

Performance Analysis of Non-linear Jacketed CSTR based on Different Control Strategies

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Abstract: This paper aims at finding the optimum controller for a jacketed Continuous Stirred Tank Reactor (CSTR) under non-ideal conditions. Various conventional control methods show poor response for non-linear processes. This paper outlines the design procedure of the Internal Model Controller (IMC) and Model Reference Adaptive Control (MRAC). The performance of the jacketed CSTR process is analyzed based on Internal Model Control and adaptive control. Simulation results have been compared with conventional PID control.

Keywords: Continuous Stirred Tank Reactor (CSTR), Model Reference Adaptive Control (MRAC), Internal Model Controller (IMC), Dead space, PID Controller

1. Introduction

Designing a controller assuming linear behaviour for the continuous stirred tank reactor (CSTR) will lead to poor performances. In the case of ideal behaviour the dead space and bypass is not considered, which affects the transient of the system and the desired output concentration.

In this paper, the following works have been done:

- Modelling of a non-linear CSTR with dead space and bypass has been shown in Section 2.
- Stability analysis of the practical system (as per modelling done in Section 2) has been shown in Section 3.
- Application of different control techniques and comparison of all the techniques for the controlled CSTR has been investigated in Section 3.

2. Mathematical Modelling of Non-Linear Jacketed CSTR

Figure 1 shows the basic schematic diagram of a jacketed CSTR, in which a simple irreversible, exothermic reaction $A \rightarrow B$ is taking place. The reactor is surrounded by a jacket where mixing is taking place at low temperature than the reactor. Energy is passed through the reactor wall into the jacket, removing the heat generated by the reaction [1,2].

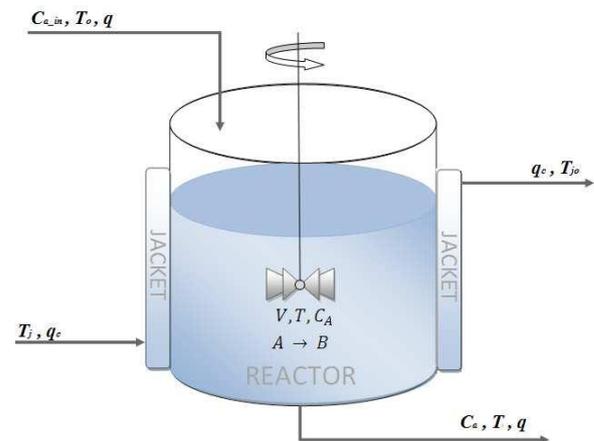


Figure 1: Schematic diagram of a continuous stirred tank reactor [2]

The feed material composition $C_{a,in}$ enters the reactor at temperature T_o at a volumetric flow rate of q . The product is withdrawn from the reactor at same volumetric flow rate q .

In a jacketed CSTR, the heat is added or removed by virtue of the temperature difference between a jacket fluid and the reactor fluid. As the reaction undergoing within the reactor is considered exothermic, heat will be evolved for the reactor and hence a coolant will flow through the jacket at a flow rate of q_c fed at a temperature of T_j .

The non-uniform mixing in non-linear CSTR results in bypassing and dead space. When perfect mixing does not takes place in the overall volume and results in less reactor volume than in case of ideal behaviour, due to which it results in rapid decay of transient than in case of ideal case. In case of bypass, the volumetric flow rate will be

less than that of the volumetric flow in the ideal behaviour case, which results in a slower decay of the transient as compared to the ideal case. The schematic representation of the non-linear CSTR combined with dead space and bypass is shown in Figure 2.

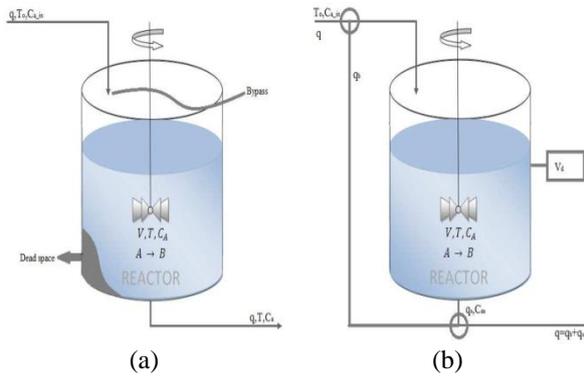


Figure 2: Non-linear CSTR: (a) Real system; (b) Model system [2]

2.1 Material balance of Component A

Considering an irreversible, exothermic first-order chemical reaction $A \rightarrow B$, taking place in non-linear condition.

$$\frac{dC_a}{dt} = \frac{q}{\alpha V} (C_{a_in} - C_a) - k_o \exp\left(\frac{-E_a}{R(T - \beta T_o)}\right) \left(\frac{C_a - \beta C_{a_in}}{1 - \beta}\right) \dots\dots (1)$$

Where C_{a_in} is the feed material concentration, C_a is the concentration of component A, k_o is the frequency factor, E_a is the activation energy, R is the gas constant, T is the temperature, α is the dead space and β is the bypass.

