Modeling and Control of a Continuous Stirred Tank Reactor (CSTR)

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Abstract

The goal of this paper is to develop a nonlinear observer-based control strategy for a jacketed continuous stirred tank reactor (CSTR). The dynamic behavior and control of CSTR has been developed where the dynamic and control system based on basic mass balance has been carried out.

The control behavior of CSTR is studied using different control strategies; conventional feedback control (PI and PID), cascade control and fuzzy-logic control (FLC).

The FLC can be chosen as the best method for controlling the CSTR process and it is clear that the auxiliary variable enables the controller to yield better control performance for highly nonlinear processes, as compared with feedback and cascade controllers.

MATLAB program is used as a tool of solution for all cases mentioned in this work.

Keywords: CSTR, Nonlinear systems, Feedback control, Cascade control, Fuzzy logic control.

الخلاصة

إن الهدف من هذا البحث هو دراسة السلوك الديناميكي وطرق السيطرة لمفاعل كيمياوي مستمر جيد الخلط ومعزول بجاكيت (CSTR) وقد تم تمثيل الموديل الرياضي للخزان ذو الخلط المستمر بمعادلات موازنة المادة والطاقة الاساسيه.

إن السلوك الديناميكي لمفاعل (CSTR) قد تم دراسته باستخدام أنواع مختلفة من المسيطرات مثل المسيطر التقليدي (PI و PID) و المسيطر ألشلالي (cascade controller)والمسيطر ذو المنطق الغير واضح .(FLC).

المسيطر ذو المنطق الغير واضح (FLC)قد تم اختياره ليكون هو الأحسن لان له اقل مقدار من الخطأ حيث تم استخدام معيار مربع الخطأ (ISE) كأساس للمقارنة بين الطرق أعلاه. والبرنامج المستخدم كأداة للحل في هذا البحث هو MATLAB .

1 Introduction

Chemical processes are often operated under high pressures, high temperatures, and with fast material flows and complex manufacturing mechanisms. Thus, their operation is always more risky, environmentally more harmful, and potentially more dangerous than other types of manufacturing activities when abnormal or destructive situations arise.

Severe nonlinearities of chemical processes influence the selection of control schemes for efficient control of a process. In recent years, a number of nonlinear control strategies have been proposed. Among them, most popular are the differential geometric based globally linearizing control (GLC). A drawback of GLC is that an exact knowledge of the system parameters is required [Amiya , 2007].

1.1 Classical Method of Control

Conventional control theory deals predominantly with linear systems having constant parameters. This is often a good approximation for systems that are regulated at fixed operating points. With moderate disturbances and a good control system the deviations will be so small that the linear approximation is sufficiently good. However, the linear constant coefficient approximation will not always be satisfactory when the operating conditions change. However, an adaptive control for example can be designed to overcome the limitations of conventional control systems [Astrom and Wittenmark, 1999].

Feedback control in general is the achievement and maintenance of desired condition by using an actual condition and comparing it to a reference value (set point), and using the difference between those to eliminate any difference between them. Most controller use negative feedback in which measured process output (control variable) is subtracted from a desired value (set point) to generate an error signal (Ei). The controller recognizes the error signal and manipulates a process input (control element) to reduce the error [Luyben , 1997].

1.2 Modern Method

A. Cascade control

Cascade control can improve control system performance over single-loop control whenever either: (1) Disturbances affect a measurable intermediate or secondary process output that directly affects the primary process output (controlled output); or (2) the gain of the secondary process, including the actuator, is nonlinear. In the first case, a cascade control system can limit the effect of the disturbances entering the secondary variable on the primary output. In the second case, a cascade control system can limit the effect of actuator or secondary process gain variations on the control system performance. Such gain variations usually arise from changes in operating point due to set point changes or sustained disturbances. [Morari and Zafiriou, 1989].

Cascade control is widely used within the process industries. Conventional cascade schemes have two distinct features:

- There are two nested feedback control loops. A secondary control loop located inside a primary control loop.
- The primary loop controller is used to calculate the set point for the inner (secondary) control loop. The block diagram of cascade control is shown in Figure (1).

B. Fuzzy Logic Control (FLC)

A fuzzy control system was developed based on fuzzy mathematics, which is a branch of applied mathematics. The fuzzy mathematics have broad applications in many fields including statistics and numerical analysis, systems and control engineering, and biomedical engineering alike [King and Mamdani, 1977].

Fuzzy controlled systems models do not require any certain model for implementation of system under consideration. These proofs stem isomorphism between an abstract algebra and linear algebra and the structure of a Fuzzy system, which comprised of an implication between actions and conclusion as antecedents and consequents. Abstract algebra incorporates systems or models dealing with groups, fields and rings. Linear algebra incorporates system models dealing with vector spaces, state vector and transition matrices. The primary benefit of fuzzy system theory is to approximate system behavior where numerical functions or analytical functions do not exist. Hence, Fuzzy systems have high potential to understand the very systems that are devoid of analytical formulations in a complex System. Complex systems can be new systems that have not been tested, they can involve with the human conditions such as biological or medical systems. The ultimate goal of the fuzzy logic is to form the theoretical foundation for reasoning about the imprecise reasoning, such reasoning is known as approximate reasoning [Farhad and Gagandeep, 2011]. It can also observe the practical implementation of fuzzy logic, in fuzzy controller, due to employ as an intelligent controller in real control application. Fuzzy logic controller emulates the behavior of the experts in controlling the system. Not needing the precise mathematical modeling is a remarkable merit, causes fuzzy controller more flexible in dealing with complex nonlinear problem [Mohd et al., 2011].

