

Soft-Sensor Based on Artificial Neuronal Network for the Prediction of Physico-Chemical Variables in Suspension Polymerization Reactions

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The possibility of employ soft-sensors for the monitoring and prediction of physico-chemical variables are useful when deals with heterogeneous polymerization systems, such as a suspension polymerization reactions. Even though, there are some well-established techniques and instruments for these off-line, on-line and in-line measurements are prolonged for control process purposes. Faced with such difficulties, even the high cost involved in the installation, maintenance and operation of these instruments, the use of soft-sensors have been widely used in the these area. An artificial neural network was trained with a dataset taken from a petrochemical plant for the production of expandable polystyrene in a batch polymerization suspension reactor. The input variables selected were: the temperatures and pressure of the reactor, and the output variables were the percent of blowing agent, residual monomer and the average molecular weight took in the final of each reaction. The artificial neural network with the Levenberg-Marquardt algorithm presented the smaller mean square error, needed less epochs and time in the training step and showed a better generalization when used a new dataset in the validation step. Finally, it was concluded that the results were very satisfactory, the developed soft-sensor was capable of predict the variables of interest at the end of each reaction.

1. Introduction

In chemical processes systems, the monitoring of the conditions of the process are very important, for these kind of measurements exist a diversity of sensors and transducers with a good accuracy and shorts delay times very affordable for the industry. However, when it deals with physical-chemical variables of monitoring the properties of the products, the situation in terms of sensors becomes more difficult. In most of these cases, there are analyzed in laboratories by collecting samples and the response time can takes minutes or even hours. Even though, providing on-line sensors, the delay in measurement can be long and the instruments very expensive for process control purposes.

Fonseca et al. (2009) presented a detailed review of the available on-line and in-line sensors and equipment used for monitoring of polymerization reactors since 1990 until today. About 600 references were included, which evidence the growth of sensor technology in the last two decades. The manuscript was divided into three main sections. The first section considers sensors developed for the operating conditions in polymer reactors, i.e. flow, level, temperature and pressure. The second part is devoted to the off line, on line and in line monitoring of polymer properties, techniques such as calorimetric, based on measurements of heat generated by a reaction can be associated with the rate of polymerization, conversion; Chromatographic techniques, such as, gas chromatography (GC) that is widely used for analysis of residual monomer, polymer conversion; Gel Permeation Chromatography (GPC) was largely used to determine the average molecular weight (MW) and molecular weight distribution (MWD), spectroscopic techniques such as middle and near infrared spectroscopy (IR) used for monitoring the conversion, reaction kinetics and MW; Raman spectroscopy (RS), such as IR, is used to obtain information about molecular structure and properties of molecules based on their vibrational transitions and an others techniques like fluorescence spectroscopy, dielectric spectroscopy, ultraviolet spectroscopy were related. The third section briefly discusses other peripheral, yet related topics such as state estimation and multivariate data analysis, fault diagnosis and sensors election and location. Unfortunately, hard sensing instruments are not available in many practical situations in the industry. In these cases, soft-sensors can be considered an option for estimating the variables of interest in these situations. This paper proposes the development of a soft-sensor using artificial neural networks (ANN) to predict the final physico-chemical properties in suspension polymerization reactors.

2. Suspension Polymerization Reactions

In a typical free radical suspension polymerization reaction, the organic phase containing monomers and initiators are dispersed in a continuous phase by the combination of vigorous agitation and the addition of suspending agents. After initiated the polymerization, all the chemical reactions inherent in this system occur strictly in the organic phase, into the dispersed droplets. Thus, it's considered that each of these droplets presented in the reaction behaves like small batch reactors (Dowding et al., 2001), surrounded by a continuous phase that acts as a cooling system (McGreavy, 1994). Moreover, it is common to assume that these droplets dispersed within the reaction kinetics behave like a bulk polymerization reaction (Yuan et al., 1991; Kricheldorf et al., 1992; Dowding et al., 2001; Odian, 2004).

Expandable Polystyrene (EPS) is a rigid cellular plastic in which the polymer is impregnated with a blowing agent, usually pentane, when subjected to heating, it provide an expansion of the polymer matrix and then can be shaped in many different forms. The EPS includes a series of features such as thermal insulation, mechanical strength being used in the manufacture of packaging for electronic products, appliances, food packaging, and applications and been used in embankment construction.

3. Soft-sensors

Soft-sensors are inferential models capable of estimate variables of interest took from instantaneously measured. The kind of sensors came from indirect control systems, in which the variables to be monitored (primary) are monitored through the behavior of other variables (secondary). The large spread of soft-sensors in industrial applications is due to the advantages facing the measurement problems of hard-sensors and particularly the economically disadvantaged, since they require high investments in the acquisition and installation, but also for the maintenance and operation.

