CHEMICAL ENGINEERING TRANSACTIONS, Volume 11, 2007
Edited by Sauro Pierucci
 ISBN 978-88-95608-00-6

Optimal Operating Conditions Of Emulsion Polymerization Process Using An Inverse Neural Network Model

Sheila Contant, Liliane M. F. Lona*
Department of Chemical Processes, School of Chemical Engineering, Campinas State University - UNICAMP
C. P. 6066, 13081-970, Campinas, São Paulo, Brazil, Tel.: +55 (19) 3521- 3954,
*liliane@feq.unicamp.br

One of the most promising tools for application in polymer reaction engineering processes is neural network. Neural networks have the ability to learn the behaviour of a process and the relationship between groups of variables, and have been widely applied to process modelling and control. This method has attracted much attention because it can handle complex and nonlinear problems, and requires less processing time than conventional methods. Data from a deterministic model were used to feed a neural network, which was used to build an inverse model of the emulsion polymerization of styrene. After training and test, neural network can help in the optimization of the process, predicting operating conditions that produce polymers and latexes with desired properties such as melt flow index, tensile strength and number of particles per litre of water.

1. Introduction

Among the techniques for the production of polymers, emulsion polymerization has a great industrial importance, accounting for a 20 million ton per year production (Asua, 2004). Examples of commercial products are styrene/butadiene rubber, polyvinyl acetate, polymethacrilates and polytetrafluoroethylene (e.g. Teflon®). Emulsion polymerization can be defined as a complex heterogeneous process in which the monomers are dispersed in a continuous phase with an emulsifier, and polymerized by free-radical mechanism. One of the greatest challenges in the polymer industry is the optimization of the polymerization reactors, especially when polymers with certain quality and productivity are required. A deterministic model is able to predict properties of a polymer for known operating conditions of the reactor, and it gives important information about the phenomenas taking place inside the reactor. In an emulsion process a deterministic model can predict for example how the average number radicals per particle are changing with conversion, or how the concentration of monomer inside the particles is decreasing with time. On the other hand, the inverse deterministic model of complex processes such as those in dispersed medium is even more difficult and optimization techniques must be involved. An inverse model could directly relate desired end-product characteristics with input reactor conditions. An interesting alternative to deterministic models is the application of trained neural networks, which

could predict the operating conditions of the reactor that could produce polymers with specific properties. Neural networks are able to deal with complex systems, and have the ability to mimic the capacity of the human brain to learn from examples. Neural networks are computational tools that are widely used both in the academic and commercial areas for the solution of several kinds of problems (Baughaman e Liu, 1995). Neural networks are able to produce fast and reliable the results to several input conditions at the same time. In this work supervised neural networks were applied to the inverse modelling of the emulsion polymerization of styrene.

2. Methodology For Network Simulation

In this work the network simulations were performed in a program implemented with the backpropagation algorithm. Many authors have shown that backpropagation is efficient to deal successfully with several complex problems, including inverse modelling (for example Savkovic-Stevanovic, 1996, Köker et al., 2004, Mikami et al., 2004). Backpropagation is an algorithm ease to implement, and require the use of only two parameters: learning rate and momentum term. The simulator was implemented with two hidden layers, two transfer functions (sigmoidal a hyperbolic tangent), and two methods for weights and bias initialization (using a Gaussian distribution or small random values). Seven variables were set in the input layer: conversion, number of polymer particles per litre of water, number-average molecular weight, weight-average molecular weight, polymer particle diameter, melt flow index and tensile strength. All the variables in the input layer, with the exception of conversion, represent properties of the latex and polymer. Conversion was included as restrictive variable in order to contribute to the reduction of the occurrence of multiple responses by the network.
The network was built to predict four operating conditions: styrene, initiator and emulsifier concentration in the feed stream and process temperature. The ranges of the variables used are shown in Table 1.

Table 1: Range Of The Variables Used In The Network Simulations.

