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Temperature control in polystyrene polymerization reactor by using neural network model predictive algorithm

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Theoretical and experimental temperature control of styrene polymerization in a batch process is searched. In MATLAB/ Simulink, heat signal is introduced to the model and reactor temperature change is recorded. An artificial neural network (NN) model was built with output changes of the disturbing process in the face of the pseudo-random binary sequence (PRBS) heat input. The neural network model predictive control algorithm is applied to maintain the desired temperature profile. Experimental control of the reactor temperature at the optimal temperature profile with the neural network model predictive algorithm was achieved successfully. Theoretical and experimental NN models utilized are compared and the representation ability of the NN models was shown.

Keywords: Neural network model, predictive control, polymerization, identification, online application.

Introduction

In the petrochemical industries, polymerization control has importance. To develop a detailed mechanistic model-based control algorithm may not be feasible. Modelling techniques based upon data might be preferable[1]. The NN approach and its training techniques have been developed in the wide sprite. The backpropagation network all neurons except the ones in the input layer are related with a bias neuron and a transfer function. These transfer functions can be linear or nonlinear. According to the purpose of the neural network the design and application of these transfer functions may differ. The computed output vectors are produced by the output layer[2]. Without actually modelling the physical and chemical laws, what happens in the process might be learnt employing neural network. Thus, they are for the understanding of the limited phenomenon[3,4]. Off-line training must be necessary for the neural networks as time limitation is considered to achieve prediction of all possible process conditions. The weights used in the network should be adapted continuously for learning about new process events in real-time. This makes the network effect for on-line process control[5]. A neural network model-based predictive control applied to a laboratory-scaled multivariable chemical reactor was reported by Yu and Gomm[6].

To meet ever-stricter product quality, the desired trajectories should follow by controlled variables. Errors in charging the process specifications to enhance the process safety management and more efficient use of materials and energy lead to batch-to-batch variations[7]. Increased profitability can be obtained by employing an efficient monitoring and control system. The online control system must be capable of quickly identifying any abnormal process behavior so that corrective actions could be taken[8].

With increasing the desired temperature in polymerization, dispersion range of product molecular weight increases. The polymerization rate is also affected by medium temperature changes. Control of polymerization rate during radical polymerization is important for obtaining constant polymer quality with a certain range of molecular weight[9].

In this work, a predictive control algorithm was developed based on experimental data taken from a real polystyrene reactor. Neural network model predictive temperature control application to a polystyrene reactor was achieved.

Models and methods

The batch jacketed polymerization reactor with the assumptions of the standard free-radical polymerization, constant density, no chain transfer, no gel effect, the quasi-steady-

state approximation for live radicals are modelled in Simulink. Optimization of the batch jacketed polymerization reactor concerning optimal temperature in minimum time is also modelled in Simulink.

Open-loop dynamic results at different optimal experimental conditions are given in Table 1. Where I_0, M_0, M_n, m^*, T, tf (s) are initial initiator concentration (mol/L), initial monomer concentration (mol/L), numerical average molecular weight, target monomer conversion, temperature (°C), and reaction time respectively.

Table 1. Dynamic and theoretical NN-MPC result in two different optimal operating conditions

Work number	Optimum parameters	Dynamic	Theoretical-NN-MPC
1	M_0 = 6,092		
	T = 97		
	I_0 = 0.0125		
	tf (s) = 7620		
	M_n = 52000	M_n = 33849	M_n* = 45814
	m^* = 0.5	m^* = 0.33	m^* = 0.45
2	M_0 = 6,092		
	T = 92		
	I_0 = 0.0150		
	tf (s) = 10200		
	M_n = 52000	M_n = 30203	M_n* = 43096
	m^* = 0.5	m^* = 0.36	m^* = 0.48

NN-MPC is implemented to track the temperature of the polymerization reactor. Neural network methodology of model identification is applied for the polymerization reactor. The control algorithm is implemented using the NN toolbox in MATLAB. The controller is shown as an independent block and the process is simulated as an analytic model.

