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Control of adiabatic continuous stirred tank reactor at an unstable operating point

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This paper describes application of temperature control to an unstable reactor. A non-adiabatic continuous stirred tank reactor simulation program was run in Matlab at a predetermined unstable operating point to attain closed loop performances. Jacket temperature was chosen as a manipulated variable. The simulated program having mass and energy balances for reactor inlet and cooling system was used to apply proportional control and to design the tuning parameters of conventional and advance control systems. A sinusoidal set point chance for a small time interval was introduced to the simulated process, the reactor temperature oscillation with a constant amplitude was monitored for proportional only control. The numerical value of the proportional controller coefficient that produces oscillatory system response was varied to rich the well-suited ultimate reactor temperature changes versus time. Ziegler-Nichols and Tyreus-Luyben evaluation technique was utilized to evaluate Proportional Integral Derivative controller parameters. Whilst retaining the computational simplicity of Matlab and the conventional control parameter evaluation techniques, the proposed method was made temperature response to follow an unstable operation set-point successfully. It is significant to note that integral action in the controller provides saddle point steady-state following without offset even if the values of the parameters of the system or of the controller change. Self-tuning Proportional Integral Derivative controller tuning parameters were also evaluated by using the proportional, integral and derivative constants and the second order parametric system model. The success of the various control actions were compared by using two performance criterions.

Keywords: Experimental Self-tuning PID application, pH control, kefir yeast, cheese whey

INTRODUCTION

All industrial chemical reactions which are either exothermic or endothermic require energy manipulation to maintain a constant temperature or a predetermined temperature profile in various types of processes [1]. Exothermic reactions in many industrial reactors which have the similar characteristic may have very interesting behaviour to investigate because of potential safety problems. A mean conversion of a reactant can be realized at a single unstable equilibrium point that can be obtained by determining the eigenvalues of this system Jacobian matrix [2]. The chemical processes such as exothermic styrene polymerization reactors are exposed to various disturbances [3]. To maintain certain set point in face of load disturbances, conventional or advance controller must be applied to a process with well-tuned control parameters [4-5]. Nonlinear oscillation of outputs, sensitivity of system parameters, ignition/extinction and interaction of responses may occur for open-loop cases in continuous stirred tank reactors (CSTR's). A steady-state analysis was used to determine operation and design parameters effects on CSTR performance [6]. The processes steady-state and dynamic characteristic behaviours and the reactor design parameters were investigated to improve feedback control efficiency. Several techniques based on process simulation were proposed to demonstrate the difficulty of control at a certain steady-state set point in some regions of operation [7].

Although the system is simulated by a set of differential equations, some applicable parametric models which include the relationship between manipulated and controlled variables were usually written in discrete- time domain for advance process control applications. The parameters identification of these models is one of the effective procedures to define the systems in a certain operation range by utilizing the best estimates of model degree and all the unknown variables of operation [8]. There are several

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methods including strategies for the tuning of the conventional controller and the selection of the best model for control application. A multi-model control strategy was proposed to identify the delay without turning the system unstable [9]. Some researchers improve control strategies to obtain a better method than conventional proportional integral derivative (PID) controllers. Several combined advance and conventional control were proposed as a novel PID controller. The performance was evaluated for the set point tracking and disturbance rejection [10].

Nomenclature	
A_R	heat transfer area
a_i	coefficients of monic polynomial in the z-domain
b_i	coefficients of polynomial in the z-domain
C_A	inlet concentration of the reactant
C	reactant concentration of the reaction mixture
Cp	average heat capacity of the reaction mixture
E_1	activation energy
e	error
F_1	feed rate to the reactor
Kc	steady-state gain for three-term controller
Ku	ultimate gain
k_0	pre-exponential for the rate constant
Pu	ultimate period
R_1	ideal gas constant
TD	derivative time
TI	integral time
T	temperature of the reaction mixture
T_1	inlet feed temperature
Tc	coolant temperature
Ts	temperature set point
r(t)	set point at time t
u(t)	input variable at time t
us	input value at initial steady-state point
U_R	overall heat transfer coefficient
V_R	volume of reaction mixture
ρ	density of the reaction mixture
(-ΔHR)	heat of reaction
y(t)	output variable at time t

An objective of this paper is to overcome the difficulty of feedback control of the CSTR when it is operated at a saddle point. PID control action was executed throughout-being considered the most likely type of control action for this application. The controller parameters were estimated using three different closed loop response tuning criteria for discrete controllers, viz. those due to Tyreus–Luyben [11] (denoted by T-L), Ziegler-Nichols [2] (denoted by Z-N), and the increased gain approach was combined by considering an application from [12]. Self-tuning proportional integral derivative (STPID) control [13-14] was also achieved by adjusting three tuning parameters with three-term PID parameters proposed by Z-N and second order system model parameters. A controlled auto regressive moving average (CARMA) model was utilized and its parameters were determined with Bierman computation procedure [15] in which data obtained by enforcing the system with a pseudo random binary sequence (PRBS).

