CHEMICAL ENGINEERING TRANSACTIONS Volume 24, 2011
Editor Sauro Pierucci

DOI: 10.3303/CET1124065

Application of Artificial Intelligence Techniques for Temperature Prediction in a Polymerization Process

Manuela Souza Leite, Brunno Ferreira dos Santos, Liliane Maria Ferrareso Lona, Flávio Vasconcelos da Silva, Ana Maria Frattini Fileti*

School of Chemical Engineering, Department of Chemical Systems Engineering, University of Campinas (UNICAMP), 13083-970, Campinas/SP, Brazil,
*frattini@feq.unicamp.br

The main feature of the polymerization reaction is its complex nonlinear behaviour, which poses a challenging control system design for the batch reactor. The present work is concerned with the development of intelligent mathematical models to predict the styrene polymerization temperature. In order to improve the final product quality, these models will be used in predictive control schemes. Two techniques from the artificial intelligence field were used: Neuro-fuzzy and artificial neural networks. The pilot plant of styrene production consisted of: a stainless steel jacketed stirred reactor, a storage tank and a variable speed pump for the thermal fluid, temperature sensors (inside reactor, inlet and outlet of the jacket), a densimeter, and a PLC (Programmable Logic Controller). The temperature of the reactor is the process variable to be predicted using the historical data acquired from the pilot plant. Software MatLab 6.0 was used to implement neural and neuro-fuzzy models. The results showed that both models were able to predict online the reactor temperature profile successfully and that they were fast enough to be used in nonlinear predictive control strategies as well.

1. Introduction

The use of polymers has been growing gradually in many industrial products, such as: automobile, electronic devices, food packaging, and building and medicine materials. Among these products stands the polystyrene, usually produced in batch or semi-batch reactors. From the technical and scientific point of view, polymerization processes are quite challenging, because they involve complex temperature-dependent chain reactions and heat transfers, described by sets of highly nonlinear algebraic and differential equations (Lepore et al., 2007). Temperature variation in polymerization reactor systems greatly affects the kinetics of polymerization and consequently changes the physical properties and quality characteristics of the produced polymer (Ghasem et al., 2007). In order to ensure the maintenance of the final product quality is crucial to keep suitable operating conditions during the polymerization reaction process. In digitally controlled systems, the use of artificial intelligence (AI) based software allows to simulate and quickly predict online the behavior of process variables based on input-output data, rendering a good alternative to this problem. Both artificial neural networks (ANN) and neuro-fuzzy systems are AI 'black-box' estimators presenting no attempt to interpret the model structure. They can be viewed as multivariate nonlinear

Please cite this article as: Souza Leite M., Ferreira Dos Santos B., Lona L.M., Vasconcelos Da Silva F. and Frattini Fileti A.M., 2011, Application of artificial intelligence techniques for temperature prediction in a polymerization process, Chemical Engineering Transactions, 24, 385-390
DOI: 10.3303/CET1124065

nonparametric estimation methods as they are typically used to approximate a function y=f(x), where the function form of f is unknown. They have been used in various models for polymerization systems (Buragohain and Mahantan, 2008).
From the above, the present paper is concerned about the development of ANN and neuro-fuzzy models to predict the reaction temperature during the styrene polymerization. The developed models were online implemented to a pilot plant.

2. Polystyrene Process Description

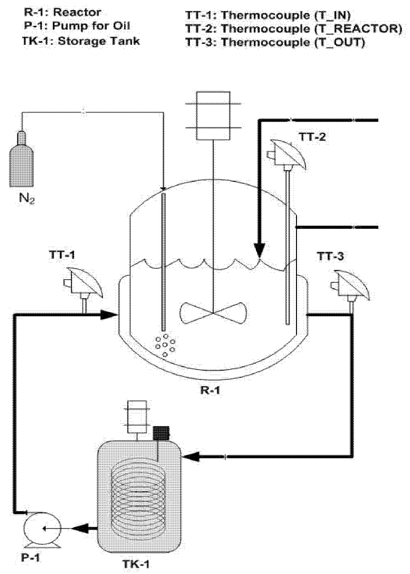


Figure 1: Schematic diagram of the experimental system.

