counts, b) Initiator percentage, c) Time of the first step polymerization. The laboratory data received by the initiator dosing method in the optimum state has been simulated by MLP ANN model and in the optimum state, the time of the polymerization has been reduced and the amount of the initiator which has been used for the process is reduced in comparison with the conventional method, the MLP ANN model has covered the laboratory data perfectly.

In our previous studies [9, 21] the goal was to implement the MID method for synthesizing expandable polystyrene (EPS). By implementing this method, the amount of used initiator and the time of the first stage polymerization has been reduced but furthermore, tests and simulations of the optimum amount of the above cases

was needed and therefore this research deals with this need besides that, the optimum number of dosings has been achieved.

EXPERIMENTAL SECTION

Materials

In this research, we used Styrene (monomer – purity 99.7%), Pentane (99%) as blowing agents, Reagent grade Calcium Phosphate (Mw= 310.18g/mol), Polyvinyl Alcohol (Mw=47000 and 98% hydrolyzed), Benzoyl Peroxide, tert-Butyl Benzoyl Peroxide and deionized water (suspension media). Styrene, pentane, and deionized water were obtained from Tabriz Petrochemical Company, and Reagent grade Calcium phosphate, Polyvinyl Alcohol, Dichloromethane, Benzoyl Peroxide, and tert-Butyl Benzoyl Peroxide were purchased from Merck.

Equipment

A 300 L stainless steel Buchi reactor equipped with baffles with a discharge valve at the bottom, and a thermostatically controlled hot oil jacket with a three-blade mixer has been used as a laboratory setup. The initiator has been supplied to the reactor at the programmed time and dosed by the dosing pump. Varian 3800CP Gas Chromatographer has been used the determination the percentage of pentane absorbed and the concentration of the monomer remaining in the sample. Testing was conducted in accordance with ASTM 5135. The mechanical strength of the prepared blocks was tested by Zwick Roll (model TI- FR010THA50) Germany according to ASTM 1621.

Preparation of benzoyl peroxide suspension

654 g Benzoyl Peroxide has been dissolved in Dichloromethane. Dichloromethane has been added until Benzoyl Peroxide has been completely dissolved. 690 g PolyVinyl Alcohol (PVA) solution was prepared in 8 L water and Stirred at 300 rpm speed. Benzoyl peroxide and dichloromethane have been added to the stirring solution. The solution was stirred for 8 h. Benzoyl Peroxide solution has been prepared in water which has more persistence.

Methods of polymerization

Conventional method

In this method semi-industrial unit has been considered, 144 kg of water was charged into a 300-Litre reactor,

followed by 336g (1.086 mol) of tricalcium phosphate and 96 kg (923.1 mol) of styrene monomer. The reaction mixture was stirred at 360 rpm. 135.6 kg (0.6984 mol) of tert-butyl benzoyl peroxide and 355.8 g (1.4688 mol) of benzoyl peroxide were added to the mixture when the reactor temperature reached 40°C. The temperature was further increased to 90°C at a rate of 0.83°C/min and kept at 90°C for 4 h. During this “low-temperature polymerization” stage, because of the existence of the risk of agglomeration of polymer beads, which might result in the formation of a two-phase system or undesirable lumps, the size and growth of the particles were regularly checked. At the end of the 4 h period of the low-temperature polymerization, 16.8912 g (0.0146808 mol) of polyvinyl alcohol (5wt %) and 7.68 kg (106.446 mol) of pentane were added and the temperature was increased to 120°C at a rate of 0.5°C/MIN (7bar). It should be noted that the boiling point of the deionized Water in 7 bar pressure is equal to 164.97°C. The reactor was kept at 120°C for 5 h and subsequently cooled to room temperature. It took about 1 h for the temperature of the reactor to reach room temperature. Finally, the reactor was evacuated, and polymer beads were filtered, washed with deionized water, and dried.

Multi-Stage initiator dosing method

As shown in Fig. 1, in this method semi-industrial unit has been considered, 144 kg of water, 336 g (1.086 mol) of tricalcium phosphate, 690 g (0.0146808 mol) of polyvinyl alcohol (5wt %), and 89.46 kg (860.19 mol) of styrene monomer were charged into the reactor. The temperature was increased to 85°C at a rate of 1.083°C/min. Then the initiator solution in 4 different states (containing 355.8 g, 284.4 g, 266.82 g and 249.06 g benzoyl peroxide in 6.54 kg (62.88 mol) styrene) was equally divided into 12, 10, 8, 6 parts and charged at the specified dosing intervals and temperatures to the reactor. The polymerization was carried out in 4, 3.5, 3, 2.5 hours of polymerization.