Variable	Neuron	Lower Value	Higher Value
T (^{o}C)	Output	50	70
Styrene (mol/l)	Output	1.05	9.60
Emulsifier (mol/l)	Output	0.016	0.087
Initiator (mol/l)	Output	0.00043	0.037
$\overline{M}_n$	Input	$6.9\text{x}10^{5}$	$5.3\text{x}10^{6}$
$\overline{M}_w$	Input	$1.2\text{x}10^{6}$	$1.2\text{x}10^{6}$
N_p (particle/l water)	Input	$7.2\text{x}10^{16}$	$3.6\text{x}10^{18}$
Particle diameter (dm^2)	Input	54	117
Conversion (%)	Input	70	99
σ = Tensile strength (psi)	Input	$6.7\text{x}10^{3}$	7.3x103
MI = Melt flow index (g/min)	Input	$8.11\text{x}10^{-5}$	$6.3\text{x}10^{-2}$

The training set used 170 data, and the test set used 30 examples arbitrarily chosen. The data used in the network simulations were obtained by a deterministic model for the homopolymerization of styrene (Contant, 2007). The reactions involved potassium persulfate (KPS) as initiator and sodium dodecil sulfate (SDS) as emulsifier. Average molecular weights were obtained by integration of the molecular weight distribution (Gilbert, 1995). Melt flow index and tensile strength were calculated by the equations shown in Valappil and Georgakis, 2002.

3. Results And Discussion

Several networks were trained with different values of hidden layers, hidden neurons, learning rate and momentum term. The best configuration, leading to the best results, was selected by the simulator, and it is shown in Figure 1. One hidden layer with 5 neurons was used. Learning rate was set as 0.3, and momentum term was defined as 0.8. The best network performance was achieved when sigmoidal transfer functions were used in all neurons, and weights and bias were initialized with small random values instead of a Gaussian distribution.

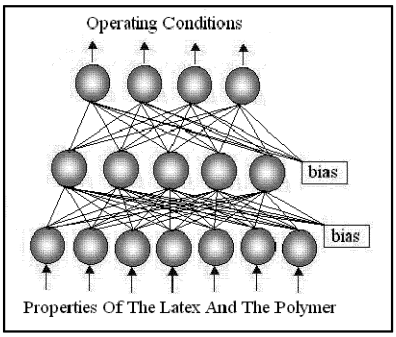

Figure 1: Configuration of the Selected Neural Network.

Figure 2 shows comparison between simulated and desired results for the four operating conditions (concentration of styrene, concentration of emulsifier, concentration of initiator and temperature). Data sets composed of 30 examples of inputs-outputs are compared in Figure 2, some of them exhibiting similar values. Determination coefficients are shown in each plot. A good agreement was found in all cases (R^2 close to 1).

The training and test error profiles are shown in Figure 3. Test errors were always diminished smoothly with iterations.

After obtaining the weights and bias in the training/test phases, the neural network is ready to suggest operating conditions to the desired properties. Several properties could be fed to the simulator at the same time, and reliable results of operating conditions could be generated quickly. Some examples of operating conditions that could be predicted by the neural network for a given set of polymer and latex properties are shown in Table 2.