2.2 Reactor Energy Balance

According to the principle of conservation of energy:

(Rate of energy accumulation) = (Rate of energy input) - (Rate of energy output) - (Rate of energy removed by the coolant) + (Rate of energy added by exothermic reaction)

$$\frac{dT}{dt} = \frac{q}{V} (T_o - T) - \alpha \left(\frac{-\Delta H}{\rho C_p}\right) k_o \exp\left(\frac{-E_a}{R(T - \beta T_o)}\right) \left(\frac{C_a - \beta C_{a_in}}{1 - \beta}\right) + \left(\frac{\rho_c C_{pc}}{\rho C_p V}\right) q_c \left[1 - \exp\left(\frac{-hA}{q_c \rho_c C_{pc}}\right)\right] (T_j - T) \dots\dots(2)$$

Where $-\Delta H$ is the heat of the reaction, UA is the heat transfer coefficient, T_o is the feed temperature, T_j is the jacketed temperature, C_p is the heat capacity, ρ is the density.

2.3 State variable form of the equation

Equations (1) and (2) are expressed in the standard state variable form as follows:

$$\frac{dC_a}{dt} = f_1(C_a, T) = \frac{q}{\alpha V} (C_{a_in} - C_a) - k_o \exp\left(\frac{-E_a}{R(T - \beta T_o)}\right) \left(\frac{C_a - \beta C_{a_in}}{1 - \beta}\right) \dots\dots (3)$$

$$\frac{dT}{dt} = f_2(C_a, T) = \frac{q}{V} (T_o - T) - \alpha \left(\frac{-\Delta H}{\rho C_p}\right) k_o \exp\left(\frac{-E_a}{R(T - \beta T_o)}\right) \left(\frac{C_a - \beta C_{a_in}}{1 - \beta}\right) + \left(\frac{\rho_c C_{pc}}{\rho C_p V}\right) q_c \left[1 - \exp\left(\frac{-hA}{q_c \rho_c C_{pc}}\right)\right] (T_j - T) \dots\dots(4)$$

2.4 Linearization

The linearization method is applied to non-linear CSTR model to obtain the state space representation. The state, input and the output vector is defined by the following:

$$x = \begin{bmatrix} C_a - C_{as} \\ T - T_s \end{bmatrix}, u = \begin{bmatrix} 0 \\ T_j - T_{js} \end{bmatrix}, y = \begin{bmatrix} C_a - C_{as} \\ T - T_s \end{bmatrix}$$

Where C_{as} is the steady-state value of effluent concentration, T_s is the steady-state value of reactor temperature, q_s is the steady-state value of feed flow rate, q_{cs} is the steady-state value of the coolant flow rate.

The state space matrices for the CSTR model are derived from the corresponding Jacobian matrix:

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

$$A_{11} = \frac{df_1}{dx_1} = \frac{q}{\alpha V} - \frac{k_o}{1 - \beta} \exp\left(\frac{-E_a(1 - \beta)}{R(T - \beta T_o)}\right)$$

$$A_{12} = \frac{df_1}{dx_2} = \frac{E_a k_o (C_a - \beta C_{a_in})}{R(T - \beta T_o)^2} \exp\left(\frac{-E_a(1 - \beta)}{R(T - \beta T_o)}\right)$$

$$A_{21} = \frac{df_2}{dx_1} = \alpha \left(\frac{\Delta H}{\rho C_p}\right) k_o \exp\left(\frac{-E_a(1 - \beta)}{R(T - \beta T_o)}\right) \left(\frac{1}{1 - \beta}\right)$$

$$A_{22} = \frac{df_2}{dx_2} = -\frac{q}{V} - \frac{\alpha \Delta H k_o E_a (C_a - \beta C_{a_in})}{\rho C_p R(T - \beta T_o)^2} \exp\left(\frac{-E_a(1 - \beta)}{R(T - \beta T_o)}\right) -$$

$$\left(\frac{\rho_c C_{pc}}{\rho C_p V}\right) \left[1 - \exp\left(\frac{-hA}{q_c \rho_c C_{pc}}\right)\right]$$

$$B = \begin{bmatrix} B_{11} \\ B_{21} \end{bmatrix} = \begin{bmatrix} \frac{\delta f_1}{\delta u_1} \\ \frac{\delta f_2}{\delta u_1} \end{bmatrix}$$

$$B_{11} = \frac{\delta f_1}{\delta u_1} = 0$$

$$B_{21} = \frac{\delta f_2}{\delta u_1} = \frac{\rho_c C_{pc}}{\rho C_p V} \left[1 - \exp\left(\frac{-hA}{q_c \rho_c C_{pc}}\right) \right]$$