At the end of the so-called “low-temperature polymerization stage”, 7.68 kg (106.446 mol) of pentane and 135.6 g (0.6984 mol) of tert-butyl benzoyl peroxide as the initiator of the second stage were added. The reaction mixture was heated to 120°C at a rate of 0.33°C/min, and polymerization was continued for 2.5 h (7 bar).

Expandable polystyrene has many applications. Therefore, due to the large-scale consumption of EPS, the preparation of this polymer is important. The process

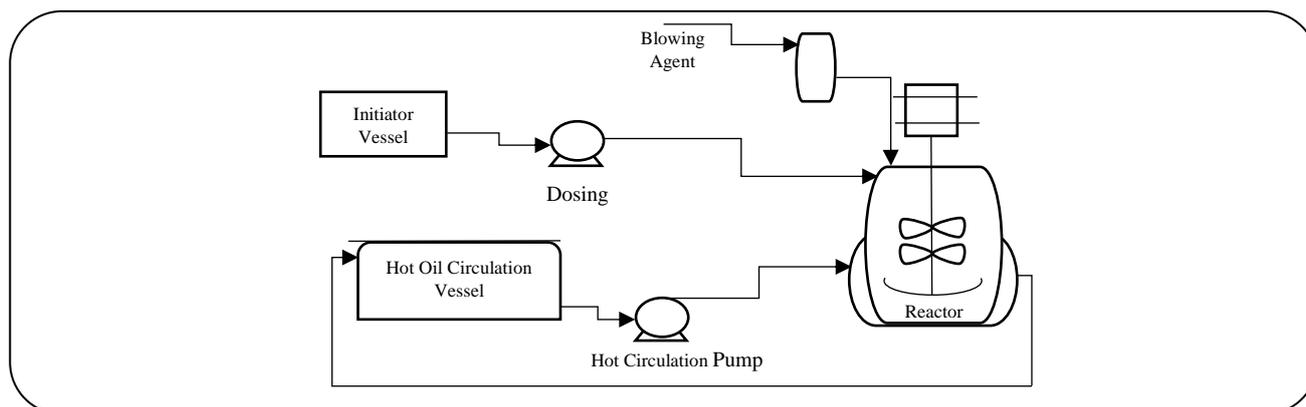


Fig. 1: Polymerization setup for MID EPS Synthesis.

of preparation of this polymer is time-consuming. So, by decreasing the needed time for polymerization, the production capacity of this polymer increases. By implementing MID method, the time of the polymerization reduces, and as a result, production capacity increases. On the other hand, the whole process is easier because of the dosings of the initiator in parts in MID method, and the amount of initiator usage is reduced.

In conventional preparation of this polymer, the initiator enters altogether into the reactor at the first stage. Therefore, during the 4-hour polymerization, the material has to be sampled from the inside of the reactor in order to see if polymeric beads are formed or not. But in the MID method, there is no need to control the bead's growth.

In Multi-Initiator Dosing (MID) method, despite In the conventional method, the initiator will be dosed into the system in several stages, therefore controlling the system will be easier in comparison to the conventional method. The first stage of polymerization in the new method happens at a higher temperature in comparison to the conventional method, which causes the time of the polymerization to be reduced. In MID method which happens at a higher temperature, in order to prevent boiling and overflow of the materials inside the reactors, the door of the reactor is closed.

Artificial Neural Network

Multi-Layer Perceptron (MLP) Network

The basic element of a Multi-Layer Perceptron (MLP) neural network is the artificial neuron performing a simple mathematical operation on its inputs. The inputs are the variables x_1, x_2, \dots, x_p , and a threshold (or bias) term. Every input value is multiplied by a weight, w_i , after which

the results are added with the bias term to produce z . finally, a known activation function, φ , performs a pre-specified (non-linear) mathematical operation on the projected inputs. Different activation functions such as sigmoid or hyperbolic tangent are traditionally used for this purpose. MLP networks can conclude many neurons are ordered in layers. While the neurons in the input and output layer merely distribute and collect the signals, the job of the neurons in the hidden layer is the actual processing. Although many hidden layers can be used, using one hidden layer network is more popular for practical applications due to its simple structure. Using multilayer hidden neurons usually leads to unnecessarily large degrees of freedom. The MLP network is trained using adapting the synaptic weights using a back-propagation technique or any other optimization procedure. During In the training phase, the network output is compared with the desired output. The error between these two signals is used to adapt the weight. This rate of adaptation may be controlled by a learning rate. A high learning rate will make the network adapt its weights quickly but will make it potentially unstable. Setting the learning rate to zero will make the network keep its weights constant. The steepest-descent optimization technique with constant step length parameters (η) was employed in this article.