A model predictive controller has good performance with a prediction horizon and small control-weighting factor. In Fig. 1, input changes versus time is given. Figs. 2 and 3 show the response of temperature controllers as plant and NN outputs to set point changes. The error is determined in the range of ± 0.03. All parameters utilized are given in Tables 2 and 3.

Theoretical NN-MPC simulating result for numerical average molecular weight values at optimal operating conditions is also given in Table 1. The reactor temperature desirably tracks the optimal temperature trajectory and this provides good numerical average molecular weight values. The neural network model was applied to the related system[10]. To identify the system, pseudo-random binary sequence type of heat input was introduced to the reactor and the reactor temperature was measured.

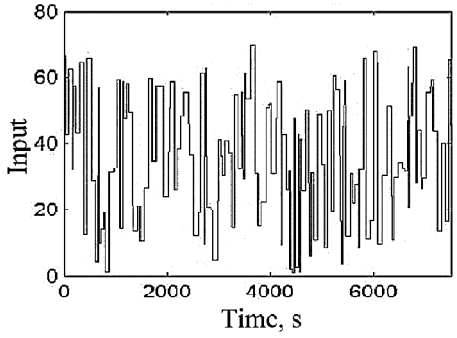


Fig. 1. Training plant input data for NN predictive control.

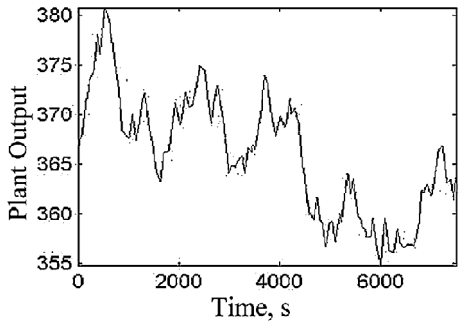


Fig. 2. Training plant output for NN predictive control.

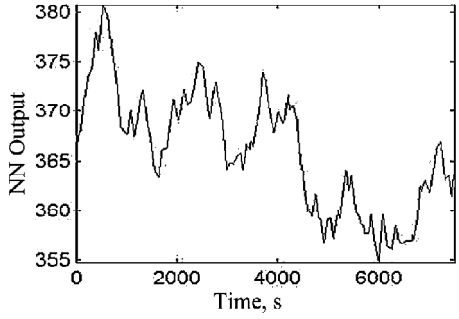


Fig. 3. Training NN output for NN predictive control.

The neural network was trained with the response data obtained from the reactor and the model representing the polymer reactor was built. The neural model had five inputs

Table 2. Parameters for NN model and NN-MPC

Size of hidden layer	2
Sampling interval	2 s
Delayed plant inputs	2
Delayed plant outputs	2
Training samples	5000
Maximum plant input	70 Cal/s
Minimum plant input	0 Cal/s
Train epochs	200
Train function	Levenberg-Marquardt
Activation function	Tansig (x)
Cost horizon (N_2)	2
Control horizon (N_u)	2
Control weighting factor (α)	0.01
Search parameter (a)	0.001
Iterations per sample time	2

Table 3. The weights and bias values of the NN for the polymer experimental system

IW{1,1}	LW{2,1}	b{1}	b{2}
	–71.0043	1.3569	95.5491
–0.020209			
0.0081864			
–0.001663			
–0.009824			
0.0039121			
	–0.50827	–88.402	
3.5582			
–40.5218			
35.4169			
9.2695			
0.50177			

and an output. The activation function was taken to be Tansig (x), Inputs (Ti-1, Ti-2, Ti-3, Ui-1, Ui-2), Target (Ti). Two neurons were found in the hidden layer of the artificial neural network. The open-loop response of the experimental artificial neural network model, the theoretical NN model and an analytical model is in good agreement with maximum error of 2.5°C.