Figure (2) shows the block diagram of fuzzy control system and Table (1) shows set of rules base corresponding to the changes in error and change of error.

A fundamental requirement for these rules is that they have to perform negative feedback control, for the sake of stability. An example of a set of rules is listed in Table (1) has to be adjusted by the experience of human operators.

Figure (3) show the membership functions selected for this problem. It can be seen that the number of membership functions for each input, e and Δe are (5) and for the controller output (7). In these figures the meaning of the adjectives are: NL= negative large, NM= negative medium, NS=negative small, ZO= zero, PS=positive small, PM= positive medium and PL=positive Large.

Now, it is necessary to define the fuzzy membership functions associated with the controller inputs: the control error and the change in the control error and with the controller output (Δu) based on prior knowledge about the process. The number of membership functions for each variable can vary, depending on the resolution required for that variable [Kwok D. P. et al., 2003].

Generally, more membership functions offer more degrees of freedom to the functional relationship of the controller**.**

2 Mathematical Model

The dynamic and steady state simulation model for continuous stirred tank reactor (CSTR) based on mass and charge balances, can be represented as [Stephanopoulos, G., 1984]

Overall Material Balance

$$\upsilon_{in}\rho_{in} - \upsilon_{out}\rho = \frac{dV\rho}{dt} \qquad \text{--------- (1)}$$

For a steady state condition, a constant amount of material in the reactor $\frac{dV\rho}{dt}$ =0, then:

$$\upsilon_{in}\rho_{in} = \upsilon_{out}\rho_{out}$$

Assuming a constant density of the input and output streams, then:

$$\upsilon_{in} = \upsilon_{out} = \upsilon$$

Component balance

The balance on component A, assuming a constant volume of reactor, is:

$$\upsilon\, C_{Ao} - \upsilon\, C_A - rV = V\frac{dC_A}{dt} \qquad \text{--------- (2)}$$

Where r is the rate of reaction per unit volume

Energy balance around tank

The energy balance, assuming a constant volume, heat capacity and density, is:-

$$(\upsilon\,\rho\, C_p(T_o - T) + (-\Delta H)rV - UA(T - T_j) = V\rho\; C_p\frac{dT}{dt} \qquad \text{--------- (3)}$$

$$\Delta H(T) = \Delta H(T_{ref}) + \Delta C_p(T - T_{ref}) \qquad \text{--------- (4)}$$

Where *(-Δ H)rV* is the rate of energy contributed by the exothermic reaction.

Energy balance around Jacket

In the energy balance around jacket, making the same assumptions as around the tank:

$$\frac{dT_j}{dt} = \frac{\upsilon_j}{V_j}(T_{ji} - T_j) + \frac{UA}{V_j\rho_j C_{p\,j}}(T - T_j) \qquad \text{-------- (5)}$$

State variable form of dynamic equations

Equations (2 and 3) can be written in a state variable form as:

$$f_1(C_A, T) = \frac{dC_A}{dt} = \frac{\upsilon}{V}(C_{Ao} - C_A) - r \qquad \text{-------- (6)}$$

$$f_2(C_A, T) = \frac{dT}{dt} = \frac{\upsilon}{V}(T_o - T) + \frac{(-\Delta H)r}{\rho C_p} - \frac{UA}{V\rho C_p}(T - T_j) \qquad \text{-------- (7)}$$

The reaction rate per unit volume (Arrhenius expression) for a first order reaction is:

$$r = k_o \exp(\frac{-\Delta E}{RT})C_A \qquad \text{-------- (8)}$$

3 Results and discussion

The present work provides the comparative performance study of the proposed control scheme and the conventional feedback (PI and PID) scheme on a simulated reactor. The control objective in this simulation-based work is to maintain the CSTR at the high conversion, and constant steady state operating conditions. The comparative performance study has been carried out between the proposed cascade and fuzzy controllers with the traditional feed controller [Mamdani E.H, (1977)]

3.1 Dynamic Behavior

In this section, the dynamic responses are carried out for different step changes in the flow rate (F_{ji})

The results are obtained by using computer simulation programs using Matlab. Figurer (4) shows the dynamic response of temperature (T) for a unit step change in jacket flow rate F_{ji}. The response shows a decrease in the reactor temperature to a new steady state value.

3.2 Control Strategies

Figurer (5) shows servo response of the temperature within reactor for PI controller to a unit step change in the jacket flow rate (F_{ji}), while Figurer (6) shows Error square versus time for PI controller. The response shows a clear oscillation behavior, this is because the effect of integral control which causes the oscillatory behavior. The value of ISE for PI control is 0.0318.

For PID control, Figurer (7) shows the behavior of the control system with a unit step change in the jacket flow rate (F_{ji}), while Figurer (8) shows Error square versus time for PID controller. The response shows better behavior with lower value of ISE (ISE = 0.0180).

Figures (9 & 10) represent the dynamic responses and the error square versus time for the primary and secondary loops of cascade controller in the case of feedback controllers (PI and PID).

Figures (11 & 12) represent the response and the square of errors ISE with time respectively for fuzzy controller.

Finally Figure (13) and Table (2) show the comparisons among feedback control, cascade control and fuzzy logic control.

Table (3) represents the variable ranges and parameters for the process, while Table (4) represents the properties of the reactor.