A pilot plant was built specifically to evaluate the polymerization reaction performance. This plant, schematically shown in Figure 1, was used to generate the input-output experimental data. It consists essentially of a 1.2-liter-stainless-steel-stirred batch reactor (R-1), an oil storage tank (TK-1), a positive displacement pump (P-1) and temperature sensors (TT). Thermal oil was used as heat transfer medium in the jacket. An electrical heater, which was connected to a thyristor, provides heating to the thermal fluid inside the storage tank.
The dissolved oxygen was purged by bubbling pure nitrogen gas through the reaction mixture. The monomer was obtained with 99% purity from Sigma Aldrich. Toluene was used as solvent and it was purchased from Ecibra with a purity of 99%. No further purification was needed. Benzoyl peroxide (BPO) from Sigma Aldrich, presenting 70% purity, was used as the initiator agent of the reaction.

Table 1. Experimental Conditions of the Styrene Solution Polymerization Reactor

V_R=800 mL	V_T=7 L	F_J= 300 L/h	I=BPO
M_R=200 rpm	M_T=200 rpm	W_T=3000 W	[I]=0.0185 mol/L

V_R – reactor volume; M_R – reactor stirring speed; V_T - tank volume; M_T – tank stirring speed; F_J – jacket flow rate; W_T – heating power; I - initiator; [I] - initiator concentration.

After loading the monomer and the solvent into the reactor, it was heated to reach the desired operating temperature, 90 °C (Ghasem et al., 2007). As soon as achieving this target, the initiator BPO was added to start the polymerization reaction. Typical experimental operating conditions are shown in Table 1. Experimental runs were conducted using several monomer/solvent ratios: 30, 50 and 70 V/V %.

3. Neural Network Modeling

An Artificial Neural Network (ANN) is composed of simple calculation elements, called neurons or nodes, operating in parallel and fully connected. Each neuron presents an activation function to determine its output (Vasickaninova et al., 2010). The ANN architecture used in this work is the feedforward with three layers. The number of operational variables needed to represent the process dynamics determines the number of input neurons. In the hidden layer, the number of neurons was defined by the smallest error criterion and the constant effective number of parameters as well. The nodes in the output layer represent the variables to be predicted. In order to modeling the polymerization process dynamics, a historical data of reactor temperature (current time and four-steps-back measurements) and also the monomer/solvent ratio were used as input signals. The output was the one-step-ahead reactor temperature.

Training of a neural network is basically the process to find a set of optimum weights of the network. In this work, the training of the neural model was carried out by using the "*trainbr*" function of the Neural Network Toolbox (MATLAB R2006a), which consists of the Levenberg-Marquardt Bayesian Regularization algorithm.

4. Adaptive Neuro-Fuzzy Inference System (ANFIS)

The ANFIS is a hybrid model in which the nodes in the different layers of the network handle fuzzy parameters, representing an useful neural network approach for the solution of function approximation problems. Data driven procedures for the synthesis of ANFIS networks are typically based on clustering a training set of numerical samples of the unknown function to be approximated. Each layer in the network corresponds to a part of the fuzzy inference system (FIS) called: input fuzzification, rule inference and fire strength computation, and output defuzzification. The main advantage of this kind of representation is that the FIS parameters are encoded as weights in the neural network and, thus, can be optimized via powerful well known neural net learning methods. This model is mostly suited to the modeling of nonlinear systems (Buragohain and Mahantan, 2008; Cosenza and Galluzzo, 2009). In this work, the training of the neuro-fuzzy estimator was performed using the ANFIS toolbox of MATLAB R2006a.

5. Results and Discussion

In order to demonstrate the effectiveness of the proposed approaches, the reactor temperature prediction from ANN model were compared to that obtained from ANFIS model, under offline and online modes.

5.1 Development of ANN model

The experimental data, obtained from three runs, were normalized in the range [-1,1]. Each run set, containing about 2000 arrays, was randomly split into sets of training data (75%) and testing data (25%). A sampling time of 1 second was used. Initially, for the prediction of the one-step-ahead temperature (Tk+1), it was proposed a network structure with two input neurons - the ratio monomer/solvent (%M) and the current reactor temperature (Tk). However, this network did not reach an acceptable value of the summation of squared error (SSE), even adding more neurons in the hidden layer. Thus, it was necessary to add dynamic information to the training: four-steps-back temperature measurements were added as inputs (Tk-1, Tk-2 Tk-3 and Tk-4).