Neural Network Model Predictive Control System used a neural network model for the prediction of a step ahead. The control process was achieved with linear optimization based on the cost function. The cost function to be minimized is given as

$$J(u,t) = E\left[\sum_{j=N_1}^{N_2}(w(t+j) - y(t+j))^2 + \alpha\sum_{j=1}^{N_u}(\Delta u(t+j-1))^2\right] \quad (1)$$

where N_1, N_2, N_u, are minimum, maximum costing horizons and control costing respectively[11].

The MPC tuning parameters were set[10]. The MPC criterion is optimized employing the gradient descent optimization technique. One-step-ahead optimization is shown as follows:

$$J = [w(t+1) - y_m(t+1)]^2 + \alpha\,[\Delta u(t)]^2 \quad (2)$$

In eq. (2) above, as $\alpha > 0$. The control weight factor, $\Delta u(t) = u(t) - u(t-1)$ and $y_m(t+1)$ is the output of a step forward ahead in the artificial neural network. To bring the controller, $y_m(t+1)$, a value in a step to the required value, $w(t+1)$, may require very much effort. For the good reconciliation between the control and the changes in the control effort in the optimization of the cost function, $\alpha \neq 0$ was assumed.

Having ensured that the artificial neural network model has been formed, the optimization of the cost function was realized using the three steps non-linear dynamic model shown below:

$$u(t) = u(t-1) - \frac{L}{1+\alpha L}\,e(t+1)\,\frac{\partial e(t+1)}{\partial u(t)} \quad (3)$$

where $L > 0$ is the optimizing step and $e(t+1) = w(t+1) - y_m(t+1)$. It has been proved that a three-layer feed-forward neural network has the capability of universal function approximation.

The formed artificial neural network model is given in eq. (4) as:

$$y_m(t+1) = \sum_{i=1}^{H} \nu_i s(.) \quad (4)$$

v is the weight. $s(.)$ is represented as follows:

$$s(.) = \sum_{j=1}^{n} \nu_{ij} y_m(t-j+1) + \sum_{j=1}^{m} \nu_{i,n+1} u(t-j+1) \quad (5)$$

The sensitivity $\partial e(t+1)/\partial u(t)$ is derived from the neural network model as follows:

$$\frac{\partial e(t+1)}{\partial u(t)} = -\sum_{i=1}^{H} \nu_i s'(.)\nu_{i,n+1} \quad (6)$$

The mathematical model description of the artificial neural network obtained upon substituting the calculated weight and bias values is given eqs. (7–9).

$$N_1 = \nu_{11}T_{i-1} + \nu_{12}T_{i-1} + \nu_{13}T_{i-3} + \\ + \nu_{14}U_{i-1} + \nu_{15}U_{i-2} + b1 \quad (7)$$

$$N_2 = \nu_{21}T_{i-1} + \nu_{22}T_{i-1} + \nu_{23}T_{i-3} + \\ + \nu_{24}U_{i-1} + \nu_{25}U_{i-2} + b2 \quad (8)$$

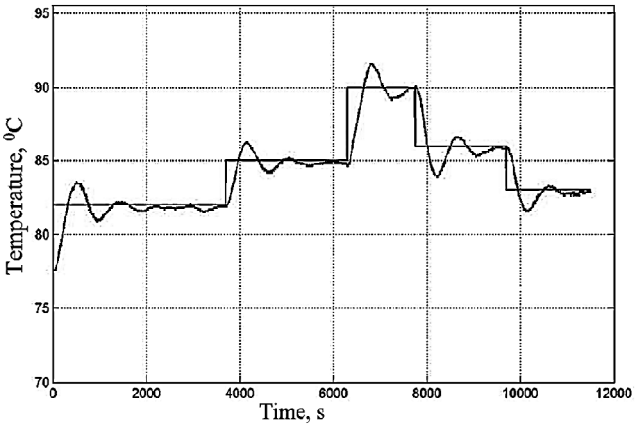
$$T_i = \nu_1\left(\frac{2}{1+\exp(-2N_1)} - 1\right) + \\ \nu_2\left(\frac{2}{1+\exp(-2N_2)} - 1\right) + b \quad (9)$$

The weight and bias values (Table 3) for the trained artificial neural network were taken and the algorithm for the predicted artificial neural network control was written in visual basic programming.

