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Discrete-time controllers for temperature control of a polystyrene polymerization reactor

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For temperature control, styrene free radical polymerization in a 1.1 l batch reactor was presented with the zero-order hold-equivalent discrete time models in the present work. Two discrete-time controllers were applied to the reactor. Firstly, a discrete-time controller with three tuning parameters was designed, and its parameters were determined by checking control performance and closed loop pole-placement in z-plane. The sixth order closed loop transfer function between reactor temperature and set point was obtained. The best tuning parameters were determined as –0.1, –0.9 and –0.1. Effect of tuning parameters to stability was investigated. Secondly, the discrete-time proportional-integral-derivative (PID) controller (2DOF) was employed. Simulink control design was utilized for tuning the six parameters of the controller as –10.75, –1.09, –19.26, 0.689, 0.1686, 4.123e-0.5 respectively. These controller performances were compared to each other for a step decrease in set point. It is noted that a very close matching was achieved and the controllers have made the closed loop system desirable and stable with the best tuned parameters determined. In order to obtain good quality 52000 g/mole polystyrene, these two different discrete-time controllers were applied theoretically for tracking previously determined optimal temperature profile. The previously published experimental data were used for validation. Cooling water flow rate was manipulated to obtain better control performance with minimum response time and reduced production cost. In the set point tracking cases studied, the best tuned controllers acted to produce non-oscillatory closed loop behaviour without offset throughout the length of the batch run.

Keywords: Polymerization, polystyrene, discrete-time model, zero-order hold, discrete-time controllers.

Introduction

Exothermic reactions in various industrial reactors that may have potential safety problems exhibit very interesting behaviour for investigation. The models based on mass and energy balances and kinetic rate relations for a styrene polymerization batch reactor was solved to provide constraint requirements, and many temperature control applications was reported for practical operation by considering the complexity of the system[1]. Polystyrene reactors are highly used in industry because of its economic importance. A well-tuned feedback control loop is essential because this process may exhibit unstable dynamic behaviours. Undesirable performances of some controllers applied to control the temperature of reaction medium were reported[2]. The polymerization reactions generate a large amount of heat which must be removed from the reactor to follow the required temperature values. The suitability of controller highly depends on the types of reaction and reactor, the process operating temperature, the processing method, and catalyst[3].

In order to provide desired polymer product, generalized predictive and traditional PID control algorithms were implemented experimentally for tracking an optimal temperature profile by manipulating heat power[1]. Polymerization temperature of styrene was controlled with fuzzy method by manipulating the heat rate obtained from electrical heater[4a]. Generalized predictive control with the neural network model between heater output and polymerization medium temperature, and neural network based model predictive control algorithms were implemented[4b,5]. For a batch polymerization reactor, a hybrid-based model was developed by using a neural network modelling strategy, and performance comparison with previously published models was achieved[6].

Without using process modelling for polystyrene polymerization, network models which are applicable to nonlinear chemical processes were developed based on datasets[7]. Hosen *et al.*[8] used the developed hybrid model which is validated with experimental data[6] to design and implement artificial neural network-based model predictive, artificial fuzzy logic, and generic model controllers for temperature control in a batch styrene polymerization reactor. The amount of heating power was manipulated by these controllers. These models and control strategies mentioned above can be applied to styrene polymerization and similar polymerization reactors. These designs have not included the energy saving aspects.

Cancelier *et al.*[9] applied a predictive control to the temperature control of a batch reactor by using an empirical model. Coolant water temperature in the reactor jacket was varied by manipulating the steam flow in the heat exchanger. Regarding cost reduction of polymerization process the minimization of steam consumption was added in the objective function of the control algorithm[9]. Malathi and Bhuvaneswari[3] implemented the continuous and discrete PID cascade controllers to temperature control of polyvinyl chloride resin production in a batch reactor by manipulating controller output percentage for two types of cooling arrangement in the jacket. The discrete cascade controller performance was found superior to the continuous controller one[3].