A hidden layer containing twenty-two neurons was determined by observing the MSE value (SSE/number of vectors). The minimum SSE obtained for the training set was 0.2011. Extracting the square root of MSE value (4.36 x10-5) and denormalizing it, the deviation of temperature was found to be 0.1°C, very close to the precision of temperature measurement. Hyperbolic tangent and linear functions were used. Using the test set to evaluate the generalization capacity of the model, a good agreement (slope=1 and linear coefficient = 0.12) was observed between predictions and unseen points in the dispersion plot (Figure 3). The developed neural model provides temperature predictions with 99.99% certainty.

An experimental run using 50% of monomer ratio was carried out, in which online predictions of temperature were performed by the digital control system. A Programmable Logic Controller communicated to the electronic devices in the polymerization plant and the acquired data were real time provided to the MATLAB software containing the neural model. Figure 4 shows that prediction curve are very close to the temperature measurements.

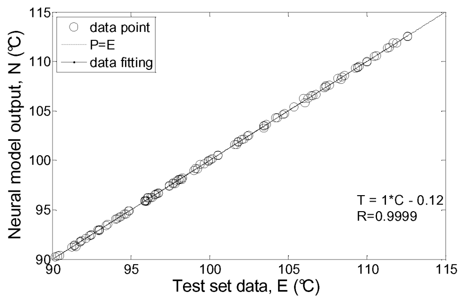


Figure 3: Neural model predictions vs. test set.

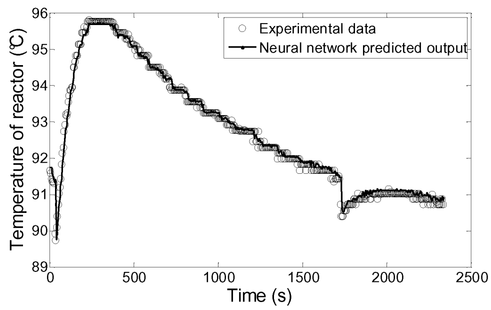


Figure 4: Online neural predictions and experimental data.

5.2 Development of ANFIS model

The same training and test sets containing six inputs were used for the ANFIS model: %M, Tk, Tk-1, Tk-2, Tk-3, Tk-4. In this paper, the fuzzy clustering algorithm was used to make a neural network system more effective. The fuzzy stage is responsible for the analysis of the distribution of data and grouping them into clusters with different membership values. The training set is reduced using ANFIS clustering, therefore, training period of the neural network decreased because of the low computational effort. In this method, parameters are tuned automatically during the learning procedure so the membership functions can suitably represent the non-linear system being studied with an optimal performance (Pan and Yang, 2007). The maximum error tolerance and epochs were set to 0.5 and 100, respectively. Test set data were fitted to the ANFIS model output, with a satisfactory error of 0.2 °C. After training, the membership function assumes a different form. Figure 5 illustrates the membership function adjusted for T_{k-4}. For all the variables of the polymerization system, the ANFIS methodology optimizes both the number of membership functions (4 MF) of the corresponding fuzzy sets and the number of rules, providing an accurate and simple model. The FIS file was make up of four membership functions (Z-zero, PS-positive small, PM-positive medium and PL-positive large). The total number fuzzy rules was four and the membership function was of Gaussian shape, defined in Equation 1, where c and σ are parameters of the Gaussian membership function.

$$f_g(x,\sigma,c)=\exp\left(-\frac{1}{2}\left(\frac{x-c}{\sigma}\right)^2\right) \quad (1)$$

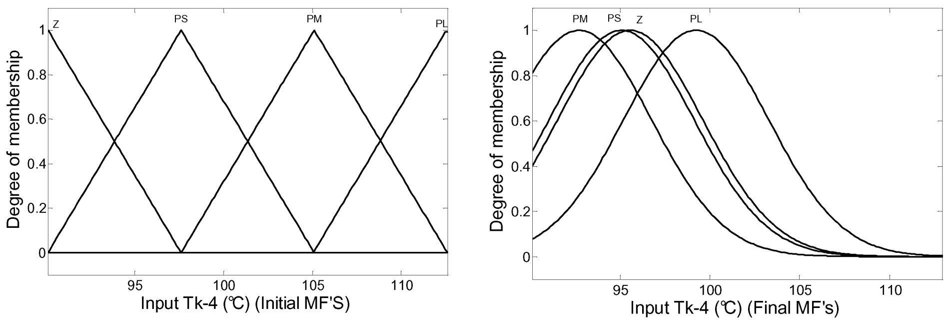
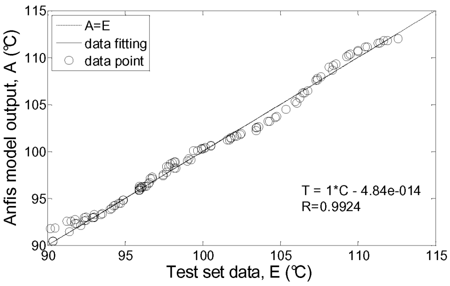