CONVENTIONAL AND SELF-TUNING CONTROLLER

The conventional three-term (PID) feedback control is the highly applied feedback control strategy because of its robustness, ease of operation and the lack of specified process knowledge required for the initial controller position or velocity form designs. When the controller parameters have been determined, sufficient and effective control is usually obtained by detuning such as increase gain approach for stability and non-oscillatory behaviour over the whole range of operating conditions. The discrete-time equivalent of three term control action may be written:

$$\frac{\Delta u}{e} = K_c\left\{\left(1+\frac{\Delta t}{2TI}+\frac{TD}{\Delta t}\right)+\left(\frac{\Delta t}{2TI}-1-\frac{2TD}{\Delta t}\right)z^{-1}+\left(\frac{TD}{\Delta t}\right)z^{-2}\right\} \quad (1)$$

Rearranging equation (1)

$$\Delta u = s_0 e(t) + s_1 e(t-1) + s_2 e(t-2), \quad (2)$$

In order to convert the position form of the PID algorithm into a self-tuning equivalent, the following equations can be written:

$$u(t) - us = e[s_0 + (s_0+s_1)z^{-1} + (s_0+s_1+s_2)z^{-2}], \quad (3)$$

The properties of the STPID closed-loop can be varied by placing the poles of the characteristic equation (T) that is the denominator of equation (4).

$$y(t) = [\frac{z^{-1}b_o(s_0+s_1z^{-1}+s_2z^{-2})}{1+t_1z^{-1}+t_2z^{-2}+t_3z^{-3}}]r(t)\,, \quad (4)$$

The system CARMA type model without control and the controller coefficients are defined respectively as:

$$y(t) = \left[\frac{z^{-1}b_o}{1+a_1z^{-1}+a_2z^{-2}}\right]u(t)\ , \qquad (5)$$

$$s_0 = \frac{t_1-a_1+1}{b_0}\ ; \quad s_1 = \frac{t_2-a_2+a_1}{b_0}\ ; \ s_2 = \frac{t_3-a_2}{b_0}, \quad (6)$$

All the coefficients of the characteristic third order T polynomial should be user defined. They can be initially determined by using the system model parameters (a_1, a_2, b_0) and Kc, TI and TD constants.

RESULTS AND DISCUSSION

To investigate the steady-state and unsteady-state behaviour of a adiabatic CSTR, the system is the model obtained from the set of the mass and energy balance equations [16]. The system parameters given in [2] are utilized as k_0 = 9703*3600 hr^{-1}, $(-\Delta H_R)$ = 5960kcal $kmol^{-1}$, E_1 = 11843 kcal $kmol^{-1}$, ρ*Cp = 500 kcal m^{-3} K^{-1}, T_1 = 298 K, CA = 10 kmol m^{-3}, V_R = 1m^3, F_1 = 1m^3 hr^{-1}, $(U_R*A_R*V_R^{-1})$ = 150kcal m^{-3} K^{-1} hr^{-1}, R_1 = 1.987 kcal $kmol^{-1}$ K^{-1}. The jacket and the reactor are assumed to be perfectly mixed and the jacket temperature is lower than the reactor temperature, T. The feasible steady-state solutions were obtained for the coolant temperature of 293 K by means of the fsolve function in Matlab software with various initial C and T values (see Table 1). The eigenvalues for the stability of a particular operating point are determined by using the eig(amat) command in Matlab (see Table 1).

At a constant coolant temperature of 293K, the phase-plane plot was obtained by using ode45 function with many initial conditions (see Fig 1). In this figure, the feasible high and low reactor temperature steady-states are also shown as ‘o’. The intermediate reactor temperature steady state was presented with the symbol ‘+’ which is unstable, since all initial conditions have diverged from it. This saddle point was chosen as the operation condition of CSTR for control cases studied.

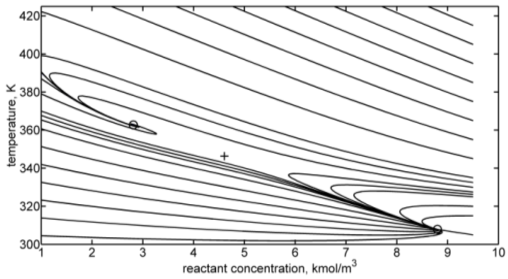

Fig. 1. Phase-plane plot for coolant temperature Tc=293K (o: stable nodes, +: saddle point).

