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Nonlinear Adaptive PID Control for a Semi-Batch Reactor Based On an RBF Network

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***Abstract*—**Control of a semi-batch polymerization reactor using an adaptive radial basis function (RBF) neural network method is investigated in this paper. A neural network inverse model is used to estimate the valve position of the reactor; this method can identify the controlled system with the RBF neural network identifier. The weights of the adaptive PID controller are timely adjusted based on the identification of the plant and self-learning capability of RBFNN. A PID controller is used in the feedback control to regulate the actual temperature by compensating the neural network inverse model output. Simulation results show that the proposed control has strong adaptability, robustness and satisfactory control performance and the nonlinear system is achieved.

***Keywords*—**Chylla-Haase polymerization reactor, RBF neural networks, feed-forward and feedback control.

I. Introduction

THE industrial polymerization reactor proposed by Chylla-Haase [1] has been discussed widely and plays an important role in batch and semi-batch reactors. It is used in many different types of products, including fine chemicals, pigments, polymer and pharmaceuticals [1]-[3]. A very precise temperature control is required as a monomer feed poses a significant demand on the control, thus it is necessary to improve the control strategy of such a process in order to ensure that the end product will have acceptable quality. Polymerization reactors are commonly controlled by a cascade controller. This method provides robust operation but lacks control performance. Efforts have been made to use advanced non-conventional control methods to develop and test alternative control schemes for improving the operational performance of exothermic batch processes.

In [2]-[3], the extension of a cascade control with a feed-forward part (Extended Kalman filter) is proposed for the polymerization reactor. The extended Kalman filter is designed to estimate the reaction heat and the heat transfer coefficient during polymerization. The feed-forward control clearly improves the control performance while maintaining the standard cascade feedback control structure.

An on-line optimization of semi-batch reaction systems through MPC in combination with state estimation can be found in [4]. Also, in [5] a nonlinear model predictive control in combination with an extended Kalman filter is applied. The MPC is used to track the set-point and the extended Kalman filter is used to estimate certain parameters, such as heat transfer and reaction heat.

In [6] the controller design methodology is based on process inverse dynamics modelling. The learning database for the controller training is generated in an open loop fashion and training of the network is carried out off-line by considering the future plant outputs as the reference set points.

A nonlinear adaptive controller consisting of a nonlinear controller (based on differential geometric concepts), coupled with an extended Kalman filter (which uses only readily available data and knowledge) is applied in [7].

An inverse neural network in a hybrid scheme is used to model and control the semi-batch polymerization process in [8]. More robust model predictive control was proposed in [9]. In addition, some contributions have aimed to minimize batch time by maximizing monomer conversion in order to save time; these can be found in literature as well. For example, a model based control scheme for batch time minimization was proposed in [10].

In this work, RBFNN is used for modelling and controlling the nonlinear semi-batch reactor. Firstly the RBFNN is used to estimate the reactor temperature and then this model is used to design the RBFNN reactor inverse model which will be used to estimate the control variable. A PID controller is used in feedback to compensate the neural RBF inverse model output. The method is designed and conducted in three stages, starting with collecting data from the Simulink model of the reactor and finishing with RBF control.

The paper is organized as follows: In Section II a process description of Chylla-Haase and the dynamic model is presented. Section III presents modelling of the system dynamics using an RBF network. The adaptive inverse model scheme is given in Section IV. Section V presents the simulation results and makes a comparison with conventional cascade control. Finally the paper is concluded in Section VI.

II. The Chylla-Haase Polymerization Reactor

A. Process Description

The industrial polymerization reactor proposed by Chylla-Haase consists of a stirred tank reactor with a working value of 30 gallons. This is used to make a specialty emulsion polymer in the process and a cooling jacket and cooling recirculation with a volume of 5.7 gallons. A common strategy is shown in Fig. 1.

The polymerization process is simulated for a product which comprises a specific recipe [1], as given below. The recipe for each batch of a specific polymer consists of a

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heating phase from 0 to 1800 s and a feed phase from 1800 to 9600 s.