An alternative to generate these inferential models are using ANN. Those models have the advantage of being computationally efficient, easily construction and implementation and also be able to incorporate some variations of the process that are not able to incorporated into a conventional mathematical model. The ability to learn from examples and generalize the learned information is undoubtedly the main attraction for the solution of problems through an ANN. One of the most known ANN are the feedforward multilayer perceptron and have been successfully applied in different problems. In this work will be preferred to use the ANN with backpropagation algorithm and Levenberg-Marquardt algorithm.

4. Methods and Materials

An important step in the development of the soft-sensor was to made a careful evaluation of the dataset collected from a petrochemical company that produce EPS in two batch suspension polymerization reactors with a capacity of 20 tons each. The input variables used in the ANN were the temperature of the reaction, it had a direct influence on the conversion rate, and the final properties of the polymer, the another variable was the reactor jacket temperature, this variable was shown as an important input data to improve the performance of the ANN, the last input was the pressure of the reactor, this variable is directly related to the addition time of the stabilizing agent and blowing agent into the reactor. The output variables of the ANN are the percent of residual monomer, the percent of blowing agent and the average molecular weight. The quantity of blowing agent in the EPS is between 6 and 10% W/W, and the residual monomer in the polymers need to be very low, this last one is necessary to fulfillment the specific regulations and legislation, to analyze this compounds was used a gas chromatograph ThermoQuest Chromatograph - CE Instruments, model Trace GC 2000 Series; packed column, model 2444 GC, Chromosorb PVAW support, 15% FFAP phase, diameter 1 / 8 ", length 15 feet. The MW of a polymer is the main property that confers useful and unique mechanical properties to a polymeric material, for analyze the MW was used a viscometer Ubbelohde type 1 (capillary diameter 0.58 mm), measurements were performed with the viscometer immersed in a thermostatic bath. The analysis procedures used are described by (Bishop, 1971).

For the development of the ANN were used the Neural Network Toolbox of the MATLAB. The dataset were about 60 reaction collected in a year of operation, 70% of dataset was for the training, 15% for the validation and 15% for the test.

5. Result and Discussions

This section was divided in two parts, in the first part will be discussed the implementation of the ANN and training step, in the second part will be discuss the validation and prediction of the ANN selected in the training step by using a new dataset constituted by five reactions, finally it is going to be chose the ANN to be used as a soft-sensor, in the table 1 are presented the architectures used in the neural networks.

Table 1: Architectures of the Feedforward ANN.

Identification	Training Algorithm	Neurons in the hidden layers	Activation function
LM-L	Levenberg-Marquardt	$4 - [N] - 3$	Logarithmic
LM-T			Hyperbolic-tangent
LM-LL		$4 - [N - N] - 3$	Logarithmic
LM-TT			Hyperbolic-tangent
BP-L	Backpropagation	$4 - [N] - 3$	Logarithmic
BP-T			Hyperbolic-tangent
BP-LL		$4 - [N - N] - 3$	Logarithmic
BP-TT			Hyperbolic-tangent

Where, (LM) Levenberg-Marquardt algorithm, (BP) backpropagation algorithm, (L) logarithmic and (T) hyperbolic tangent are the activation functions, N is the number of neurons in each hidden layer.

In table 2 are described the structures of the hidden layer and the number of neurons used in each one of these ANN.

Table 2: Structure of the hidden layers in each feedforward ANN.

Structure	Artificial Neuronal Networks										
	1	2	3	4	5	6	7	8	9	10	11
$4 - [N] - 3$	5	8	10	12	15	18	20	25	30	35	40
$4 - [N - N] - 3$	3-3	5-5	10-5	5-10	10-10	10-15	15-10	15-15	20-15	15-20	20-20

As shown in Fig. 1(a) all the ANN trained, LM-L had the lowest MSE if compared with the others LM algorithm. By another hand, the ANN with the BP algorithm Fig. 1(b) the lowest MSE were observed in the ANN with a single hidden layer BP-L and BP-T. The Fig. 1(c) shows the MSE of the ANN that had the lowest MSE selected from the Fig. 1(a) e Fig. 1 (b). Analyzing the Fig. 1(c) can be concluded that the ANN11 with LM algorithm and 40 neurons in the hidden layer had the smallest MSE. In contrast, the others ANN with the BP algorithm the lowest MSE had 15 neurons in the hidden layer with logarithmic activation function named ANN 5.