Table 1. The steady-state solution and the eigenvalues of the continuous stirred tank reactor.

Initial values, C , kmol/m^3 , T, K	The feasible solution of the steady-state equations for coolant temperature, Tc=293K	
3 370	C=2.81 T=362.73	The eigenvalues : -0.48+0.70i, -0.48-0.70i Spiral sink (stable focus)
4 360	C=2.81 T=362.73	
5 350	C=4.60 T=346.30	The eigenvalues : -0.76, 0.48 Saddle point (unstable)
6 330	C=4.60 T=346.30	
7 320	C=8.79 T=307.85	The eigenvalues: -0.88, -0.65 Sink (stable node)
8 310	C=8.79 T=307.85	
9 300	C=8.79 T=307.85	

2	380	× ×	C=2.81 T=362.73
1	390		C=2.81 T=362.73
1	450		C=2.81 T=362.73

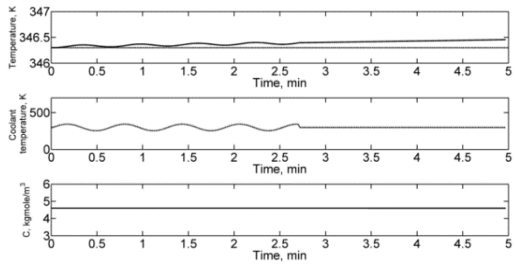

Fig. 2. The reactor temperature response of proportional only control with K_C=0.5 in the face of the set-point change as 90 sin(600t)

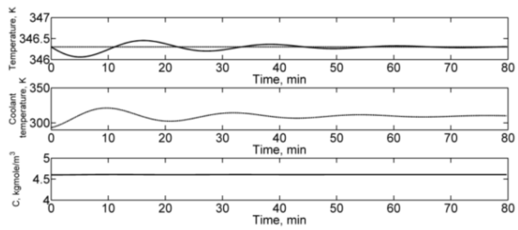

Fig. 3. PID control of the reaction temperature (the T-L settings with increase gain applied as K_C=22.5, TI=1.37min, TD=0.1min).

The conventional controller settings were estimated based on the continuous cycling method. To obtain the ultimate gain (Ku) and period (Pu) at the middle operation point, a sinusoidal temperature set point change (Ts = 346.3+90*sin(600t)) was introduced to the closed loop system with various steady-state gain (Kc) for proportional controller in a short time interval. The well suited Kc value of 0.5 that produces continuous cycling within a certain range was found by monitoring coolant temperature and reactor temperature changes versus time (see Fig 2). The Ku and Pu values are evaluated as 0.5 and 0.6228min respectively. The Ziegler-Nichols and Tyreus-Luyben settings were evaluated based on Ku and Pu values. These numerical values of Kc multiplied by 100 to obtained the well-suited increase gain for PID controller.

For the simulation of the closed loop behaviour of the controlled reactor at the saddle point, the PID controllers based on the T-L settings with increase gain (K_C=22.5, TI=1.37min, TD=0.1min) and the Z-N settings with increase gain (K_C=30, TI=0.3min, TD=0.08min) were used. The controlled temperate of reactor and the manipulated coolant temperature changes versus time were shown in Fig 3 and Fig 4 respectively. The magnitude of temperature sampling time was 1.08s which influences the stability of the controlled output. Comparison of PID performances using two different parameter settings were made by considering set point following in Figures 3-4. The control algorithm using the Z-N settings with increase gain were preferred to bring the reactor temperature to the set point.

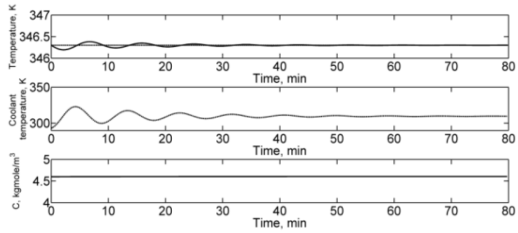

Fig. 4. PID control of the reaction temperature (the Z-N settings with increase gain applied as K_C=30, TI=0.3min, TD=0.08min)

A pole-placement based STPID algorithm application was also achieved to obtain better performance. Firstly, a second order system transfer function of the CARMA form was considered. Secondly, the PRBS of the certain magnitude given in Fig. 5 was applied to the coolant temperature. The simultaneous input and output data were obtained for the system model parameters identification. Finally, Bierman algorithm in Matlab was utilized to evaluate the three model parameters as given in the equation below:

$$y(t) = \frac{0.00003\,u(t-1)}{1+0.669z^{-1}+0.332z^{-2}}, \qquad (7)$$

These system model parameters a_1 = 0.669, a_2 = 0.332, b_0 = 0.0003 and the Z-N settings as Kc=0.3, TI=0.3min, TD=0.08min were used to determine the closed loop real denominator coefficients as t_1=-0.33, t_2=-0.337, t_3=-0.33 for the STPID controller tuning. Figure 6 shows the STPID control of reactor temperature in the face of an exothermic reaction in unstable operation condition with t_1=-0.33, t_2=-0.337 and t_3=-0.33 for the CSTR.