- Initial charges of solids (polymer, monomer) and water are placed into the reactor at ambient temperature T_{amb}.
- The temperature of the initial charge is raised to the reaction temperature set point T, set at 1800 s.
- After 1800 s, pure monomer is fed into the reactor at 0.00648 kg/s until 9600 s for Product B.
- After the feed addition has stopped, the temperature of the reaction is held at its set point value T.

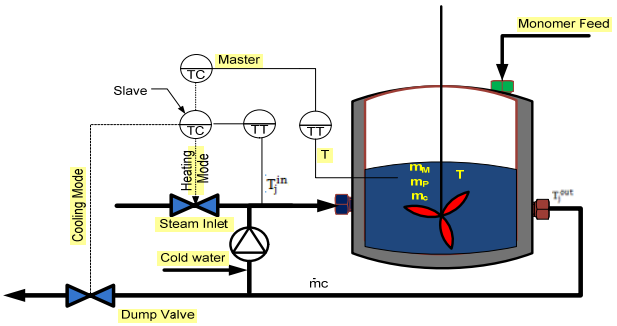

Fig. 1 Schematic Chylla-Haase reactor

The temperature of the reactor is often ramped up from the ambient reactor charge conditions to a temperature where the reaction begins to take off. The heat released through the reaction must be removed by circulating cold water through the jacket, where both hot and cold jacket steams are available. When the jacket temperature controller output is between 0 and 50%, the valve is opened and cold water is inserted; and when the jacket controller output is between 50 and 100%, the valve is opened and steam is inserted [2]-[11].

B. Reactor Dynamic Model

The reactor simulation model used here has been developed using MATLAB/SIMULINK (2010). The dynamic model can be described by a set of five ordinary differential equations (ODE) as follows:

$$\frac{dm_M}{dt} = \dot{m}_M^{in} - R_p \tag{1}$$

$$\frac{dmp}{dt} = R_p \tag{2}$$

$$\frac{dT}{dt} = \frac{1}{\sum_i mi\ \mathrm{Cp,i}}[\dot{m}_M^{in}\ C_{p,M}(T_{Amb} - T) - UA(T - T_j) - (UA)_{loss}(T - T_{Amb}) + Q_{Rea}] \quad (i = M, P, W). \tag{3}$$

$$\frac{dT_j^{out}}{dt} = \frac{1}{m_c C_{P,c}}[\dot{m}_c\ C_{P,c}(T_j^{in}(t-\theta_1) - T_j^{out}) + UA(T - T_j)] \tag{4}$$

$$\frac{dT_j^{in}}{dt} = \dot{T}_j^{out}(t-\theta_2) + \frac{T_j^{out}(t-\theta_2) - T_j^{in}}{\tau_P} + \frac{K_p(c)}{\tau_P} \tag{5}$$

The reactor model includes the material balances (1) and (2) for the monomer mass $m_M(t)$ and the polymer mass $m_p(t)$, the energy balance (3) with the reactor temperature $T(t)$, plus the energy balances (4) and (5) of the cooling jacket and the recirculation loop with the outlet and inlet temperatures $T_j^{in}(t)$ and $T_j^{out}(t)$ of the coolant C [2]. Further variables and parameters are defined in Tables I-III.

TABLE I
NOTATION OF THE CHYLLA-HAASE REACTOR

$\dot{m}_M^{in}$	Monomer feed rate [kg/s]
$Q_{Rea} = -\Delta H \bullet R_P$	Reaction heat [kw]
R_P	Rate of polymerization [kg/s]
$-\Delta H$	Reaction enthalpy [kj/kg]
U	Overall heat transfer coefficient [kw/mk]
A	Jacket heat transfer area [m2]
$(UA)_{loss}$	Heat loss coefficient [kw/k]
$C_{P,M}, C_{P,c}, C_{P,p}$	Specific heat at constant pressure []
θ_1, θ_2	Transport delay in jacket and recirculation loop [s]
$T_j = (T_j^{in} + T_j^{out})/2$	Average cooling jacket temperature [k]
$K_P(c)$	Heating/cooling function [k]
τ_P	Heating/cooling time constant [s]