4 Conclusions

The present work represents a simulation programs in MATLAB language used to study and develop a mathematical model of the dynamic behavior of a continuous stirred tank reactor (CSTR), and the process control implemented using different control strategies. The following conclusions can be drawn:

1. In this work PID feedback controller is better than PI feedback controller because of the small ISE in the first one.
2. In this work the cascade controller is better than the feedback (PI, PID) controller for the same reason.
3. Fuzzy logic controller gives a marked improvement over cascade controller. However the fuzzy logic controller is preferable since it does not require an accurate mathematical model for the process to be controlled, while all other strategies require very wide knowledge about the dynamic behavior and an accurate mathematical model of the process.
4. Conclusively we can confidently say the controller designed for the problem was stable. The network was successfully used to model and solve the CSTR problem keeping the system at its optimum.

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Table (1) Rule base for fuzzy inference engine

e \ Δe	negative	zero	positive
negative	**negative**	**negative**	**positive**
zero	**negative**	**zero**	**positive**
positive	**negative**	**positive**	**positive**

Table (2) Comparison among feedback control and fuzzy logic control

Controllers	ISE
PI controller	0.0318
PID controller	0.0180
Cascade controller	0.0116
Fuzzy controller	0.0084

Table (3) Variable Range and Parameters

Area for heat exchange	23.23 (m^3)
Ideal gas constant	8.314 (kJ/kmol K)
Heat of reaction	-69780 (kJ/kmol)
Activation energy	69780 (kJ/kmol)
Overall heat transfer coefficient	3066.3 (kJ/h m^2 K)
Heat capacity	3.14 (kJ/kg K)
Heat capacity for jacket	4.19 (kJ/kg K)
Density	800.95 (kg/m^3)
Density for jacket	997.98 (kg/m^3)
Pre exponential factor	$7.08*10^{10}$ (h^{-1})

Table (4) Properties

Reactor output flow rate	1.13 (m^3/h)
Jacket feed flow rate	1.41 (m^3/h)
Jacket output flow rate	1.41 (m^3/h)
Reactor feed temperature	294.44 (K)
Reactor feed temperature	294.44 (K)
Jacket feed temperature	294.44 (K)
Temperature of reactor	333.33 (K)
Temperature of jacket	330.33 (K)
Concentration inlet	8.01 (kmol/m^3)
Concentration	3.92 (kmol/m^3)
Volume of liquid in reactor	1.36 (m^3)
Coolant volume in jacket	0.11 (m^3)