For comparison of the performances of the all controllers applied, the integral square of the error (ISE) and the integral of absolute value of error (IAE) criteria were evaluated by using the following formula:

$$ISE = \sum (T - Ts)^2, \tag{8}$$

$$IAE = \sum |T - Ts|, \tag{9}$$

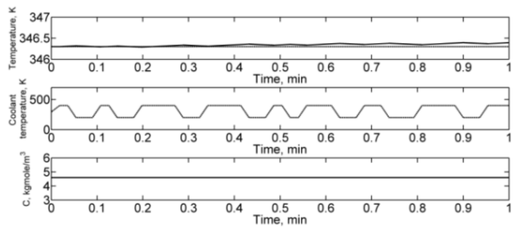

Fig. 5. The temperature response obtained in the face of the pseudo-random binary sequence given to the coolant temperature.

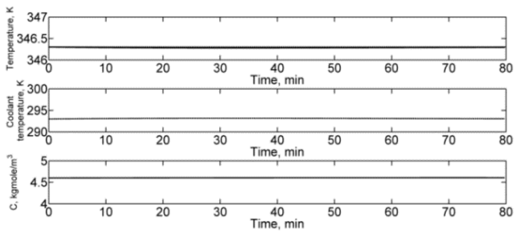

Fig. 6. Self-tuning PID control of reactor temperature by using the coolant temperature as the controlling variable.

Table 2. ISE and IAE values obtained for PID and Self-tuning PID control of the reaction temperature.

Controller	ISE	IAE	Figure number
PID with Tyreus-luyben increased gain	29.7	248.5	Fig 3
PID with Ziegler-Nichols increased gain	3.5	72.7	Fig 4
Self-tuning PID with second order ARMAX model	1.1	67.1	Fig 6

Table 2 lists the ISE and IAE criteria values for each controlled variable response. By using STPID, improvement in the control is clearly seen in Fig 6. There is no doubt that the introduction of STPID reduces the ISE and IAE values for the controlled reactor temperature response (see Table 2).

CONCLUSION

The modelling equations of the CSTR were solved simultaneously by using ode45 function in Matlab. For the identification, the magnitude and generation of PRBS forcing function was well-determined for operating conditions of the system. The simulation result obtained without control was used for the system model parameters identification. The PID control parameters were estimated by using the proportional control response in the face of a momentary sinusoidal set point change with well-chosen amplitude and radian frequency. Both sets of parameters were found by using the data obtained in a sort time domain. These parameters were used successfully to evaluate the tuning parameters of STPID controller. The position form of PID and STPID controller were applied to the CSTR by accepting the heat release during the reaction as a disturbance of the system. Although the control was stable in all cases the STPID action was found to give smaller closed-loop ISE and IAE values than the PID action when applied to the CSTR at an unstable operating saddle point.

For the operating point studied, the performance of the position form STPID control have been shown in Fig 6 to be superior to the velocity form of STPID control results given in Fig 7. It was found that the performance of velocity form controller algorithm was unacceptably poor (see Appendix A).

Appendix A. *Velocity form of STPID control application to a adiabatic CSTR*

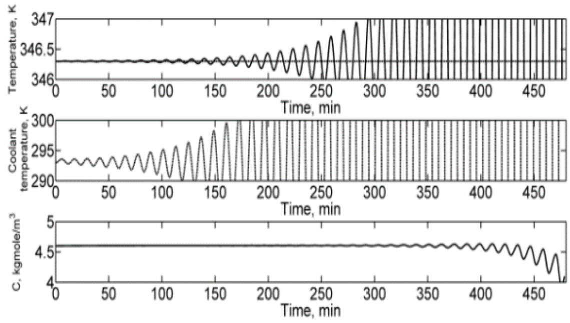

Fig. 7. Velocity form self-tuning PID control of reactor temperature by using the coolant temperature as the controlling variable.

The velocity form STPID control was applied to the CSTR. The controller tuning parameters were used as t_1 = -0.33, t_2 = -0.337, t_3 = -0.33. Fig 7 shows the reactor temperature response during the velocity form control application at the unstable operating saddle point.

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