The heating/cooling function $K_P$is defined by (6) and is a function of the valve position c (t), [2]-[11]:

$$K_p(c) = \begin{cases} 0.8 \cdot 30^{-c/50}(T_{inlet} - T_j^{in}(t)), & C < 50\% \\ 0 & C = 50\% \\ 0.15 \cdot 30^{-c/50-2}(T_{steam} - T_j^{in}(t)), & C > 50\% \end{cases} \tag{6}$$

TABLE II
EMPIRICAL RELATIONS FOR THE POLYMERIZATION RATE R_p, THE JACKET HEAT TRANSFER AREA A, AND THE OVERALL HEAT TRANSFER COEFFICIENT U

$R_P = iKm_M$	i Impurity factor
$K = K_0 \exp(-\frac{E}{RT}) \cdot (K_1\mu)^{K_2}$	Kinetic constant
$\mu = c_0 \exp(c_1 f) \cdot 10^{c_2(a_0/T - c_3)}$	Batch viscosity
$f = m_p/(m_M + m_p + m_c)$	Mass function
$A = (\frac{m_M}{\rho_M} + \frac{m_P}{\rho_P} + \frac{m_W}{\rho_W})\frac{P}{B_1} + B_2$	jacket heat transfer area
$U = \frac{1}{h^{-1} + h_f^{-1}}$ with $h = d_0 \exp(d_1 \mu_{wall})$	Heat transfer coefficient

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TABLE III
PARAMETER VALUES OF CHYLLA-HAASE REACTOR

Symbol	Unit	Values of Polymer B
$m_{M,0}$	kg	0
$m_{p,0}$	kg	11.010
m_w	kg	41.2825
ρ_M	kgm^{-3}	900
ρ_p	kgm^{-3}	1040
ρ_w	kgm^{-3}	1000
$C_{p,M}$	$kJkg^{-1}k^{-1}$	1.675
$C_{p,P}$	$kJkg^{-1}k^{-1}$	3.140
$C_{p,W}$	$kJkg^{-1}k^{-1}$	4.187
MW_M	$kgkmol^{-1}$	106.0
m_c	kg	42.996
$\dot{m}_c$	kg/s	0.9412
$C_{p,C}$	$kJkg^{-1}k^{-1}$	4.187
K_0	S^{-1}	20
K_1	$m\,s\,kg^{-1}$	1000
K_2		0.4
E	$kJkmol^{-1}$	29560.89
c_0	$kgm^{-1}S^{-1}$	3.2×10^{-5}
c_1		19.1
c_2		2.3
c_3		1.563
a_0	k	555.556
ΔH_p	$kJkmol^{-1}$	65593.2
d_0	$kW\,m^{-2}k^{-1}$	0.814
d_1	$m\,s\,kg^{-1}$	-5.13
$m_M^{in,max}$	kg/s	6.048×10^{-3}
$[t_{M,0}^{in}, t_{M,1}^{in}]$	min	[30,90]
$[t_{M,2}^{in}, t_{M,3}^{in}]$	min	[120,160]
T^{set}	K	353.160

C. Modelling of Uncertainty

The main uncertainties and disturbances that affect the process are condensed into two variables: the purity factor i and the fouling factor $1/h_f$. The purity factor i varies from 0.8 to 1.2 and describes the fluctuations in the reaction rate caused by impurities in the row materials. It is constant during one batch, but it changes randomly from batch to batch. The fouling factor $1/h_f$ varies from 0 to 0.704 m^2K/KW in order to simulate the decrease in U due to the formation of a polymer film on the reactor wall during successive batches [1], [2], [11]. While data for two different products, A and B, are given in [1]-[3], this work is restricted to product B only.

TABLE IV
SCENARIO CONSIDERED FOR CONTROL ANALYSIS

Scenario	$i[-]$	$1/hf[m^2K/KW]$
1	0.8	0.0
2	1.2	0.704

III. RBF NEURAL NETWORK INVERSE MODEL

The radial basis function neural network (RBFNN) has an ability to model any nonlinear function. However, this kind of neural network can need many nodes to achieve the required approximating properties [12]. The first step in the reactor modelling is the generation of a suitable training data set. The accuracy of the neural network modelling performance will be influenced by the training data. For RBF neural network training, the K-means algorithm is used to choose the centers, the P-nearest neighbor algorithm decides the widths and the recursive training algorithm calculates the weights for the output layer [13]. Here, the RBFNN based inverse model is used to predict the valve position $Cv(k)$ which is the manipulated variable in the next sample time. The RBFNN block diagram is illustrated in Fig. 2.

