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Simulation of Response Performance of a CSTR Process with Digital Compensator

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***Abstract*—*This paper has presented simulation of response performance of a continuous stirred tank reactor (CSTR) process with digital compensator. It is required to improve the response performance of a CSTR process. A nonlinear dynamic model of CSTR is obtained and then linearized. A digital compensated is designed using Matlab software. The designed compensator was integrated with the CSTR model. Simulation was performed in Matlab environment. The result obtained shows that the response performance of the compensated process was highly improved considering a unit step input.*

Keywords*— *CSTR, Dgital Compensator, Response, Simulation.

I. INTRODUCTION

A Continuous Stirred Tank Reactor (CSTR) is one in which the chemical reaction taking place is such that the reactant are added and product are continuously removed at a steady rate while maintain continuous stirring of the reaction mixture using internal components [3]. In CSTR, chemical reactions taking place can either be an endothermic or exothermic. This means that energy can be added or removed from the system so as to keep the temperature constant. The running of CSTR is normally at steady state and is usually operated to have a well-mixed [2]. The fact that CSTR is run at steady state has made the modelling of the system to having no special variations in concentration, temperature or rate of reaction throughout the system arrangement [2].

Nowadays, there is rise in the number of industries has resulted to increase in water and chemical into the environment. As a result of government regulation policy on disposable water or chemical to prevent environmental hazard has given rise to installation of CSTR for waste water treatment [3].

There is a need to improve the response performance of a CSTR such that product concentration is treated and maintained within acceptable level suitable for disposal. The object of this paper is to design a compensator for a CSTR system to improve the response performance.

The characterization of a five-litre continuous stirred tank reactor (CSTR) is presented in [5]. An experimental study on the effect of operating conditions on the conversion and specific rate constant was studied [4]. Antonelli and Astolfli [6] designed bounded control laws for the temperature stabilization of a class of continuous stirred tank reactors with exothermic or endothermic reactions using methodologies and tools from Lyapunov theory. Controller design for continuous stirred tank reactor is presented by Prabhu and Bhaskaran [7]. It studied the problem of temperature control of CSRT using adaptive controller. DI Ciccio et al. [8] proposed a novel digital control law for continuous stirred reactor tank. Rubi et al. [1] presented temperature control of CSTR using PID controller. A simulation work on implementation of a Kalman-Bucy filter for estimating product concentration of a CSTR process is presented in [10].

II. IDEAL CSTR PROCESS DESCRIPTION

A Continuous stirred tank reactors (CSTR) is shown in Fig. 1. The dynamic model of a CSTR using first principle of the CSTR and the operating data as stated in [9] for simulations. It is common in chemical industries to have nonlinear CSTR process. In order to perform simulation studied in this paper, a non-reversible, exothermic reaction $A \rightarrow B$ occurs in reactor whose volume is constant and cooled by a single coolant stream. A feed waste material of concentration C_{Ao} enters the reactor at temperature T_o at a constant volume of f flow rate q . It is assumed that the mixing taking place in the reactor is sufficient enough to ensure that the liquid content in the reactor is homogeneous.

Heat is added or removed by the means of the difference between the jacket fluid and the reactor fluid for a jacketed CSTR [2]. Heat transfer takes place through the wall of the reactor into the jacket [1]. The objective is improve the response performance of the system.

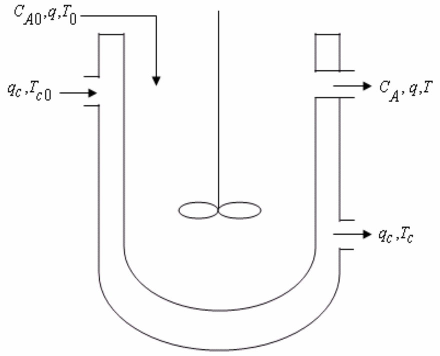

Fig. 1. Typical diagram of a CSTR [2].

III. DYNAMIC MODELING AND SYSTEM CONFIGURATION

In order to perform the modeling of the dynamic equation of the process, it is necessary to make the following assumptions for a simplified dynamic equations of an ideal CSTR as in [2]:

a. The mixing in the reactor and jacket is perfect
b. The volume of the reactor and jacket is constant

The formulation for the process dynamic model is presented as follow using energy conservation principle as follows:

A. Mass Balance of Reactor

The reactor mass balance equation is given by [2]:

$$\mathrm{V}\frac{dC_A}{dt} = q\left(C_{Ao} - C_A\right) - \mathrm{V}r_A \tag{1}$$

where C_A is the product concentration of component A in the reactor and r_A is the rate of reaction per volume. The Arrhenius equation is often used for the rate of reaction. A reaction of a first order will result to the following equation:

$$r_A = K_o \exp\left(-\frac{E}{RT}\right)C_A \tag{2}$$

B. Energy Balance Equation

The reactor energy balance equation is given by [2]:

$$\mathrm{V}\rho C_p\frac{dT}{dt} = q\rho C_p\left(T_o - T\right) - \left(-\Delta H\right)\mathrm{V}r_A + \rho_c C_{pc} q_c\left[1 - \exp\left(-\frac{hA}{q_c\rho_c C_{pc}}\right)\right]\left(T_{co} - T\right) \tag{3}$$

where $\left(-\Delta H\right)$ is the heat of reaction, hA is the heat transfer coefficient, T_o is the feed temperature and T_{co} is the inlet coolant temperature. Equations (1) to (3), are further simplified to give the mass and energy balance Equations of the CSTR as follows [2]:

$$\frac{dC_A}{dt} = \frac{q}{\mathrm{V}}\left(C_{Ao} - C_A\right) - K_o C_A \exp\left(-\frac{E}{RT}\right) \tag{4}$$

$$\frac{dT}{dt} = \frac{q}{\mathrm{V}}\left(T_o - T\right) - \left(\frac{-\Delta H}{\rho C_p}\right)K_o C_A \exp\left(\frac{-E}{RT}\right) + \left(\frac{\rho C_{pc}}{\rho C_p \mathrm{V}}\right)q_c\left[\frac{-hA}{q_c\rho_c C_{pc}}\right]\left(T_{co} - T\right) \tag{5}$$

The dynamic equations of a CSTR such as (4) and (5) contain nonlinear functions T and C_A [2]. It is impossible to solve one Equation separately from the other because they are coupled. Equations (4) and (5) are further transform into state variable form.

C. State Variable Formulation

$$\frac{dC_A}{dt} = f_1\left(C_A, T\right) = \frac{q}{\mathrm{V}}\left(C_{Ao} - C_A\right) - K_o C_A \exp\left(-\frac{E}{RT}\right) \tag{6}$$

$$\frac{dT}{dt} = f_2\left(C_A, T\right) = \frac{q}{\mathrm{V}}\left(T_o - T\right) - \left(\frac{-\Delta H}{\rho C_p}\right)K_o C_A \exp\left(-\frac{E}{RT}\right) + \left(\frac{\rho_c C_c}{\rho C_p \mathrm{V}}\right)q_c\left[1 - \exp\left(\frac{-hA}{q_c\rho_c C_{pc}}\right)\right]\left(T_{co} - T\right) \tag{7}$$

D. Linearization of Nonlinear Dynamic Equation

Equations (6) and (7) are linearized and represented in the state variable form as stated below:

$$\dot{x} = Ax + Bu \tag{8}$$

$$y = Cx + Du \tag{9}$$

where matrices A and B represent the Jacobian matrices corresponding to the nominal values of the state variables and input variables and x, u, and y represent the deviation variables. The output matrix is given as C. The disturbance matrix is D.

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} C_A - C_{As} \\ T - T_s \end{bmatrix} \tag{10}$$

$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} q - q_s \\ q_c - q_{cs} \end{bmatrix} \tag{11}$$

$$y = \begin{bmatrix} C_A - C_{As} \\ T - T_s \end{bmatrix} \tag{12}$$

where C_{As}, T_s, q_s, q_{cs}, are the steady state values of the product concentration, reactor temperature, feed flow rate and coolant flow rate respectively.

The Jacobian matrices A and B are given is given by:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} \tag{13}$$

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix} \tag{14}$$

The objective is to design a compensator to improve the response performance of a CSTR so as to ensure the product concentration is maintained at an acceptable level. Hence (14) is reduced into a 2 × 1 matrix as in (15):

$$B = \begin{bmatrix} B_{11} \\ B_{21} \end{bmatrix} = \begin{bmatrix} \frac{\partial f1}{\partial u_1} \\ \frac{\partial f_2}{\partial u_1} \end{bmatrix} \tag{15}$$

where

$$A_{11} = \frac{-q}{\mathrm{V}} - K_s \tag{16}$$

$$A_{12} = -C_{As}K_{so} \tag{17}$$

$$A_{21} = -\left(\frac{\Delta \mathrm{H}}{\rho C_p}\right)K_s \tag{18}$$

$$A_{22} = \frac{-q}{\mathrm{V}} + \left[\frac{(-\Delta \mathrm{H}) C_{As}}{\rho C_p}\right] K_{s1} + \left[\frac{-\rho_c C_{pc}}{\rho C_p \mathrm{V}}\right] q + \left[\frac{\rho C_{pc}}{\rho C_p \mathrm{V}}\right] q_c \times \exp\left[-\frac{hA}{q_c \rho C_p}\right] \tag{19}$$