In this work, additional linear weights (α 's, as shown in Fig. 2) were used to accelerate the network convergence. The optimal values of these linear parameters are updated after each back-propagation iteration using the following set of linear equations:

$$(\phi^T \phi)^{\alpha} = \phi^T \underline{y} \quad (1)$$

Where $\phi_{i,j} = \varphi(z_{i,j})$, $i = 1, \dots, N$ & $j = 1, \dots, M$ and \underline{y} is the $N \times 1$ vector of measured values. The parameters N and M

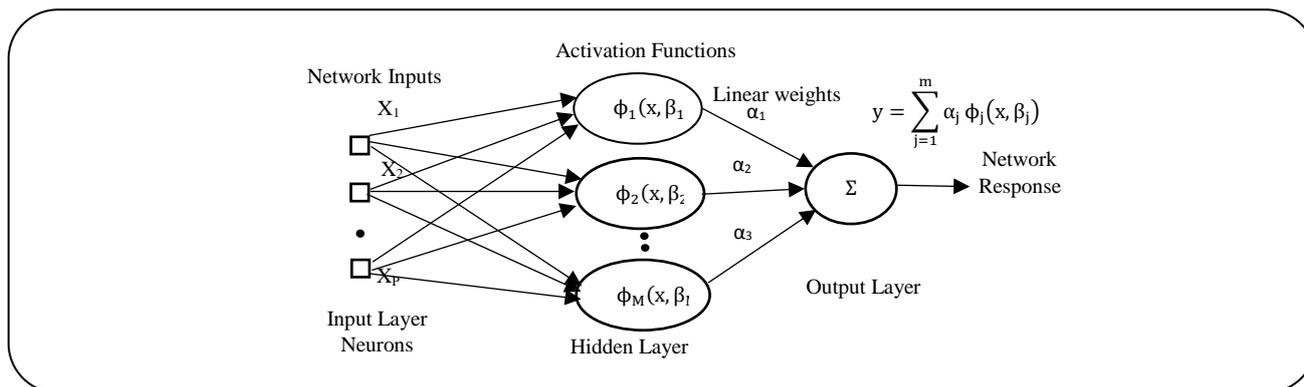


Fig. 2: The regularization network.