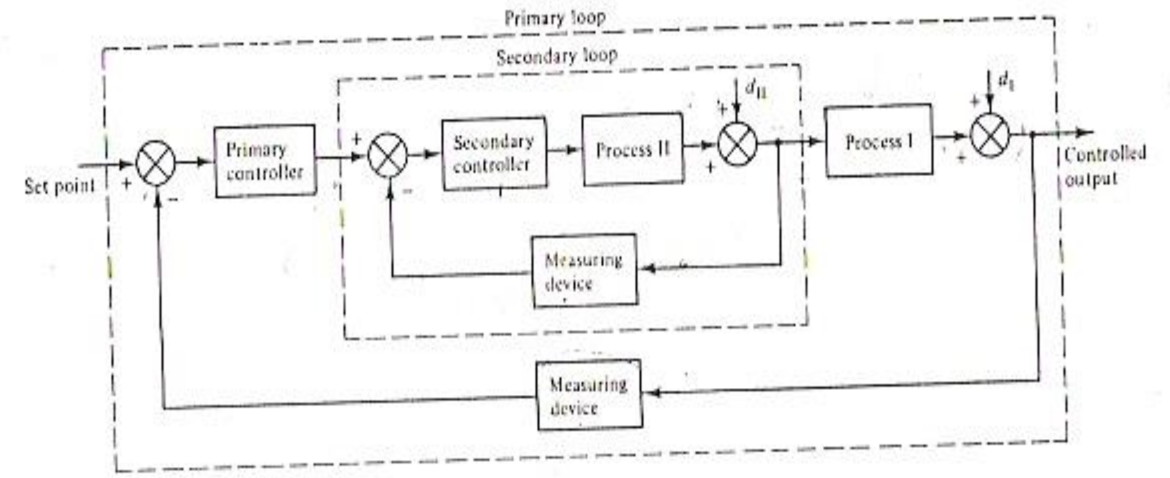


Figure (1) The block diagram of cascade controller

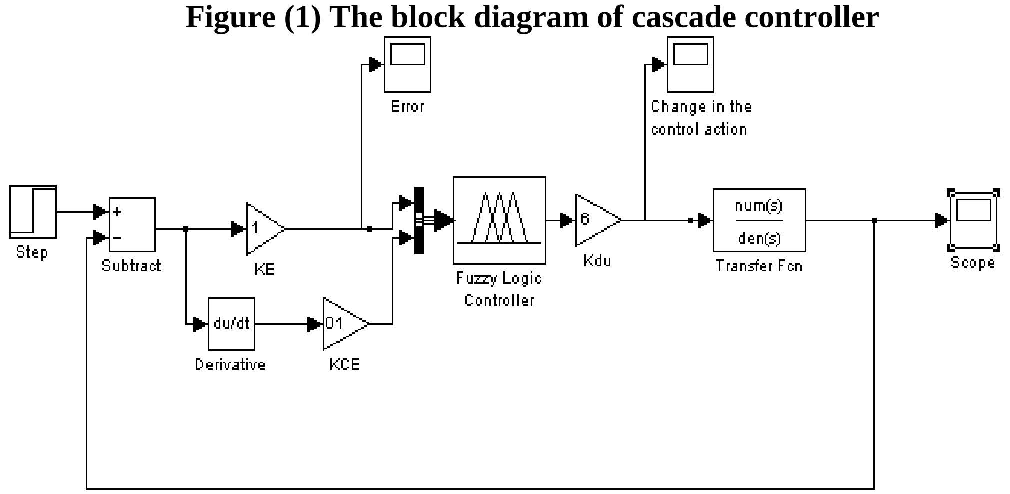
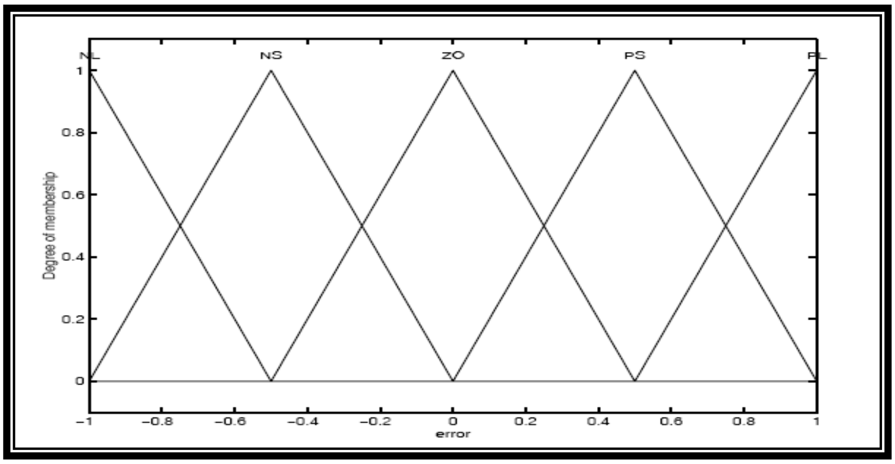
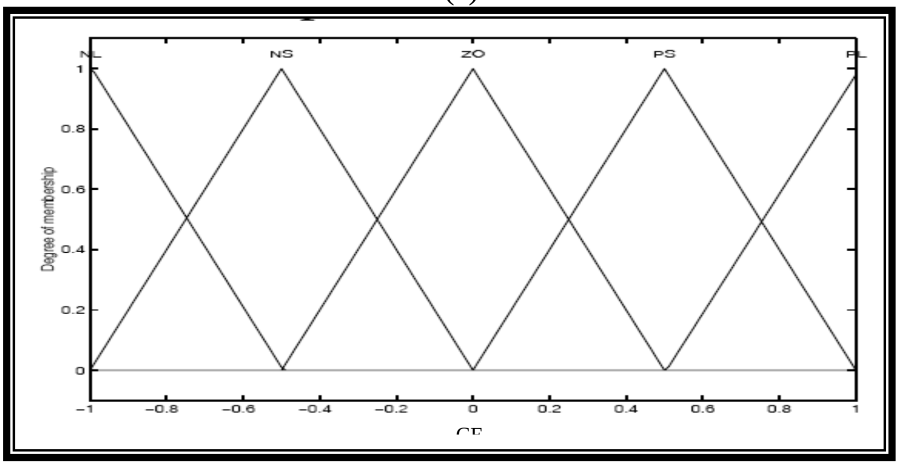


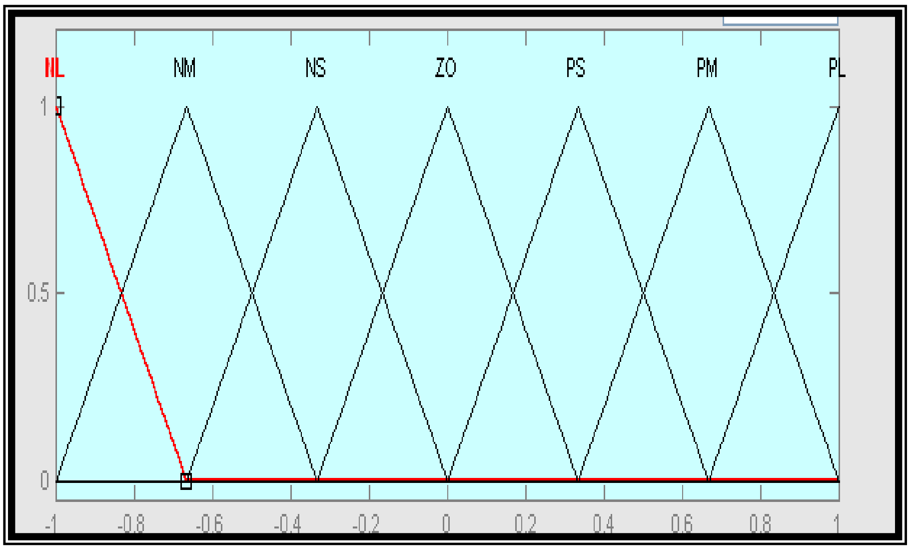
Figure (2) MATLAB file generated for the fuzzy controller.



(a)



(b)



(c)

Figure (3) Membership functions (a) for the control error (b) for the change of control error (c) for the output of fuzzy controller.