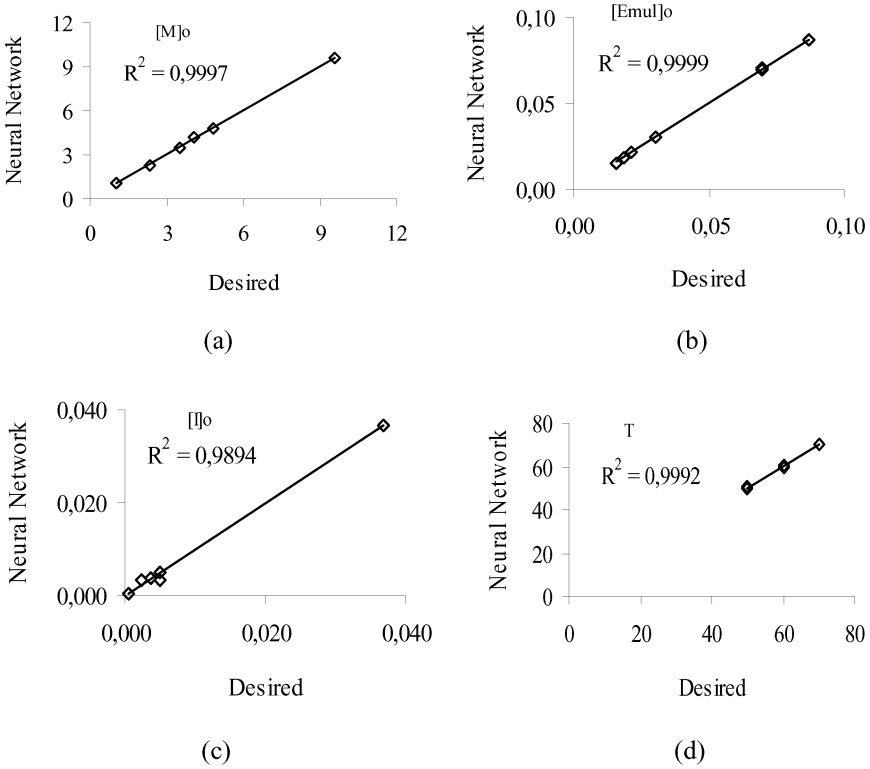

Figure 2: Neural Network Results Versus Desired Values In The Emulsion Polymerization Of Styrene: (a) Styrene Concentration, (b) Emulsifier Concentration, (c) Initiator Concentration and (d) Temperature.

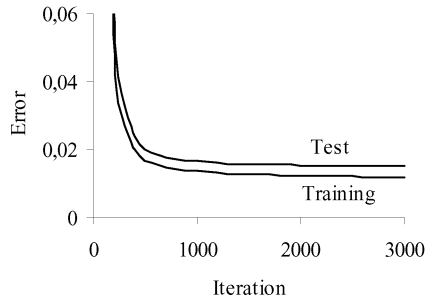

Figure 3: Evolution of Training And Test Errors In The Neural Network Simulations.

Table 2: Examples of Operating Conditions That Could Be Predicted By Trained Networks.

Network Inputs							Network Output			
x (%)	N_p/l_{water}	$\overline{M}_w$	$\overline{M}_n$	d_p (dm^2)	MI (g/min)	σ (psi)	$[M]_o$ (mol/l)	$[I]_o$ (mol/l)	$[Emul]_o$ (mol/l)	T (^oC)
99	$5x10^{17}$	$3x10^6$	$1x10^6$	93	$3.4x10^{-3}$	$7x10^3$	2.4	$3.4x10^{-3}$	$3x10^{-2}$	60
71	$7x10^{16}$	$1x10^5$	$7x10^5$	117	$6.3x10^{-2}$	$7x10^3$	1.1	$4.3x10^{-4}$	$2x10^{-2}$	70
91	$4x10^{17}$	$4x10^6$	$3x10^6$	95	$1.3x10^{-3}$	$7x10^3$	4.8	$5x10^{-3}$	$2x10^{-2}$	50

4. Conclusion

In this paper is illustrated how neural networks could be used to deal with an inverse modelling of a polymerization process. Homopolymerization of styrene at different temperatures was studied. Neural networks were trained and tested using data from a deterministic model previously developed. An interesting option could be to feed and train the networks with data from an industrial plant. In this case, the application of neural networks would be very interesting because neural networks are able to deal with data with noise or outliers that common in industrial data, and the training of the networks may require large data-bases, with are easily available in industrial operations.

5. Acknowledgment

The authors wish to thank FAPESP (proc. 02/09366-3).

6. References

Asua, J.M., 2004, J. Pol. Sci.: Part A: Pol. Chem., 42, 1025.
Baughman, D.R. and Y.A. Liu, 1995, Neural Networks in Bioprocessing and Chemical Engineering. Academic Press, USA.
Contant, S., 2007. PhD. Thesis, Campinas State University – UNICAMP, Brazil (in Portuguese).
Köker, R., C. Öz, T. Çakar and H. Ekiz, 2004, Robot. Auton. Syst., 49, 227.
Mikami, D., T. Ohki, K. Yamaji, S. Ishihara, D. Citterio, M. Hagiwara and K. Suzuki, 2004. Analyt. Chem., 76, 5726.
Savkovic-Stevanovic, J., 1996, Comp. Chem. Eng., 20, S925.