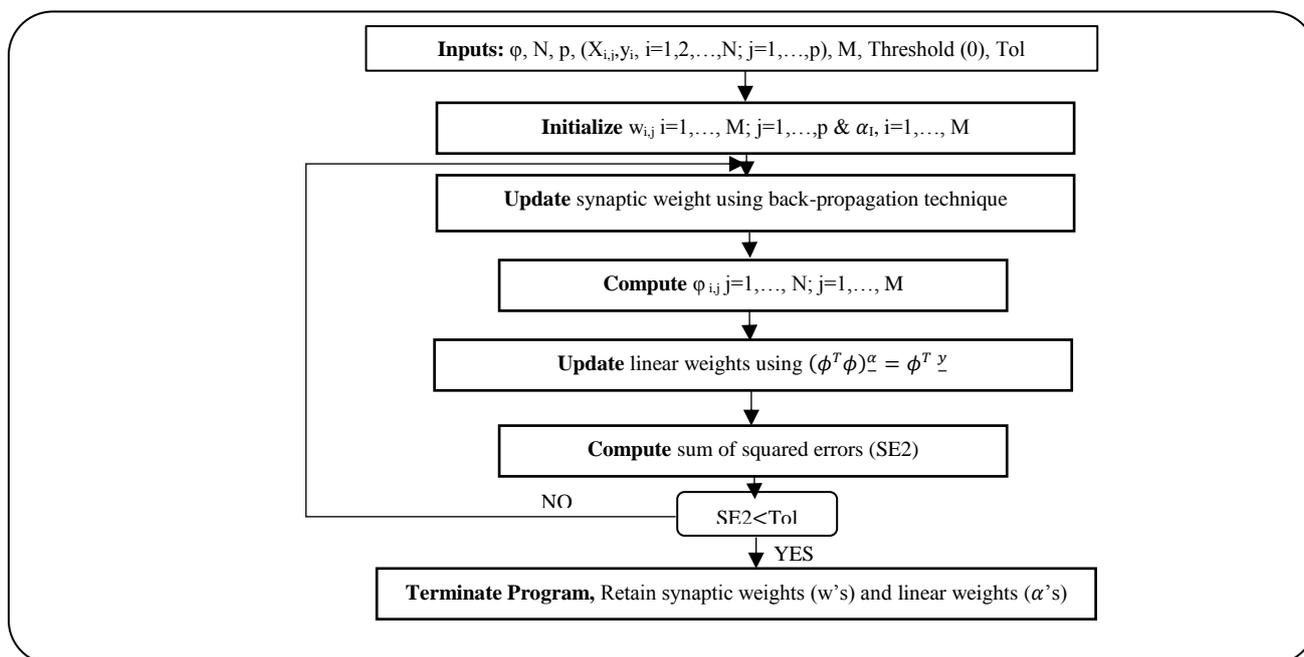


Fig. 3: Learning algorithm for MLP Networks.

represent a number of training data and a number of neurons, respectively. The training flow chart of such MLP network is given in our previous articles.

Similarly, other quadratic methods (e.g. Newton-like techniques) may be used to compute the optimal performances of the MLP networks. The so-called “line search” technique is usually used to predict the optimum learning rate compared to Newtown step length⁴ ($\Delta x = -G^{-1}g$). Evidently, the quadratic methods converge faster at near-optimal points and are not necessarily far from them. This is one of the reasons why quasi-Newton techniques such as Levenberg-Marquardt or Gauss-Newton are used [30]. Finally, the steepest-descent methods (such as back-propagation)

are more robust than the quadratic techniques when a proper step length control is used. In practice, almost never Newton-like optimization methods are used for efficient neural network training because they can easily trap into sub-optimal solutions. The algorithm of the MLP network is shown in Fig. 3.

RESULTS AND DISCUSSION

EPS was prepared by conventional and multi-stage dosing methods. In the multi-stage dosing method, different counts of dosing and time of the polymerization, and amount of the initiator was tested. The stress-strain ratio of these tests is shown in Figs. 4, 5, 6.

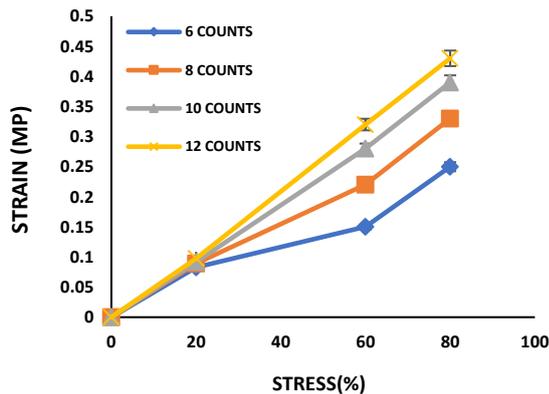


Fig. 4: Stress-Strain ratio in different dosing counts.

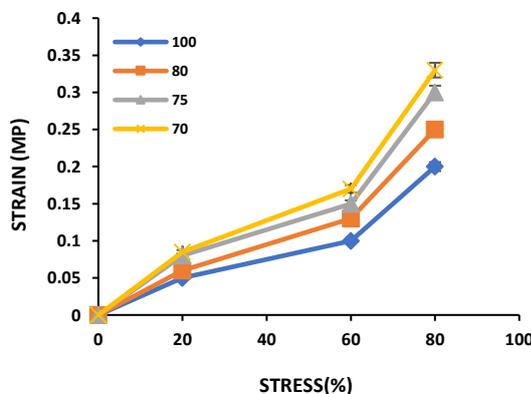


Fig. 5: Stress-Strain ratio in different initiator percentages.

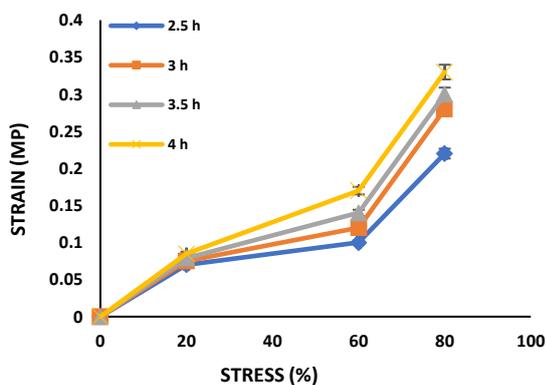


Fig. 6: Stress-Strain ratio at different times of the first step polymerization.