Controllers structured simply such as a sampled-data PID controllers has been highly implemented in industry. Many design methods are available to determine optimal parameters of these controllers. For the design of controller, stability is the most critical factor besides its set profile tracking performance. Tajika *et al.*[10] designed a discrete-time PID controller to control a discrete first-order plus dead time system by achieving a desired robustness level. Kurokawa *et al.*[11] designed a sampled-data PID controller to control a second-order plus dead-time sampled-data system by means of optimal normalized PID parameters. Sharma and Janardhanan[12] designed a discrete-time higher-order sliding mode (DHOSM) controller by considering matched uncertainty. They proposed also a DHOSM controller for an uncertain discrete-time linear time invariant system in the presence of unmatched uncertainty[13]. Khan *et al.*[14] proposed a detailed design of a cost-effective discrete-time proportional integral (PI) controller with a proper anti-windup structure by using two tuning parameters to control temperature of a heating pad. The P and I parameters were estimated by placing the poles of the closed-loop system. Hinkkanen *et al.*[15] applied an analytical discrete-time pole-placement design method for two-degrees-of-freedom (2DOF) PI current controller by verifying experimentally. Dincel and Soylemez[16] designed a new digital PI-PD controller via dominant pole placement approach. In this method the dominant pole pair is placed to the desired points in z-plane and the remaining poles are kept a certain times away from the dominant poles.

In this study, the discrete-time transfer function which relates batch polymerization reactor temperature as output and the flow rate and initial temperature of the coolant as inputs was developed to capture the dynamic behaviour of the process. The feedback controller and zero-order hold element were used to map output to corresponding set point with the actual process data and knowledge. Two discrete-time controllers were used for performance comparison. The three tuning parameters of the first discrete-time controller designed were tuned by checking the closed-loop pole locations. The six parameters of the second discrete-time PID controller (2DOF) were tuned by means of Simulink control design.

Discrete-time control system

Modelling approach applied to industrial processes has moved from use of differential and algebraic equations to data-driven transfer functions to describe the operation range. Discrete-time transfer function of the polystyrene polymerization batch reactor was obtained by using zero-order hold element and 1s sampling time (t_s). The process transfer function parameters were fitted according to measured characteristics of the system. Reactor temperature related with coolant flow rate and coolant jacket inlet temperature was given in deviation variable form (eqs. (1)–(2)).

$$T' = G_{p1}m'_c + G_{p2}T'_{ci} \quad (1)$$

$$\frac{T'}{m'_c} = \frac{-0.0055z^2}{z^4 - 1.655z^3 + 0.682z^2 - 1.749\times10^{-7}z + 1.285\times10^{-6}} \quad (2)$$

where T', G_{p1}, m'_c, G_{p2}, T'_{ci} are temperature of the reaction mixture in deviation variable form, discrete-time process transfer function relating T' and m'_c, coolant flow rate in deviation variable form, discrete-time process transfer function relating T' and T'_{ci} and coolant jacket inlet temperature in deviation variable form respectively.

Two different discrete-time controllers were applied. The first proposed controller transfer function was defined between error and coolant flow rate in eq. (3).

$$\frac{m'_c}{e} = \frac{(B)z^2}{z^2 + (A1)z + (A2)} \quad (3)$$

$$e = T' - T'_R \quad (4)$$

where $A1$ and $A2$ are coefficients of monic polynomial in the z-domain. B represents coefficients of polynomial in the z-domain. T'_R and e are set point temperature in deviation variable form and error in deviation variable form respectively.