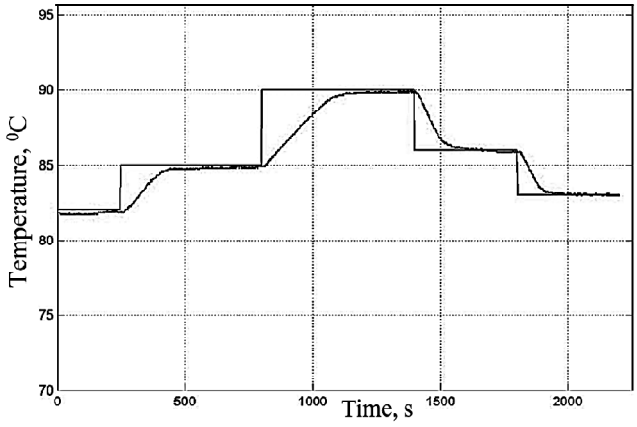
Results and discussion

The following experiments were performed to verify the sensitivity of the control systems and calculate the control and system parameters. The parameters like weighting factor, sampling interval, the number of iterations within a sampling interval were determined using the trial and error method. Typical set point tracking results are shown in Fig. 4. Settling time of response with $(\lambda/(1 + \alpha\lambda)) = 5$ was found to be much shorter than the one obtained with $(\lambda/(1 + \alpha\lambda)) = 0.1$. The best values of the set of tuning parameters for the NN-MPC method were selected and also the most suitable value of the parameter was taken $((\lambda/(1 + \alpha\lambda)) = 5$. This group of parameters value was used to carry out the required experiments.

Since the controlled variables were chosen as the reaction temperature the control was, therefore, aimed at making the reaction occur at the optimal temperature profile. When the reactor solvent medium was at the steady-state condition with definite values of heating and cooling flow rate, benzoyl peroxide was added. Furthermore, the temperature, being an exothermic property of the reaction, increased and



(a) $(\lambda/(1 + \alpha\lambda)) = 0.1$



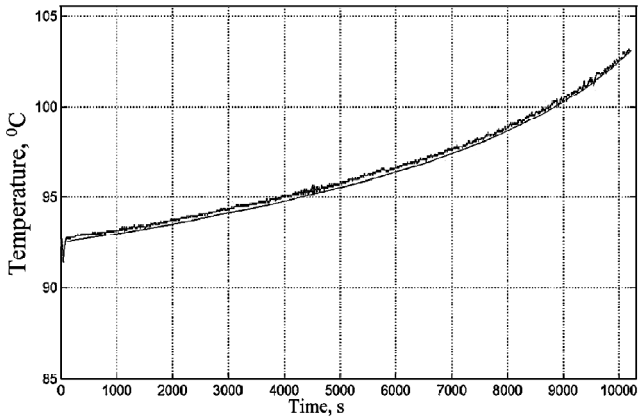
(b) $(\lambda/(1 + \alpha\lambda)) = 5$

Fig. 4. The response of temperature controller to set point changes.

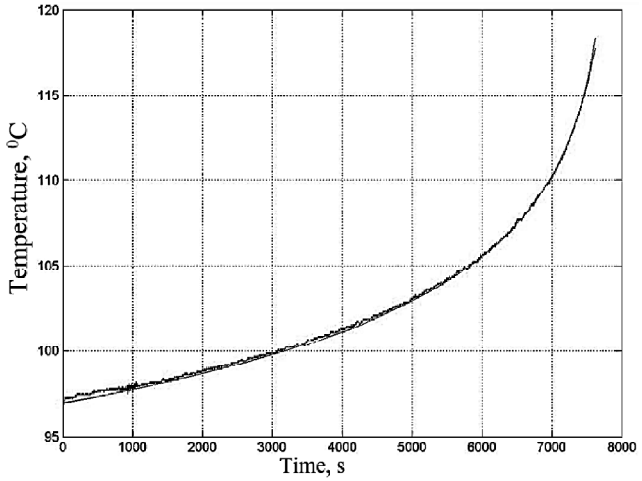
the NN-MPC algorithm was applied to control the reactor temperature at the optimal trajectory.