In Fig. 4, the stress-strain ratio in different counts of initiator dosing is shown. The results indicate that the 6 counts of initiator dosing have a better slope between 20% and 60% strain in comparison with other counts of

initiator dosing. By studying figures for different states, it becomes clear that for 3 states of initiator dosing times (12, 10, 8) by increasing stress, the amount of strain increases with a higher slope and causes the obtained blocks from EPS production to be fragile. But for the state with 6 dosing times, the figure has a gentle slope. Therefore, the state with 6 dosing times is better than the other states.

In Fig. 5, stress strains for different initiator percentages are shown. The results show that all 4 charts have a similar slope and the chart with 70% initiator has better mechanical friction and better condition. Investigations declare that the growth chart is almost the same for all 4 states. All 4 figures have 3 stages: 0 to 20% with a normal slope, 20 to 60% with a lower slope, and 60 to 80% with a steep slope. Because of having the most strain in the state with 70% of initiator amount in comparison to other states with the same stress, and economically, having less amount of initiator is better and makes the product have higher quality, the state with 70% of initiator amount is more acceptable in comparison with the conventional method.

In Fig. 6 stress-strain ratios for different times of the first step of polymerization are shown. Because of the mechanical friction condition being similar in all 4 charts, the prepared polymer in 2.5, 3, 3.5, 4 hours of the polymerization in the first step, has a similar condition to other polymers.

For different stresses in states with 4, 3.5, 3, 2.5 hours, the ratio chart of stress to strain behavior is almost the same and only the chart growth of 3 states (3, 3.5, 4 hours) is higher in between 60% to 80%. According to the main objective of this research (reducing the time of the polymerization) and the chart has no unusual behavior for the state with a lower time of first stage polymerization, the state with a lower first stage polymerization time has no problem in terms of stress to strain.

In order to obtain the optimal condition, the following steps have been taken.

The first step is to reach the optimal size of the used initiator; therefore, the optimization has been studied in 4 hours for polymerization and 12 times of initiator dosing and in 4 states for initiator size. 4 states respectively are 70% of the primitive size, 75% of the primitive size, 80% of the primitive size, and unchanged size (100%).

For the 4 states, the polymerization has been done, EPS blocks have been prepared, and the stress-strain test has been done.

The results of the simulated laboratory data have been reported in Figs. 7, 8, 9 respectively.

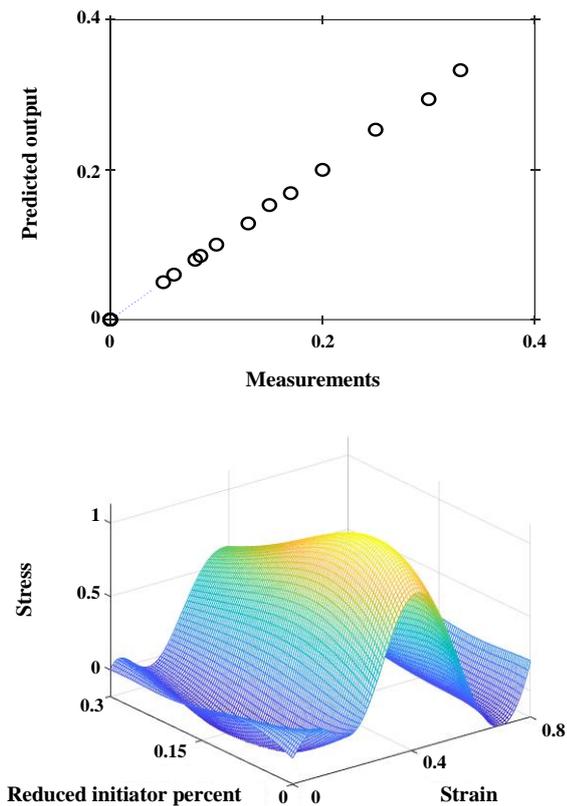


Fig. 7: MLP results for reducing Initiator Percentage.

The goal is to decrease the number of initiators for two reasons: 1) Economical reasons, 2) Reducing the number of initiators who remained in the final product. These results show that the state with 70% of the initiator is the best state. From the results, the reduction of the initiator up to 70% has not differed much, and the result of the state with 70% of the initiator size was acceptable.

In the next step, with 70% of the amount of the initiator, the optimization of the time of the polymerization is the goal. The time of the polymerization has been set to 4, 3.5, 3, 2.5 hours, and after the polymerization and preparation of the polymer blocks, the respective test has been done, and the result of the simulation has been reported in Fig. 8. Results show that the polymerization time of 3 hours is better than the other times of the polymerizations, according to the figures of the other simulations.