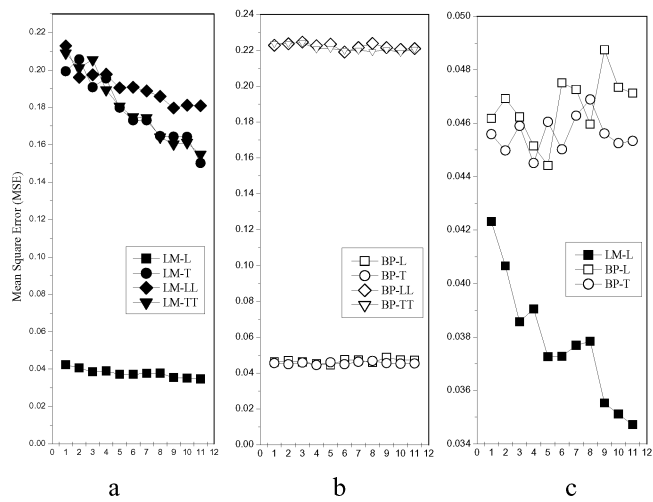


Figure 1: Mean square error (MSE) of the ANN in the training step.

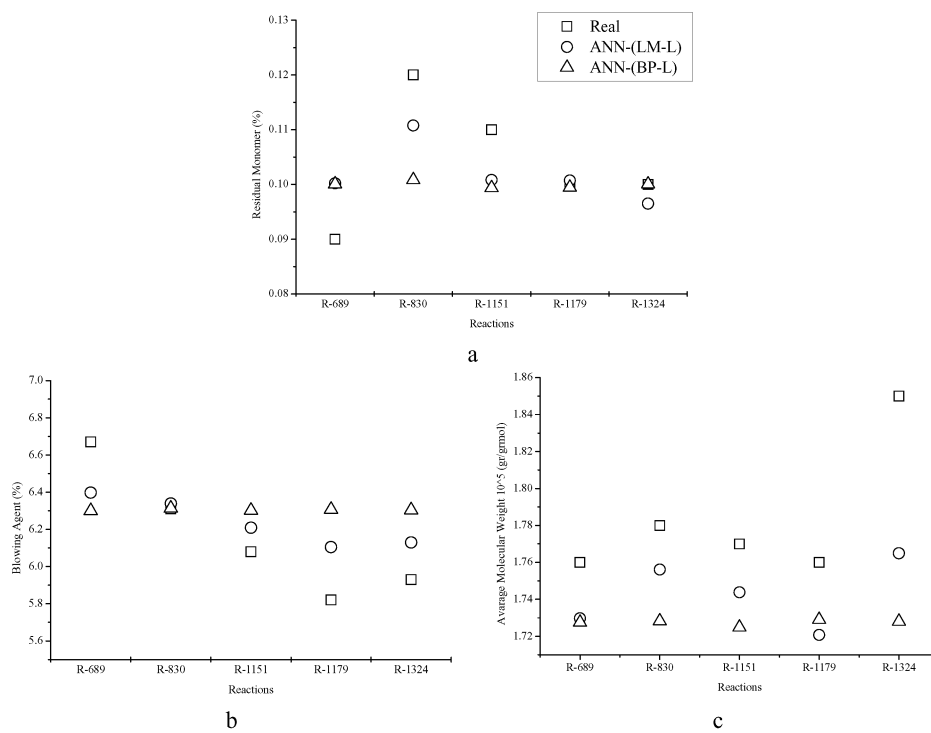


Figure 2: Values predicted by the ANN in the validation step.

Analyzing the predicted values of the ANN (Fig. 2) selected from the training step, can be concluded that, both ANN have a good predictive ability. Analyzing the values predicted for monitoring the residual monomer was observed that ANN with LM algorithm Fig. 2 (a) shown a better performance if compared with the BP ANN. The same conclusion can be observed with the LM ANN for the prediction the blowing agent Fig. 2 (b), as the same as the others variables, the LM ANN had a good predictive ability for the monitoring of the MW Fig. 2(c). The better performance of the ANN with LM algorithm can be related to the method used to adjust the synaptic weight in the training step of the ANN. Since the LM algorithm use the modified method of Gauss-making taking less time and few epochs to learn and avoiding the overfitting.

6. Conclusions

After made a careful analysis of the collected dataset and a carefully selection of the operational variables (inputs) used to determine the variables of interest (outputs) to predict the properties of the EPS, different types of ANN with a variety of topologies and structures had been implemented and tested. The training step and selection of the best ANN was obviously the most exhaustive and long of his study. The most appropriate ANN to be used as a virtual sensor has been with four neurons in input layer, forty neurons in hidden layer and 3 neurons in the output layer ([4] - [40] - [3]). The training algorithm was the Levenberg-Marquardt algorithm showing an excellent generalization and therefore a better predicting capacity. Finally, it was concluded that the results were very satisfactory, since the soft-sensor presented a good ability and accuracy to predict the properties when used a new dataset.

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