In the control of the polystyrene reactor, NN-MPC algorithms which was written in a visual basic programming language was used and the most appropriate NN architecture was obtained by using 2 neurons in the hidden layers. The parameters, weighting factor, sampling interval, the number of iterations within a sampling interval were chosen by utilizing trial and error technique. The best method of the training of NN was selected as the Levenberg-Marquardt algorithm and used in the control step. Many data which were used in the training were collected using the experimental system. To obtain the polymer with the desired characteristics, the temperature control of the reactor was carried out over the

optimum temperature profile by NN-MPC algorithm and the results of the control are presented in Fig. 5. PID control result for I_0 = 0.00125 is given in Fig. 6. PID parameters were found using Cohen-Coon method as K_c = 18.55, τ_I = 2.428, τ_D = 0.361. Where K_c, τ_I, τ_D represents controller gain, derivative time, and integral time respectively. In comparison with NN-MPC control result, the fluctuations occurred are more rapid and large. So, NN-MPC controller for tracking temperature path is more effective than the PID controller.



(a) I_0 = 0.0150 mol/L, Exp. number (1)



(b) I_0 = 0.0125 mol/L, Exp. number (2)

Fig. 5. Temperature NN-MPC control profile.

Numerical Average Molecular Weight determined from the experiment NN-MPC, PID is given in Table 4. As can be seen from Fig. 6, the reactor temperature closely follows the optimal temperature trajectory without exhibiting significant fluctuations, and this provides to obtain molecular weights showed a very high tendency of approaching the controlled one. That is to say that, the targeted polymer in this work, which was the one with the numerical average molecular weight of 52000 g/mole, has been approximately achieved. As can be seen from Table 4, Numerical Average Molecular Weight in the NN-MPC system is better than the one in the PID controller.

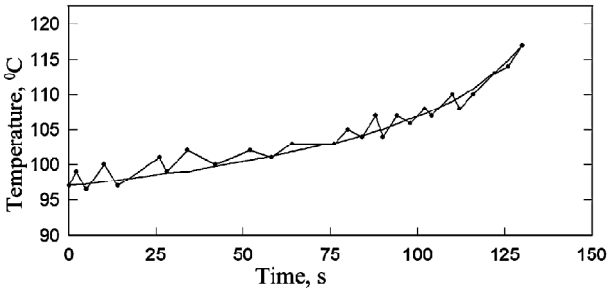


Fig. 6. Temperature PID control profile (I_0 = 0.0125 mol/L).

Table 4. Experimental NN-MPC and experimental PID for two different optimal operating conditions

Exp. number	Optimum parameters	Experimental NN-MPC	Experimental PID
1	M_0 = 6,092		
	T = 97		
	I_0 = 0.0125		
	tf (s) = 7620		
	M_n = 52000	M_n = 51739	M_n* = 38428
	m* = 0.5	m* = 0.63	m* = 0.44
2	M_0 = 6,092		
	T = 92		
	I_0 = 0.0150		
	tf (s) = 10200		
	M_n = 52000	M_n = 56215	M_n = 50299
	m* = 0.5	m* = 0.66	m* = 0.65

Conclusions

Experimental and theoretical implementation of NN-MPC algorithm was achieved successfully to track the temperature on a predetermined trajectory in a batch polymerization reactor. The results obtained from the Neural Network Model Predictive Control were found very satisfactory by comparing with the experimental results of the work carried out by

Özkan *et al.*[12]. In the cases studied, the temperature control with the NN-MPC algorithm was performed better than the one obtained using the PID controller.

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