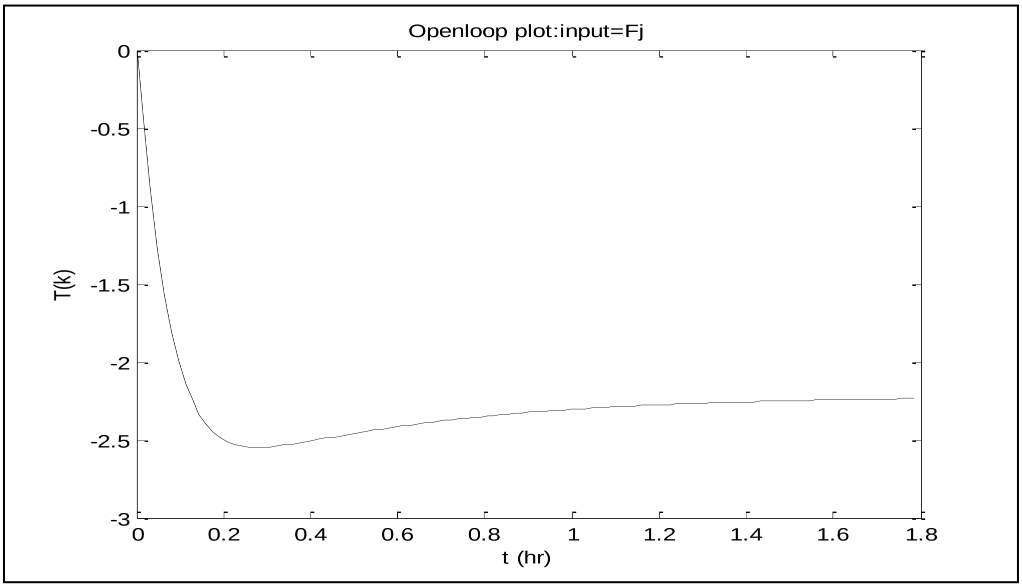


Figure (4) Dynamic response for flow rate step change (open loop system).

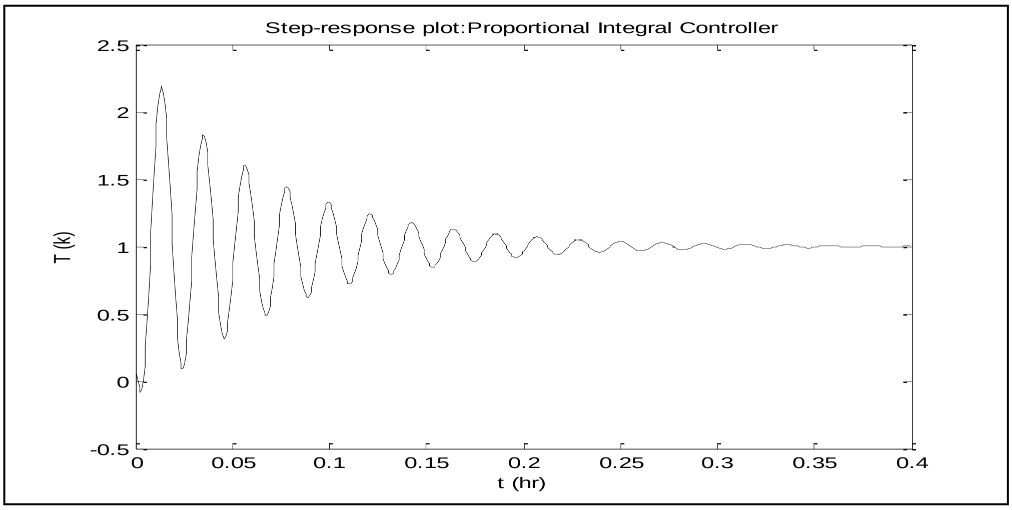


Figure (5) Servo response of the temperature within reactor for PI controller to a unit step change in (F_{jo})

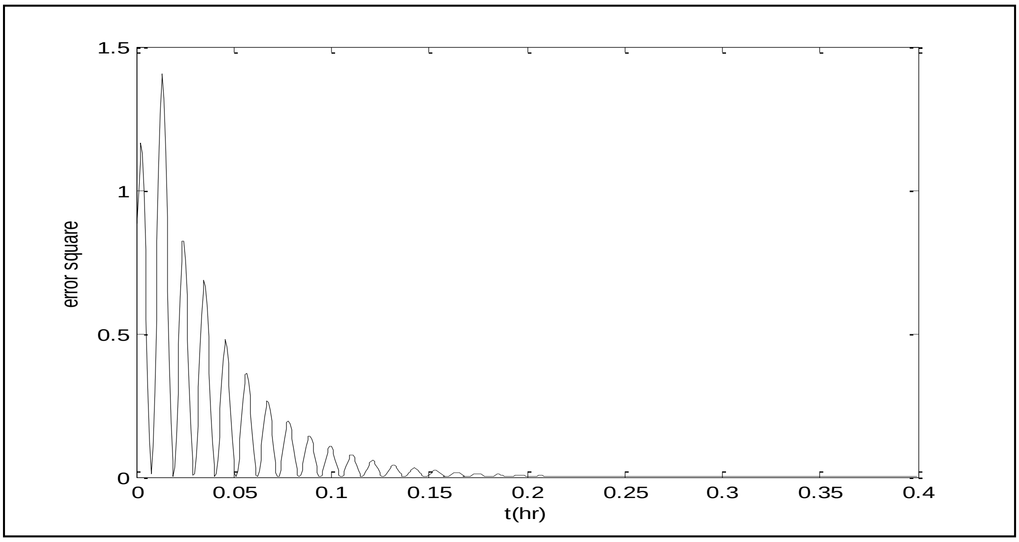


Figure (6) Error square versus time for PI controller.