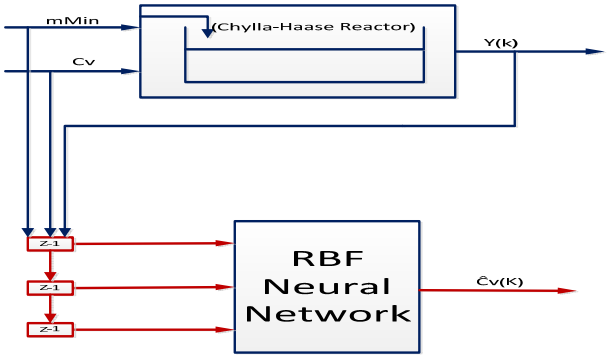

Fig. 2 RBFNN model structure

The dynamics between the actual reactor output (temperature) and the control variable (valve position Cv), can be represented by:

$$T(k) = f[T(k-1), T(k-2), Cv(k-1), Cv(k-2), \dot{m}_M^{in}(k-1)] \quad (7)$$

$$Cv(k-1) = g[Cv(k-2), T(k), T(k-1), T(k-2), \dot{m}_M^{in}(k-1)] \quad (8)$$

$$Cv(k) = g[Cv(k-1), T(k+1), T(k), T(k-1), \dot{m}_M^{in}(k)] \quad (9)$$

$$Cv(k) = g[Cv(k-1), r(k+1), r(k), T(k-1), \dot{m}_M^{in}(k)] \quad (10)$$

So the RBF network input will be:

$$X_1 = [Cv(k-1), r(k+1), r(k), T(k-1), \dot{m}_M^{in}(k)] \quad (11)$$

where X_1 is the vector input for the RBF model, Cv is the valve position for the reactor, T is the reactor temperature, $\dot{m}_M^{in}$ is monomer feed rate and r is the reference signal. Generally, $\hat{C}v$, which is the estimated valve position, is a weighted sum of the hidden node outputs.

$$\hat{Cv} = \sum_{j=1}^{nh} \phi_j(t) \bullet W_{ji} \qquad i = 1,.....q \quad (12)$$

where ϕ_j is defined by (13), w represents the output layer weights and q is the number of outputs. The method that is used in this work to calculate the Euclidean distance between the center and the network input vector X_1 is Gaussian basis function [12]-[14]:

$$\phi_j(t) = \exp\left(-\frac{\left\|X_1(t) - c_j(t)\right\|^2}{\sigma_j^2}\right), \qquad j = 1,..,nh \quad (13)$$

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where σ_j is a positive scalar called width and c_j is the number of centers.

RASs were applied to only the first reactor input Cv (valve position) and the second input here is considered to be the monomer feed rate, which is a fixed value at a specific time. Data for the reactor were collected for reactor temperature at each sample time. The raw data were scaled using the following equation before training:

$$xscale(k) = \frac{x(k) - \min\{x(i)\}}{\max\{x(i)\} - \min\{x(i)\}} \qquad i \in [1, N] \tag{14}$$

The training data set with 3000 samples are used to train the RBFNN model. Then, the test is set with different RAS samples, as displayed in Figs. 3 and 4. The mean square error (MSE) is used to evaluate the modelling and control performance in this work, which is given by the following equation:

$$MSE = \frac{1}{N}\sum_{k=1}^{N}\left|\hat{C}v(k) - Cv(k)\right| = \frac{1}{N}\sum_{k=1}^{N}\left|e(k)'*e(k)\right| \tag{15}$$

where $\hat{C}v(k)$ is the output prediction of the neural network model and $Cv(k)$ is the inverse output of the reactor. The Cv in Figs. 3 and 4 is the normalized value.

$$\sigma = 11,\ p(0) = 1.0 \times 10^{-2} \times \mathrm{I}_{nh \times nh},\ w(0) = 1.0 \times 10^{-2} \times \mathrm{U}_{nh \times 1},$$

where σ is the width of the hidden layer and p and w are RLS parameters which are used for weight updating [13]. $\mathbf{I}$ is an identity matrix and $\mathbf{U}$ stands for a matrix whose components are ones.