When the parameters B, $A1$, $A2$ were –0.1, –0.9 and –0.1 respectively, the closed feedback loop transfer function was given below.

$$\frac{T'}{T'_R} = \frac{-0.00055z^4}{z^6 - 2.555z^5 + 2.072z^4 - 0.448z^3 - 0.068z^2 - 1.1\times10^{-6}z - 1.2\times10^{-7}} \quad (5)$$

The second discrete controller was obtained from Simulink Library in MATLAB. This discrete PID controller (2DOF) was presented in eq. (6).

$$\frac{m'_c}{e} = P\,(b\times T'_R) + I\times t_s \frac{1}{(z-1)}\,(T'_R - T')$$

$$D\frac{N}{1 + N\times t_s \frac{1}{(1-z)}}(c\times T'_R - T') \quad (6)$$

where b, c, D, I, P, N, t_s are the first and second set point weights, derivative, integral, proportional terms for discrete-time PID controller, filter coefficient, sampling time respectively.

This controller block has some unconventional features such as windup protection, desired value tracking, and external reset. The controller parameters can be tuned by means of Simulink facility which requires Simulink Control Design.

Results and discussion

The stability of polystyrene polymerization batch reactor without control was guaranteed experimentally and theoretically through the desired temperature range[1]. This data bank and the modelling knowledge[1] were used to obtain the discrete-time transfer function of the process in eq. (1). The temperature of 85°C was chosen as initial steady state reactor temperature that was used as bias value for deviation variable form. This transfer function characteristic polynomial roots were evaluated as 0.8800 + 0.0000i, 0.7750 + 0.0000i, –0.0000 + 0.0014i, and –0.0000 – 0.0014i which are in unit circle of z-plane. The discrete-time controller with three tuning parameters (eq. (3)) was applied to control the batch reactor medium temperature. The best controller parameters were determined by using closed loop transfer function pole-placement technique in unit circle of z-plane (Fig. 1). The controller tuning parameter values of B, $A1$ and $A2$ were changed to investigate their effect on the closed-loop stability (Table 1). The well-tuned B, $A1$, and $A2$ values were detected as –0.1, –0.9 and –0.1 respectively in Table 1.

For discrete-time closed loop, to test the bias reactor temperature value when error is zero, temperature set point of

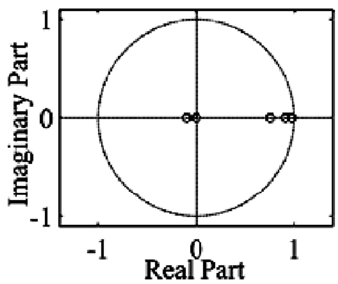

Fig. 1. Closed loop transfer function pole-placement in z-plane by using the best controller tuning parameters, B = –0.1, $A1$ = –0.9, $A2$ = –0.1.

Table 1. Closed loop transfer function poles obtained by using various set of controller tuning parameters, *B*, *A*1, *A*2

Controller tuning parameters			Closed loop transfer function poles	Stability
B	*A*1	*A*2		
–0.1	–0.9	–0.1	0.9777 + 0.0000i	Stable
			0.9144 + 0.0000i	
			0.7629 + 0.0000i	
			–0.1000 + 0.0000i	
			–0.0000 + 0.0014i	
			–0.0000 – 0.0014i	
–1.0	–0.9	–0.1	40.9737 + 0.1281i	Stable and oscillatory
			0.9737 – 0.1281i	
			0.7075 + 0.0000i	
			–0.0999 + 0.0000i	
			–0.0000 + 0.0014i	
			–0.0000 – 0.0014i	
–4.0	–0.9	–0.1	1.0094 + 0.2369i	Unstable
			1.0094 – 0.2369i	
			0.6359 + 0.0000i	
			–0.0998 + 0.0000i	
			–0.0000 + 0.0014i	
			–0.0000 – 0.0014i	
–0.1	–0.99	–0.1	1.0733 + 0.0000i	Unstable
			0.8989 + 0.0000i	
			0.7652 + 0.0000i	
			–0.0924 + 0.0000i	
			–0.0000 + 0.0014i	
			–0.0000 – 0.0014i	
–0.1	–0.9	–0.3	1.1544 + 0.0000i	Unstable
			0.8911 + 0.0000i	
			0.7684 + 0.0000i	
			–0.2589 + 0.0000i	
			–0.0000 + 0.0014i	
			–0.0000 – 0.0014i	