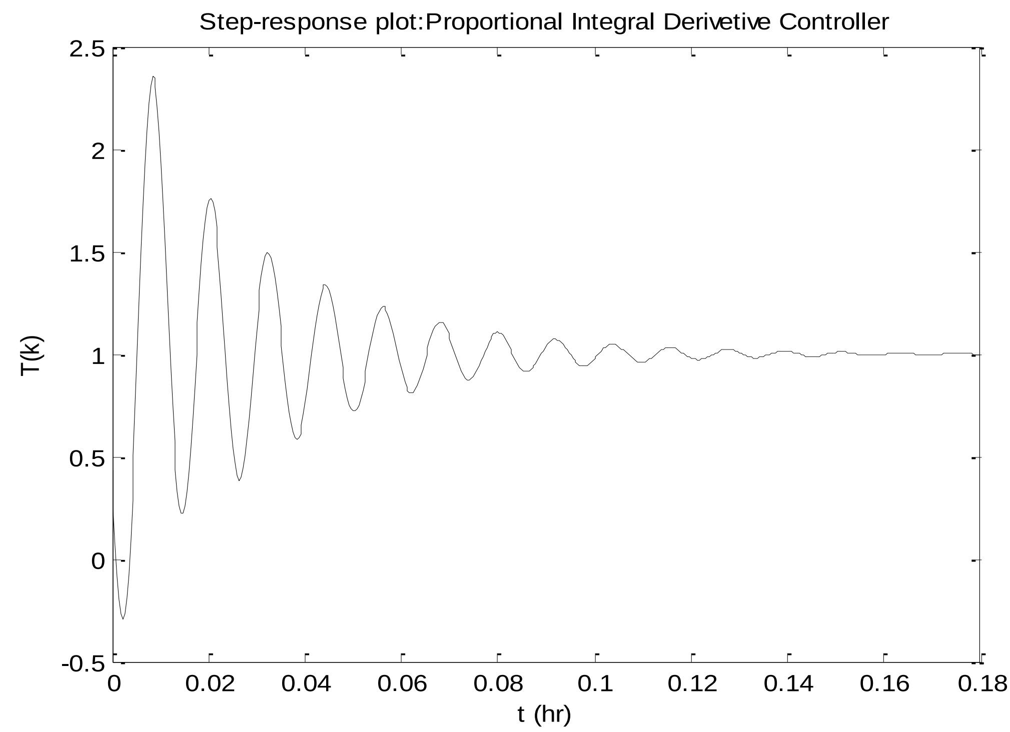


Figure (7) Step response for the temperature of reactor with PID controller

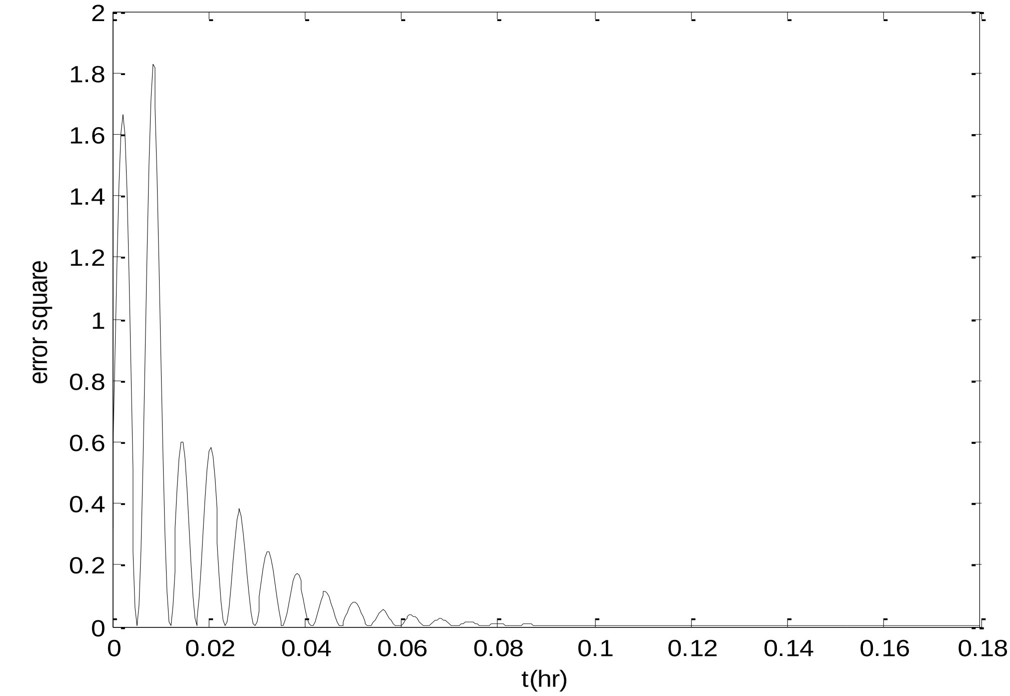


Figure (8) Error square versus time for PID controller.

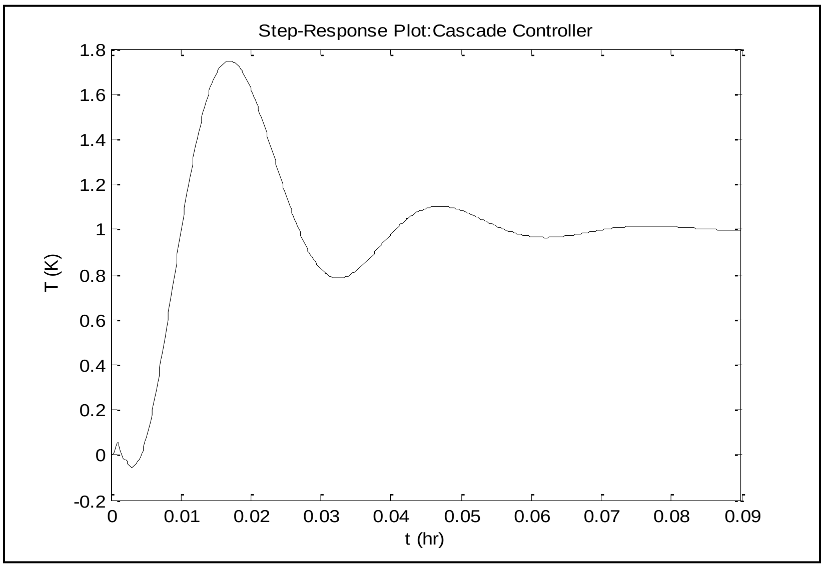


Figure (9) Step response for the temperature of reactor with cascade controller PID controller.