IV. Adaptive Inverse Control Scheme

In the previous section the RBFNN model used to estimate the control variable (Cv) was presented and satisfactory results were obtained, as shown in Figs. 3 and 4. In this section the inverse model will be used in the reactor feed-forward path in order to maintain the temperature of the reactor. The structure of adaptive FF with FB based on the RBFNN is shown in Fig. 5. After training the RBFNN inverse model a satisfactory result was obtained. The Recursive Least Square parameters, widths and weights will be updated at each sample time (on-line) and then this model will be used in the feed-forward path to predict the valve position $Cv(k)$.

The PID controller is added to form the feedback controller. In this case the activating valve position is the sum of two controller output variables; one is from the RBF based feed-forward neural network controller, the other from the feedback PID controller.

The algorithm of the basic PID Controller based on the RBF neural network is as follows [13]-[15]:

$$Cv(k) = Cv(k-1) + [K_p * e(k-1) + K_i * e(k) + K_d * (e(k) - e(k-1)/T_s] \tag{16}$$

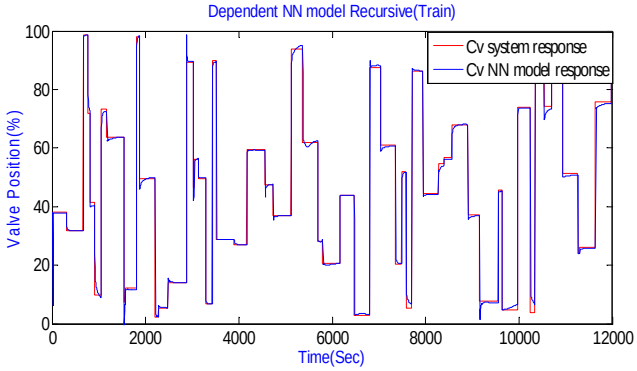

Fig. 3 Cv training data for RBFNN model MAE (Mean Absolute Errors = 0.453)

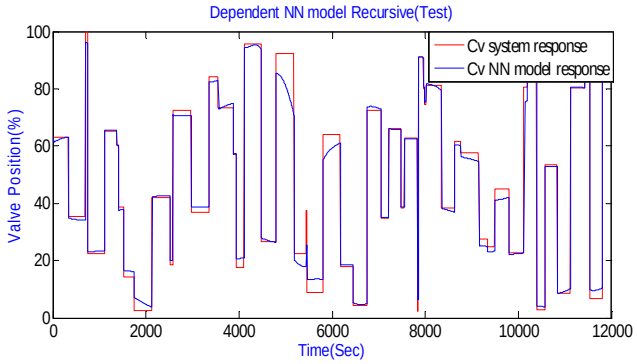

Fig. 4 Cv validation data for RBFNN model MAE (Mean Absolute Errors = 0.501)

After fine tuning, the PID controller that is used here with the RBF based neural network controller for the Chylla-Haase reactor is:

$$Cv(k) = Cv(k-1) + [35 * e(k-1) + 0.008 * e(k) + 150 * (e(k) - e(k-1)/4] \tag{17}$$