In the 3rd step, with choosing 70% of the initiator size and 3 hours for the polymerization, the goal is to optimize the injection counts. 4 states for the injection

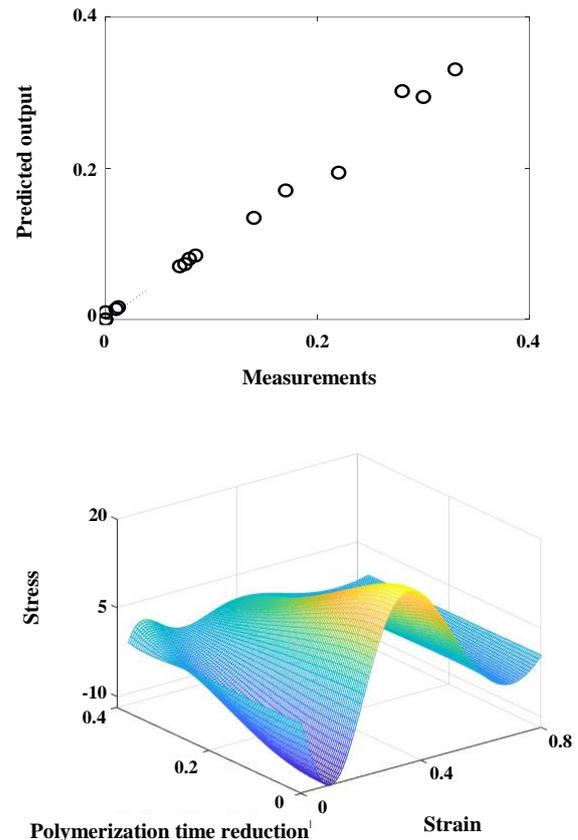


Fig. 8: MLP results for polymerization time.

counts have been selected. The states were with 12, 10, 8, 6 injections. The results of the simulations are reported in Fig. 9.

The results have shown the state with 6 injections and 3 hours of polymerization and 70% of the initiator size is the most optimal state possible.

CONCLUSIONS

Expandable polystyrene synthesis by a new method causes the processing time to be reduced and production capacity to be increased. By adding the initiator in several stages, the control of the process becomes easier in comparison to the conventional method. In order to achieve the optimum state for MID method, first stage polymerization has been done in 4 states (4, 3.5, 3, 2.4 hours), amount of used initiator has been done in 4 states in comparison to the conventional method (100, 80, 75, 70 percent) and also number of dosings has been done in 4 states (12, 10, 8, 6 times). EPS polymerization with conventional and MID methods are stimulated by MLP ANN. In the MID method

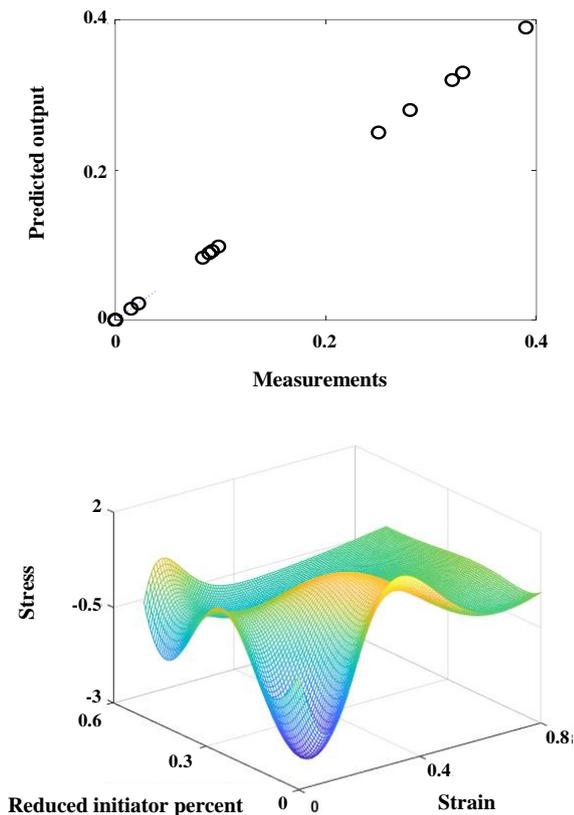


Fig. 9: MLP results for injection counts.

by polymerization in higher temperatures and initiator doings in several shares, the problems of the conventional method have been solved. In order to optimize MID method, MLP method of the ANN has been used, and the results of the simulation showed that the time of the first step of the polymerization was reduced from 4 to 3 hours, and the amount of the used initiator was reduced to 70% and the count of the dosing times reduced to 50%. This is the most optimized state, and therefore the time of the EPS polymerization is reduced to 60% of the conventional method.