85°C was introduced for 1000 s. Then a set point step decrease from 85°C to 82°C was given at time 1000 s. The obtained reactor temperature as closed loop output versus time was shown in Fig. 2. This set point tracking performance of the discrete-time controller with three well-tuned parameters was found successful with response time of 214 s. By tuning *B* parameter of the controller as –1.0, a pair of closed loop poles that created oscillatory reactor temperature behaviour was placed in stability region (Fig. 3). In this figure, system output tracked the set point with smaller rise time and larger response time than the tracking obtained in Fig. 2. By changing controller parameter *B* from –0.1 to –1.0, the system output behaviour moved from overdamped case (Fig. 2) to underdamped case (Fig. 3) by reducing rise time and increasing response time.

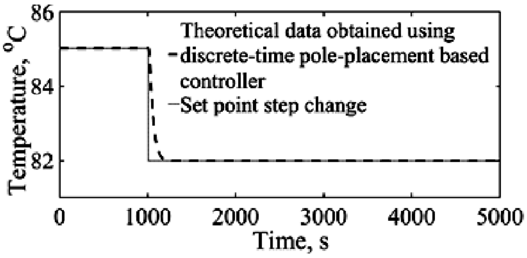

Fig. 2. The controlled reactor temperature response obtained using the discrete-time controller with three tuning parameters, *B* = –0.1, *A*1 = –0.9, *A*2 = –0.1.

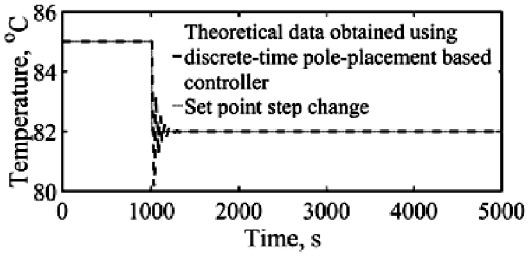

Fig. 3. The controlled reactor temperature response obtained using the discrete-time controller with three tuning parameters, *B* = –1.0, *A*1 = –0.9, *A*2 = –0.1.

In Fig. 4, the discrete PID controller with six parameters tuned using Simulink control design was implemented. The feedback temperature control response of the reactor was obtained through a set point step change to 82°C at time 1000 s. The performance of controller with three parameters given above was compared with the effectiveness of discrete PID controller (2DOF) that is available in Simulink library. The second controller with the response time of 7 s produced successful set point tracking without oscillation (Fig. 4).

For initial initiator concentration (I_0) = 0.02 mole/L, desired number average molecular weight (M_{nd}) = 52000 g/mole, and target monomer conversion (X_d) = 0.5, the optimal set temperature profile previously reported[1] was used in the present study (Figs. 5 and 6). Experimental validation

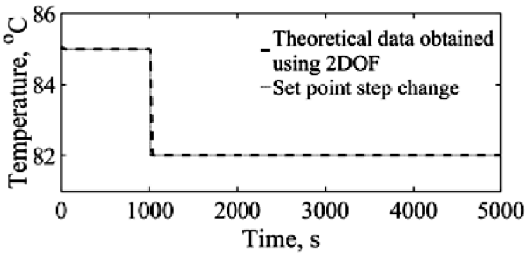

Fig. 4. The controlled reactor temperature response obtained using the discrete-time PID controller (2DOF) with six tuning parameters, $P = -10.75$, $I = -1.09$, $D = -19.26$, $N = 0.689$, $b = 0.1686$, $c = 4.123e\text{-}0.5$.