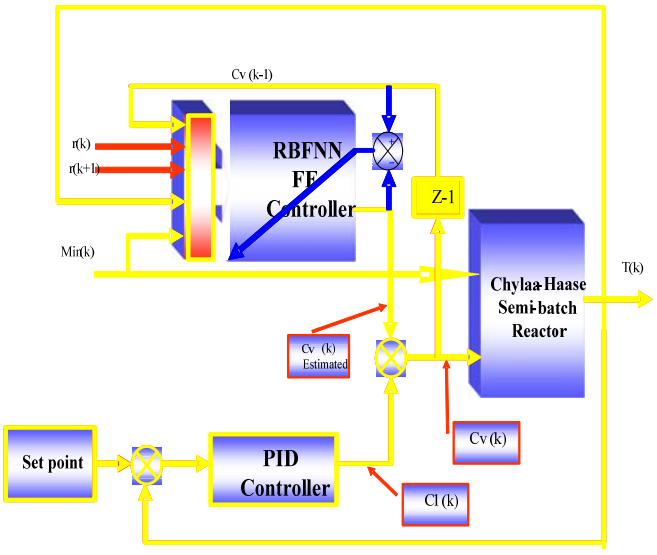

Fig. 5 RBFNN FF and PID controller for Chylla-Haase reactor

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V. Simulation Results and Analysis Comparison

In this paper the simulation adopted a nonlinear semi-batch polymerization reactor. The performance of the RBFNN in tracking control was compared to the conventional cascade control controller with different disturbance effects, impurity factors and fouling factors with two scenarios: the first and fifth batch of the process.

In the RBF tuning of PID control, the three parameters of PID control were given as follows: K_p was 35, K_i was 0.008 and K_d was 150. The sampling time was 4 s, network weights and the network structure was 5-15-1.

The results after using a cascade PID control method are shown in Figs. 6 (a)-(c). The results of the RBF tuning PID control strategy are shown in Figs. 7 (a)-(c). In Fig. 6 (a) it is clear that the reactor temperature in the fifth batch reached the lower bound, which will in fact have a big impact on the quality of the product and goes beyond the limited tolerance ($\pm$0.6K).

Significant improvement can be seen in terms of the reactor temperature in Fig. 7 (a) using the RBFNN inverse model based on PID control; even in the fifth batch, which had a big disturbance effect on temperature, the RBFNN can still maintain the temperature within the tolerance range (which is $\pm$0.6K) from the set point.

The mean square error used here to evaluate the control performance shows that the cascade controller has less capability (MSE = 0.7427 for the first batch and MSE = 5.7543 for the fifth batch) than the adaptive RBF controller (MSE = 0.0682 for the first bath and MSE = 1.0181) for the fifth batch.

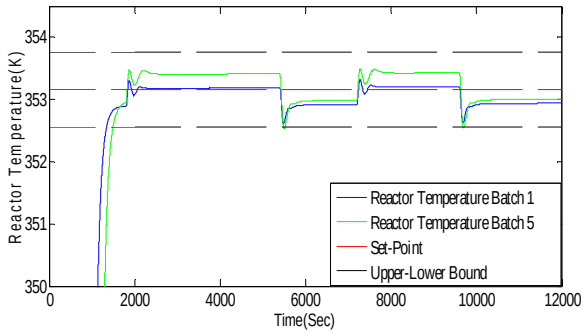

Fig. 6 (a) Reactor temperature based on cascade control for first and fifth batches