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REFERENCES

- [1] Wang L., Wang C., Liu P., Jing Z., Ge X., Jiang Y., The Flame Resistance Properties of Expandable Polystyrene Foams Coated with Cheap and Effective Barrier Layer, *Construction and Building Materials Elsevier*, **176**: 403-414 (2018).
- [2] Huang J., Zhao Z., Chen T., Zhu Y., LV Z., Gong X., Niu Y., MA B., Preparation of Highly Dispersed Expandable Graphite/Polystyrene Composite Foam via Suspension Polymerization Non-Covalently Compatibilized by Polystyrene with Enhanced Fire Retardation, *Carbon 13944*, (2019).
Doi: 10.1016/j.carbon.2019.02.029.
- [3] Yuan B., Wang G., Bai S., Liu P., Preparation of Halogen-Free Flame-Retardant Expandable Polystyrene Foam by Suspension Polymerization, *Journal of Applied Polymer Science*, **136(29)**: 47779 (2019).
Doi: 10.1002/app.47779.
- [4] Kannan P., Biernacki J. J., Visco Jr D. P., Lambert W., Kinetics of the Thermal Decomposition of Expandable Polystyrene in Different Gaseous Environments, *Journal of Analytical and Applied Pyrolysis Elsevier*, **84**:139-144 (2009)
- [5] Li M., Yan Y., Zhao H., Jian R., Wang Y., A Facile and Efficient Flame-Retardant and Smoke-Suppressant Resin Coating for Expanded Polystyrene Foams, *Journal of Composites Part B Elsevier*, **185** (2020).
<https://doi.org/10.1016/j.compositesb.2020.107797>
- [6] Kwak J. I., An Y. J., Iced Block Method: An Efficient Method for Preparation of Micro-Sized Expanded Polystyrene Foams, *Journal of Environmental Pollution Elsevier*, **263**: 114387(2020).
<https://doi.org/10.1016/j.envpol.2020.114387>
- [7] Battulga B., Kawahigashi M., Oyuntsetseg B., Behavior and Distribution of Polystyrene Foams on the Shore of Tuul River in Mongolia, *Environmental Pollution Elsevier*, **260**: 113979 (2020).
<https://doi.org/10.1016/j.envpol.2020.113979>
- [8] Scheirs J., Priddy D., "Modern Styrenic Polymers", Wiley Series in Polymer Science, England, (2003).
- [9] Derakhshanfard F., Vaziri A., Fazeli N., Heydarinasab A., Optimization of Synthesis of Expandable Polystyrene by MultiStage Initiator Dosing, *Iranian Journal of Chemical Engineering*, **13 (1)**: 20-31(2016).
- [10] Herman H. A., Enschede O., Bart F., et al *US Pat. 069983* (2011).
- [11] Moghaddam H., Sargolzaei J., Asl M. H., Derakhshanfard F., Effect of Different Parameters on WEPS Production and Thermal Behavior Prediction Using Artificial Neural Network (ANN), *Journal of Polymer-Plastics Technology and Engineering*, **51**: 480-486 (2012).
DOI: 10.1080/03602559.2011.651243.