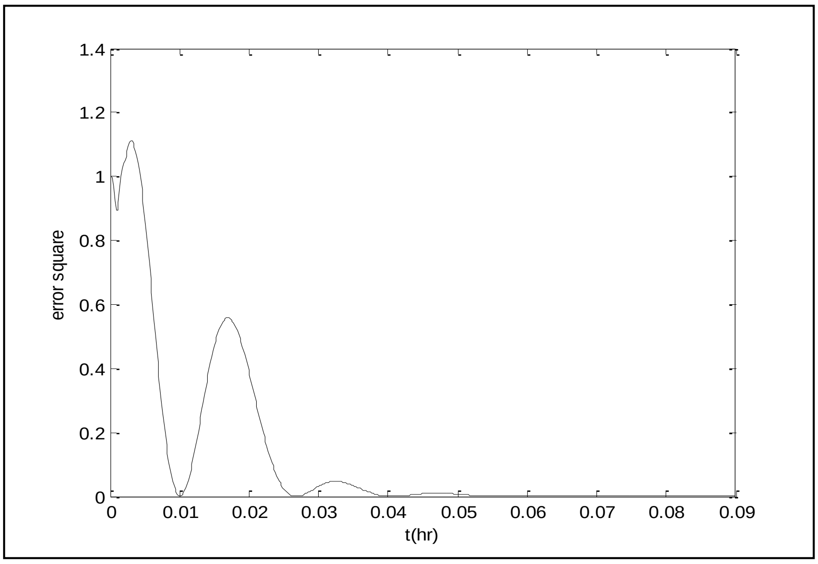


Figure (10) Error square versus time for cascade controller

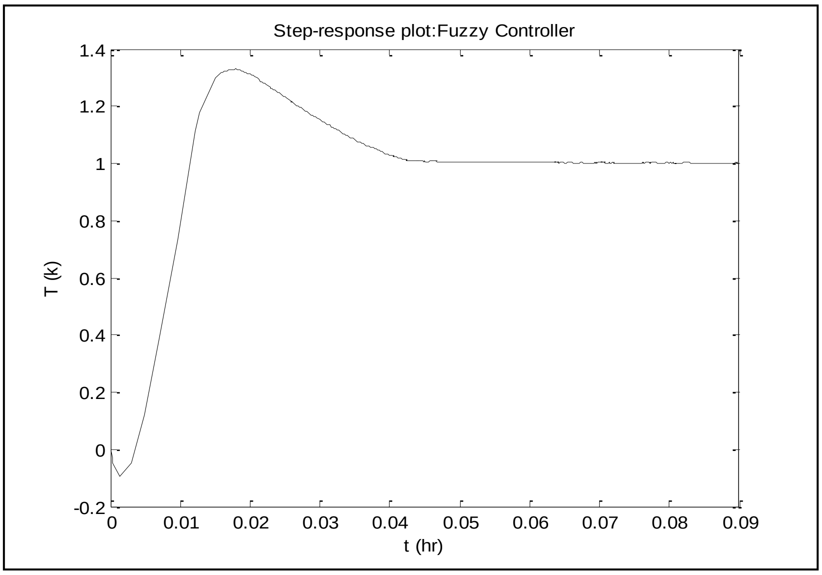


Figure (11) Step response for the temperature of reactor with fuzzy controller

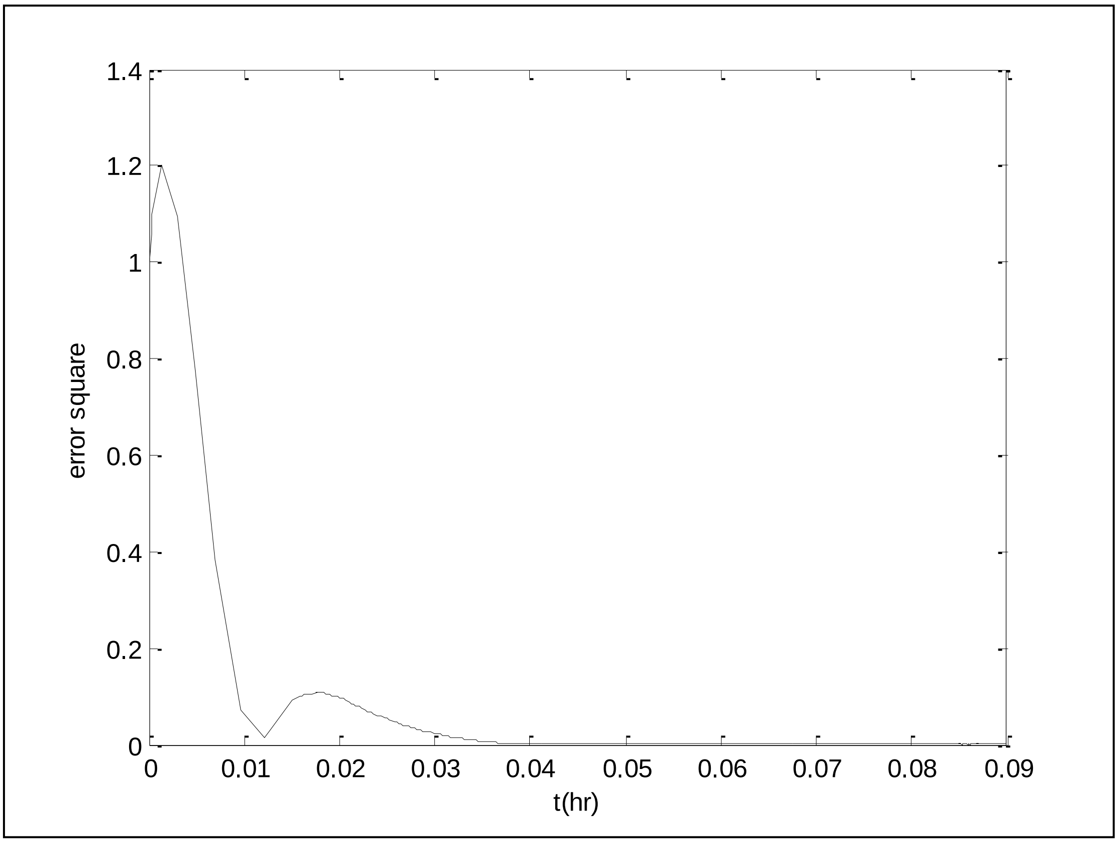


Figure (12) Error square versus time with fuzzy controller

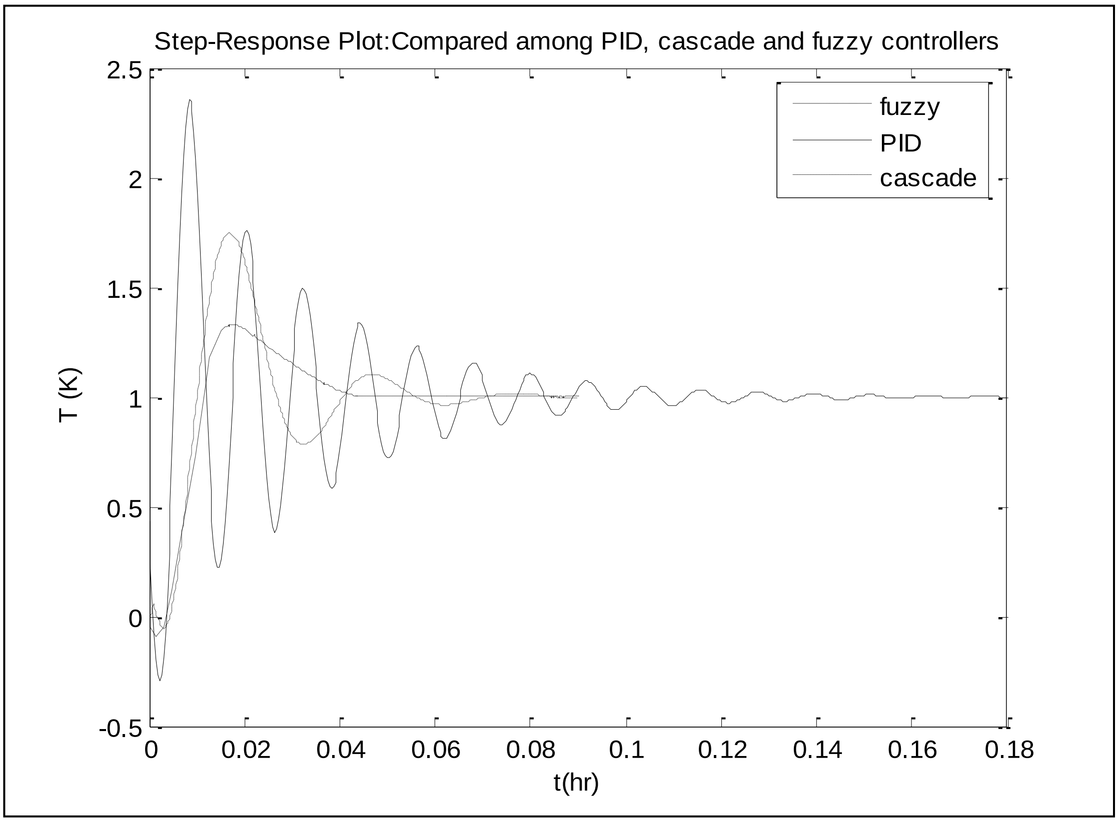


Figure (13) Compare among PID, cascade and fuzzy controllers

Nomenclature

A_H Area for heat exchange (m^2)
C_A Concentration of propylene oxide in reactor ($kmol/m^3$)
C_{Ao} Concentration of propylene oxide in feed stream ($kmol/m^3$)
C_p Heat capacity (kJ/kg K)
C_j Heat capacity for jacket (kJ/kg K)
E Activation energy (kJ/kmol)
F_0 Reactor feed flowrate (m^3/h)
F Reactor output flow rate (m^3/h)
H Heat capacity (kJ/kg K)
H_j Heat capacity for jacket (kJ/kg K)
F_{ji} Jacket feed flow rate (m^3/h)
F_{jo} Jacket output flow rate (m^3/h)
α Pre exponential factor ($time^{-1}$)
R Ideal gas constant (energy/mol*temperature) (kJ/kmol K)
r Rate of reaction per unit volume (mol/volume*time)
t Time (h)
T_0 Reactor feed temperature (K)
T Reactor output temperature (K)
T_{jo} Jacket feed temperature (K)
T_j Jacket output temperature (K)
U Overall heat transfer coefficient (kJ/h m^2 K)
V Volume of liquid in reactor (m^3)
V_j Coolant Volume in jacket (m^3)
($-\Delta H$) Heat of reaction (kJ/h m^2 K)
ρ Density (kg/m^3)
ρ_j Density for jacket (kg/m^3)
$_i$ Inlet
$_j$ Jacket
$_{ji}$ Jacket inlet
$_{ref}$ Reference
e Error
Δe Change of error
Δu controller output