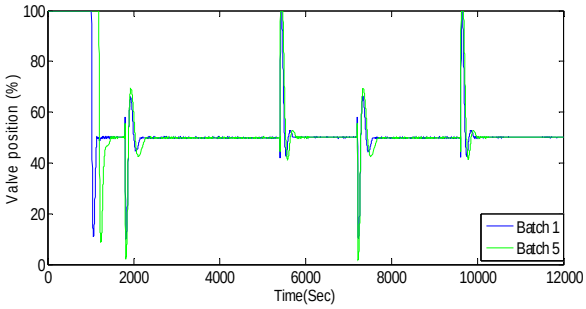

Fig. 6 (b) Valve positon based on cascade control for first and fifth batches

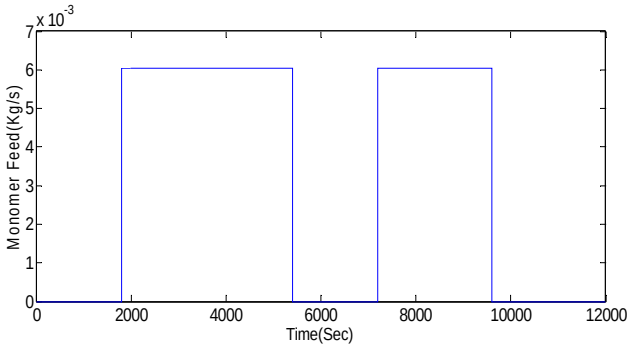

Fig. 6 (c) Monomer feed rate

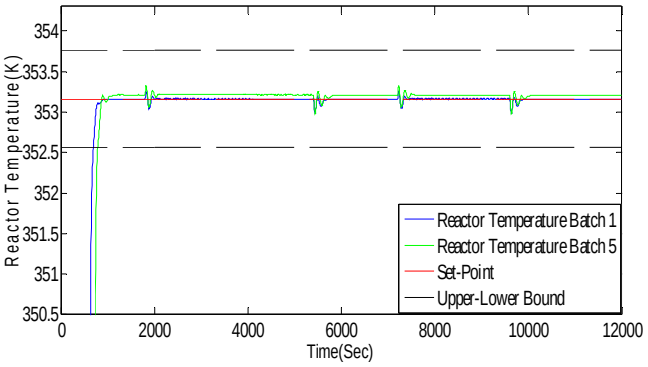

Fig. 7 (a) Reactor temperature with adaptive RBFNN inverse model for first and fifth batches

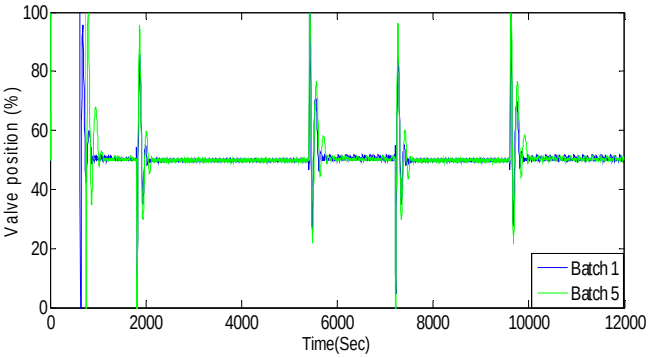

Fig. 7 (b) Valve position with adaptive RBFNN inverse model for first and fifth batches

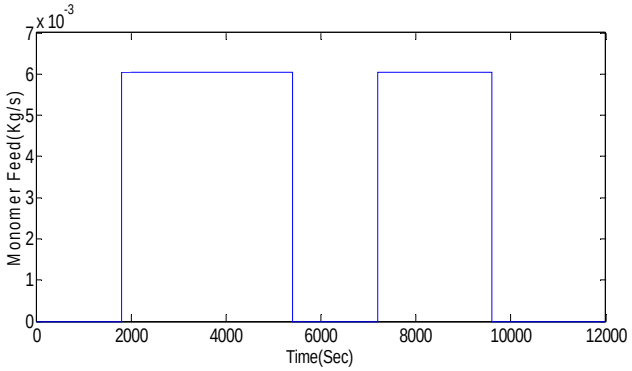

Fig. 7 (c) Monomer feed rate

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VI. Conclusion

It is anticipated that PID controllers will continue to play a key role in process control for a long time to come. Therefore, in this work we have attempted development of control strategies that maintain the PID structure while enhancing its performance capabilities. This is done by combining the conventional control techniques with evolving RBFNN methodologies.

The general framework observed throughout this paper can be summarized as follows. First, we have tried to combine NN modelling techniques, in particular RBF, with classical PID control strategies so that we can augment the capabilities of this technique and improve the overall control for the Chylla-Haase reactor. Secondly, we have attempted to preserve, as much as possible from a practical perspective, the PID structure, for easy design and implementation. Thirdly, we have developed a strategy for controller tuning to maintain the temperature with specific tolerance against monomer feed inlet effect and disturbance. The effect of the proposed method is clear from simulation results and by evaluating the control performance using the mean square error: the cascade controller has less capability than the adaptive RBF controller.

Further work will cover control ability for more uncertainties and disturbances and the issue of the monomer feed rate being constant which leads to long durations of batch run. Another optimization scheme is needed in order to make the monomer feed vary to reduce batch run.

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