where

$$K_s = K_o \exp\left(-\frac{E}{RT_s}\right) \tag{20}$$

$$K_{s1} = \left[K_o \exp\left(-\frac{E}{RT_s}\right)\right]\left(\frac{E}{RT_s^2}\right) \qquad (20)$$

$$B_{11} = \left(\frac{C_{Ao} - C_{As}}{\mathrm{V}}\right) \tag{21}$$

$$B_{21} = \left(\frac{T_o - T_s}{\mathrm{V}}\right) \tag{22}$$

The matrix of the output is given by:

$$C = [1 \quad 0], \; D = 0 \tag{23}$$

Table 1 shows the steady state operational parameters and their values use for simulations performed using MATLAB software.

TABLE 1 Steady state operational data for simulation [9]

Parameter	Symbol	Value
Product concentration	C_A	0.0882 moll^{-1}
Reactor temperature	T	441.2 K
Coolant flow rate	q_c	100 lmin^{-1}
Feed flow rate	q	100 lmin^{-1}
Feed concentration	C_{Ao}	1 moll^{-1}
Feed temperature	T_o	350 K
Inlet coolant	T_{co}	350 K
CSTR volume	V	100 l
Heat transfer term	hA	7×10^5 $\mathrm{Cal(mink)}^{-1}$
Reaction rate constant	K_o	$7.2 \times 10^{10} \mathrm{min}^{-1}$
Activation Energy term	$\frac{E}{R}$	1×10^4 K
Heat of reaction	$-\Delta \mathrm{H}$	-2×10^5 Calmol^{-1}
Liquid densities	$\rho,\ \rho_c$	1×10^3 gl^{-1}
Specific heat	$C_p,\ C_{pc}$	1 $\mathrm{cal(gK)}^{-1}$

Substituting that data in Table 1 into matrices A and B yields:

$$A = \begin{bmatrix} -11.3241 & -0.0478 \\ 2064.8 & 7.3562 \end{bmatrix} \tag{24}$$

$$B = \begin{bmatrix} 0.0091 \\ -0.9120 \end{bmatrix} \tag{25}$$

Converting the state space equations to equivalent form into transfer function gives:

$$G(s) = \frac{0.0091s - 0.02335}{s^2 + 3.9679s + 15.3951} \tag{26}$$

Using a sampling time of 0.2 seconds, the equivalent discrete time transfer function of the process model is:

$$G(z) = \frac{0.0007853z - 0.001398}{z^2 - 1.048z + 0.4522} \tag{27}$$

E. Design Specifications

It is desired that the process meets the following performance criteria.

i. Rise time of less than 0.8 seconds
ii. Settling time of less than 10 seconds
iii. Overshoot of less than 10%

F. Compensator Design

The compensator implemented in this paper is designed using MATLAB software. The compensator in continuous time (28) and the equivalent digital compensator (29) are given by:

$$G_c(s) = \frac{-315s - 358}{s} \tag{28}$$

$$G_c(z) = \frac{315(1-z) - 358}{z - 1} \tag{29}$$

A sampling time of 0.2 seconds is used.

G. System Configuration

The system configuration is shown in Fig. 2. It has the digital compensator and the process in the forward path of the closed loop system. The response C_A is compared to a unit step input.

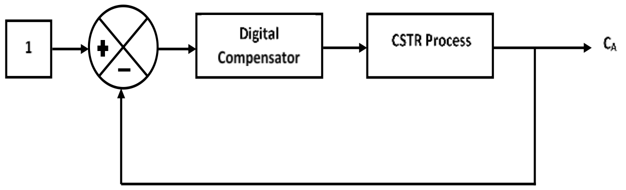

Fig. 2. CSTR process compensator loop.

IV. SIMULATION RESULTS AND DISCUSSION

A. Simulation Results

The results obtained from the simulations performed using MATLAB software are presented in Fig. 3 and 4. Fig. 3 is the result of the simulation carried out when the designed digital compensator is not in the loop. Fig. 4 is the result obtained when the compensator is integrated into the loop of the process.

B. Discussion

The results of the simulations carried out for a typical continuous stirred tank reactor (CSTR). It is carried out to improving the response performance and maintaining the product concentration within acceptable level of concentration. Fig. 3 is the step response performance of the process when it has not been compensated. The system gives a large response magnitude to a unit step input. The system seems sluggish and unable to track the step input.