Figure 5: Initial membership function (5a) and final membership function (5b) for Tk-4 input for the prediction model using ANFIS clustering.

The ANFIS model was considered acceptable because the dispersion plot in Figure 6 presented a slope equal to the unity and the linear coefficient vanished.



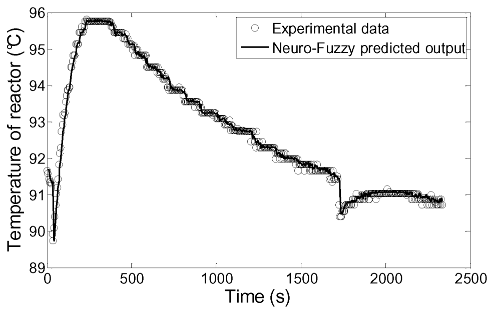


Figure 6: ANFIS predictions vs. test set.

Figure 7: Online ANFIS predictions and experimental data.

Another experimental run using 50% of monomer ratio was carried out, in which online predictions of temperature were performed by the ANFIS model. Figure 7 shows that prediction curve are very close to the temperature measurements. A commercial SCADA system was used for the management and data acquisition monitoring.

6. Conclusions

In the present work, two techniques from artificial intelligence field were applied for the prediction of the styrene polymerization temperature: artificial neural network and neuro-fuzzy system. The main feature of this polymerization reaction is its complex nonlinear behaviour, which poses a challenging control system design for the batch reactor. Some solution properties change drastically during the batch reaction (density, viscosity and heat capacity) turning the linear control strategies unsuitable for this process. In this context, the main goal of the present work is to provide precise and fast models for subsequent application in control strategies.

Based on several experimental runs - under different operating conditions - the models were built in order to predict the one-step-ahead reactor temperature. Implementing of such modeling strategies in this system is very promising because, based on the prediction model, optimal and/or predictive control schemes can be developed so that the end-of-batch product quality is optimised.

The neural network and the neuro-fuzzy model showed to be very effective in the dynamic modeling of this nonlinear batch process, offering accurate long-range predictions as well. The difference between the results vanished and it was proved that ANN and ANFIS are powerful tools for online predicting the temperature in styrene polymerization reaction. Both models did not demanded high computational costs, so that they can be used as internal models in advanced control strategies.

Acknowledgements

The authors are grateful to CAPES and FAPESP (Grant no. 2008/10710-7).

References

Buragohain , M. and Mahantan, C., 2008, A novel approach for ANFIS modelling based on full factorial design, Applied Soft Computing 8:609–625.

Cosenza, B. and Galluzzo, M., 2009, Development of a predictive Type-2 neurofuzzy controller, Chemical Engineering Transaction 17, 1203 – 1208.

Ghasem, N. M., Sata, S. A. and Hussain, M. A., 2007, Temperature Control of a Bench-Scale Batch Polymerization Reactor for Polystyrene Production, Chemical Engineering Technology 30, 9: 1193–1202.

Lepore, R., Wouwer, A. V., Remy, M., Findeisen, R., Nagy, Z. and Allgower, F., 2007, Optimization strategies for a MMA polymerization reactor. Computers and Chemical Engineering 31: 281–291.

Pan, L. and Yang, S., 2007, Analysing livestock farm odour using an adaptive neuro-fuzzy approach, Biosystems Engineering 97, 387 – 393.

Vasickaninova, A., Bakosova, M., Meszaros, A. and Klemes, J., 2010, Neural network predictive control of a heat exchanger, Chemical Engineering Transaction 21, 73 – 78.