- [12] Sun Q., Ertekin T., [Screening and Optimization of Polymer Flooding Projects Using Artificial Neural Network \(ANN\) Based Proxies](#), *Journal of Petroleum Science & Engineering*, **185**: 106617 (2019).
Doi: 10.1016/j.petrol.2019.106617.
- [13] Bispo V.D.D.S., Scheid C.M., Calcada L.A., Meleiro L.A.D.C., [Development of an ANN-Based Soft-Sensor to Estimate the Apparent Viscosity of Water-Based Drilling Fluids](#), *Journal of Petroleum Science & Engineering*, **150**: 69-73 (2017).
Doi: 10.1016/j.petrol.2016.11.030.
- [14] Babakhani S. M., Bahmani M., Shariati J., Badr K., Balouchi Y., [Comparing the Capability of Artificial Neural Network \(ANN\) and CSMHYD Program for Predicting of Hydrate Formation Pressure In Binary Mixtures](#), *Journal of Petroleum Science & Engineering*, **136**: 78-87 (2015).
Doi: 10.1016/j.petrol.2015.11.002.
- [15] Shahsavand A., Ahmadpour A., [Application of Optimal RBF Neural Networks for Optimization and Characterization of Porous Materials](#), *Computers & Chemical Engineering*, **29**: 2134-2143 (2005).
- [16] Ketabchi N., Naghibzadeh M., Adabi M., Esnaashari S.S., Faridi-Majidi R., [Preparation and Optimization of Chitosan/Polyethylene Oxide Nanofiber Diameter Using Artificial Neural Networks](#), *The Natural Computing Applications Forum*, **28**: 3131-3143 (2017).
DOI: 10.1007/s00521-016-2212-0.
- [17] Adibifard M., Tabatabaei-Nejad S.A.R., Khodapanaz E., [Artificial Neural Network \(ANN\) to Estimate Reservoir Parameters in Naturally Fractured Reservoirs Using Well Test Data](#), *Journal of Petroleum Science and Engineering*, **122**: 585-594 (2014).
- [18] Hanna P., Hazaim H., Cotton W., Brooks J., [Process for Making Gray Expanded Polystyrene](#), *US Pat. 20190112447A1* (2007).
- [19] Speikamp H. D., Kuhnle A., Bretschneider J., [Process for controlling the Particle Size in the Preparation of Expandable Styrene Polymers by Suspension Polymerization](#), *US Pat. 5189069A*, (1991).
- [20] Yang J., Yen S., Chiou N., Gou Z., Daniel T., Lee L.J., [Synthesis and Foaming of Water Expandable Polystyrene-Activated Carbon \(WEPSAC\)](#), *Journal of Polymer*, **50(14)**: 3169-3173 (2009).
Doi: 10.1016/j.polymer.2009.05.007.
- [21] Derakhshanfard F., Fzeli N., Vaziri A., Heydarinasab A., [Kinetic Study of the Synthesis of Expandable Polystyrene via "Multi-Stage Initiator Dosing Method"](#), *J. Polym. Res*, **22**: 118 (2015).
DOI: 10.1007/S1096-015-0766-7.
- [22] Bijhanmanesh M. J., Etesami N., Esfahany M. N., [Continuous Dosing of Fast Initiator During Suspension Polymerization of Vinyl Chloride for Enhanced Productivity](#), "Mathematical Modeling and Experimental Study, Chemical Engineering Communications", Tylor & Francis Group (2016).
Doi: 10.1080/00986445.2016.1205981.
- [23] Meulenbrugge L., Swieten A. P. V., Vanduffel, K. A. K., Westmije H., [Polymerization Process Involving the Dosing Initiators](#), *US Pat. 7173095B2* (2006).
- [24] Littmann D., Finette A.A., Mohrbutter J.P., Wolfram S.G., [Ethylene Polymerization in a High-Pressure Reactor with Improved Initiator Feeding](#), *US Pat. 8217124B2* (2010).
- [25] Derakhshanfard F., Mehralizadeh A., [Application of Artificial Neural Networks for Viscosity of Crude Oil-Based Nanofluids Containing Oxide Nanoparticles](#), *Journal of Petroleum Science and Engineering*, **168**: 263-272 (2018).
DOI: 10.1016/j.petrol.2018.05.018.
- [26] Shahsavand A., DerakhshanFard F., Sotoudeh F., [Application of Artificial Neural Networks for Simulation of Experimental CO₂ Absorption Data in a Packed Column](#), *Journal of Natural Gas Science and Engineering*, **3(3)**: 518-529 (2011).
- Agwu O E., Akpabio J.U., Alabi S.B., Dosunmu A., [Artificial Intelligence Techniques and Their Applications in Drilling Fluid Engineering: A Review](#), *Journal of Petroleum Science and Engineering*, **167**: 300-315 (2018).
doi: 10.1016/j.petrol.2018.04.019.
- [28] Enab K., Ertekin T., [Artificial Neural Network-Based Design for Dual Lateral Well Applications](#), *Journal of Petroleum Science and Engineering*, **123**: 84-95 (2014).
<https://doi.org/10.1016/j.petrol.2014.09.004>
- [29] Moradi G., Nazari M., Sahraei S., [Investigation of Various Characterization Methods Using Generalized Distribution Model and Artificial Neural Network](#), *Journal of Petroleum Science and Engineering*, **127**: 286-296 (2015).
<http://dx.doi.org/10.1016/j.petrol.2015.01.002>.

- [30] Girosi F., Poggio T., "Networks and the Best Approximation Property, Artificial Intelligence Laboratory, Center for Biological Information Processing", Massachusetts Institute of Technology, Cambridge, MA 02139, USA, (1989).