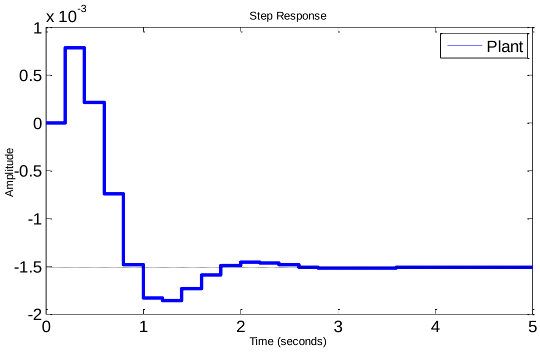

Fig. 3. Step response for uncompensated process.

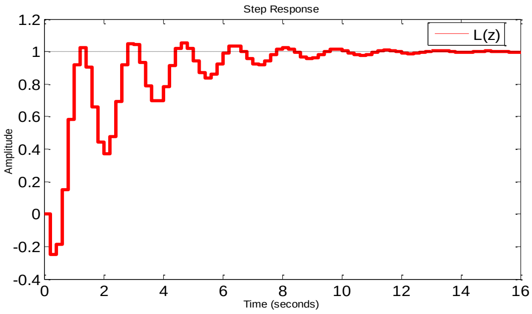

Fig. 4. Step response for compensated process.

This results to the following performance: rise time of 0.29 seconds, settling time of 2.23 seconds, and overshoot of 23 %. In Fig. 4, the designed compensator is added to the loop. It can be seen that the performance of the system is improved as the response track the unit step input. The compensated system performance is: rise time of 0.4 seconds, settling time of 9.2 seconds, and overshoot of 5.56 %. This shows that the digital compensator improved the response performance of the process.

V. CONCLUSION

This paper has presented simulation of response performance of a continuous stirred tank reactor (CSTR) process with digital compensator. The dynamic model of a typical CSTR process was obtained in nonlinear form and then linearized. The linearized system was initially represented in state space form and then transformed into the equivalent transfer function model. The transfer function of the process in continuous time was converted into its equivalent discrete time form considering a sampling time of 0.2 seconds. A digital compensator was designed and integrated with the process. Simulation result showed that the response performance of the system was highly improved.

REFERENCES

[1] Rubi, V. Agarwal, A. Deo, and N. Kumar, “Temperature control of CSTR using PID Controller,” *International Journal of Engineering and Computer Science*, vol. 4, issue 5, pp. 11902-11905, 2015.

[2] Anonymous, “Mathematical modeling of a continuous stirred tank reactor,”

[3] Persistence Market research, “Continuous flow stirred tank reactor (CSTR) market: Global industry analysis and forecast 2016-2026” https://www.persistencemarketresearch.com/market-research/continuous-flow-stirred-tank-reactor-market.asp

[4] M. Danish, M. K. Al Mesfer, and M. Rashid, “Effect of operating conditions on CSTR Performance: an experimental study,” *Int. Journal of Engineering Research and Applications*, vol. 5, issue 2, pp. 74-78, 2015.

[5] P. K. Igbokwe, J.T. Nwabanne, and S. W. Gadzama, “Characterization of a 5 litre continuous stirred tank reactor,” *World Journal of Engineering and Technology*, vol. 3, pp. 25-40, 2015.

[6] R. Antonelli and A. Astolfi, “Continuous stirred tank reactors: Easy to stabilize,” *Automatica*, vol. 39, pp. 1817-1827, 2003.

[7] K. Prabhu and V. M. Bhaskaran, “Controller design for continuous stirred tank reactor using adaptive control,” *Research Journal of Applied Sciences*, vol. 9, pp. 489-495, 2014.

[8] M. P. Di Ciccio, M. Bottini, and P. Pepe, “Digital control of a continuous stirred tank reactor,” Hindawi Publishing Corporation, Mathematical Probles in Engineering, vol. 2011, Article ID 439785, pp. 1-18, 2011.

[9] M. Pottman and D. E. Seborg, “Identification of nomlinear process using reciprocal multiquadratic functions,” *J. Process Control*, vol. 2, pp. 189-203, 1992.

[10] P. C. Eze, C. Muoghalu, J. Amabikutol, F. A. Aigbodioh, E. A. Okoronkwo, and B. O. Ekengwu, “Implementation of a Kalman-Bucy filter for estimating product concentration of a CSTR process,” *International Research Journal of Advanced Engineering and Science*, vol. 3, issue 1, pp. 97-100, 2018.