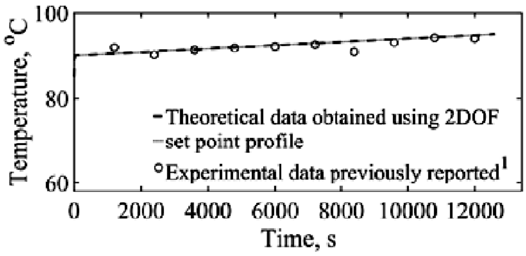

Fig. 6. The controlled reactor temperature response obtained using the discrete-time PID controller (2DOF) with six tuning parameters, $P = -10.75$, $I = -1.09$, $D = -19.26$, $N = 0.689$, $b = 0.1686$, $c = 4.123e\text{-}0.5$ for optimal temperature profile (I_0 = 0.02 mol/L).

was realized by using previously published closed loop output data[1] obtained by manipulating power of an immersed heater. In Fig. 5, the theoretical temperature control results obtained by manipulating coolant flow rate were shown for application of the discrete-time controller including three tuning parameters. The parameters of discrete-time pole-placement based controller were used as $B = -1.0$, $A1 = -0.9$, and $A2 = -0.1$. With this well-tuned controller, reactor temperature closely tracked the optimal set profile and the desired robustness was achieved.

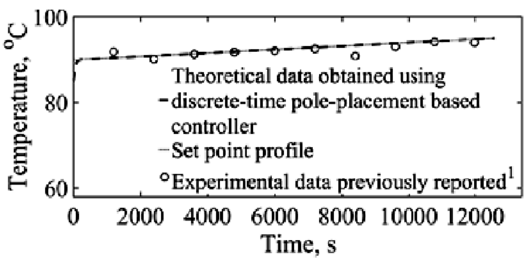

Fig. 5. The controlled reactor temperature response obtained using the discrete-time controller with three tuning parameters, $B = -0.1$, $A1 = -0.9$, $A2 = -0.1$ for optimal temperature profile (I_0 = 0.02 mol/L).

In Fig. 6, from Simulink library, the discrete PID controller with well-tuned six parameters was used to obtain reactor temperature control response that follows the desired temperature profile by manipulating reactor jacket coolant flow rate. Both performance of discrete-time controllers utilized was close to each other and introduced successful set point tracking (Figs. 5 and 6). The present reactor temperature responses given in Figs. 5 and 6 was also compared with the previously published experimental standard PID closed-loop response obtained using the immerse heater power as the manipulated variable[1]. The discrete controllers applied in the present study performed the control objective of keeping the batch reactor temperature within a tight tolerance level of the optimal temperature profile. With a constant jacket inlet temperature of 21°C, the discrete-time controllers successfully quenched out excess heat energy occurring from the reaction by manipulating the jacket coolant flow rate in a cost-effective way.

The advantages of the controllers used in the cases studied were low rise time, low settling time, and very smooth transient responses which have importance during the polymerization period. The desired level of performance was guaranteed using suitable tuning technique for controller parameters.

Conclusions

Some small changes in a batch reactor temperature may lead to poor product quality. Therefore reactor temperature as a fast sampling intermediate variable was controlled to obtain the desired molecular weight of the polystyrene produced. The monomer styrene free radical polymerization using toluene as solvent, and benzoyl peroxide as a monomer soluble initiator was modelled in discrete-time domain for closed loop application. The experimental data were consistent with the discrete-time model so that the problem of mechanisms nonlinearity not modelled was eliminated within the acceptable truncation error range. Two discrete time controllers with three and six tuning parameters were used respectively using digital computers without discretization error.

It is important to keep the batch reactor mixture at the optimal temperature profile by reducing the energy consumption of the polystyrene polymerization. The robustness of the controller applied is also important. For this reason, the closed-loop system poles are located in a region without tight tuning of poles. The proposed controller with three parameters can easily be implemented in the process industry because of its effectiveness and ease. This controller performance has been successfully investigated by comparing with the effectiveness of the PID controller in which the six terms are positioned by using Simulink control design. The theoretical cost-effective performances of controllers used are verified by means of the experimental standard PID controller performance previously obtained[1] in a real environment.

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