Table 1: Steady state operating data

Symb ol	Parameters	Values
C_a	Reactor Concentration	0.0882 mol / l
T	Reactor temperature	441.2K
q_c	Coolant flow rate	100l / min
q	Feed flow rate	100l / min
C_{a_in}	Feed concentration	1mol / l
T_o	Inlet temperature	350K
T_j	Inlet jacket temperature	350K
V	CSTR volume	100l
hA	Heat transfer coefficient	$7 \times 10^5 \text{ cal / (min K)}$
k_o	Reaction rate constant	$7.2 \times 10^{10} \text{ min}^{-1}$
$\frac{E_a}{R}$	Activation energy term	$1 \times 10^4 \text{ K}$
$-\Delta H$	Heat of reaction	$-2 \times 10^5 \text{ cal / mol}$
ρ, ρ_c	Liquid densities	$1 \times 10^3 \text{ g / l}$
C_p, C_{pc}	Specific heat	1 cal / (g / K)

The operating points for the local linear models of the non-linear CSTR for both the cases are presented in Table 2.

Table 2: The operating points for the local linear models of the non-linear CSTR

Feed flow (l/min)	Coolant flow (l/min)	Effluent Conc. (mol/l)	Reactor Temp. (K)
103	97	0.2442	427.9

The matrices A and B can be determined using the values mentioned in the above table and the transfer function that relate the input and output.

$$A = \begin{bmatrix} -16.64 & 0.486 \\ 3528 & -11.75 \end{bmatrix}, B = \begin{bmatrix} 0 \\ 0.99908 \end{bmatrix}, C = [0,1], D = 0$$

The continuous time transfer function is given as:

$$g_p(s) = \frac{0.991s + 16.62}{s^2 + 28.39s + 24.06}$$

2.5 Stability Analysis of Non-Linear CSTR

Stability analysis of nonlinear continuous CSTR system is done by using Lyapunov stability.

Given a nonlinear differential equation,

$$\dot{x} = f(x, t)$$

And a scalar function $V(x)$,

If

1. $V(x)$ is positive definite, and
2. $\dot{V}(x)$, the derivative of $V(x)$, is negative definite, and
3. $V(x) \rightarrow \infty$, as $\|x\| \rightarrow \infty$

Then, the system $\dot{x} = f(x, t)$ is globally asymptotically stable.

To derive the necessary condition for stability $\dot{x} = Ax$ using the method of Lyapunov, the above-mentioned steps should be followed where the possible Lyapunov function in quadratic form is chosen as: $V(x) = x^T P x$

The Lyapunov function will be positive definite if the matrix P is symmetric positive definite. The time derivative is given by:

$$\dot{V}(x) = x^T (A^T P + AP) x$$

Where the convenience matrix $Q = -(A^T P + AP)$

So, if ‘ $-Q$ ’ is negative definite, (or alternatively Q is positive definite, $Q > 0$), then the system is stable [4,5].

In the case of non-linear CSTR the value of ‘ P ’ is:

$$P = \begin{bmatrix} 144.28 & -0.6807 \\ -0.6807 & 0.0144 \end{bmatrix}$$

Positive definiteness can be found using MATLAB software by a doing Cholesky decomposition using the function $[R,p] = \text{chol}(A)$. In this given case, ‘ P ’ is 1. Hence, P is positive definite and therefore the system is stable.

3. Control Strategies for Non-Ideal CSTR

3.1 Adaption Law

The adaption law attempts to find a set of parameters that minimizes the error between the plant and the model outputs. To do this, the parameters of the controller are incrementally adjusted until the error has reduced to zero [12]. A number of adaption laws have been developed to

date. The two main types are the gradient and the Lyapunov approach [12], and we have used the gradient approach [7].

3.1.1 Model Reference Adaptive Control

Model Reference Adaptive Control (MRAC) is considered to be an important adaptive controller. In the case of MRAC, the desired performance is expressed in terms of a reference model that provides a desired response to the command signal.

The standard implementation of MRAC is shown in Figure 3. It is composed of two loops. The first loop is the ordinary feedback loop that consists of the process and the controller, which is known as the inner loop. The second loop, also known as the outer loop comprises of the adjusting mechanism. The difference between the plant output and the reference model output provides the error signal and parameter change will be based upon that error signal [8,9].

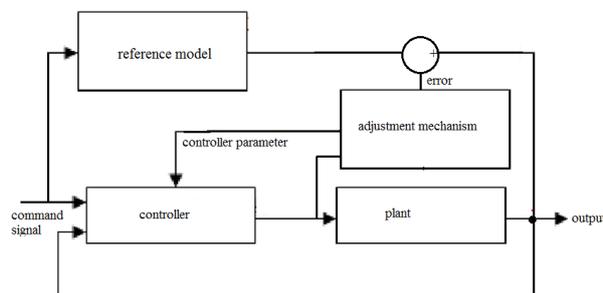


Figure 3: Model Reference Adaptive Controller

The adjusting mechanism will be based upon two methods, the gradient method and the Lyapunov method [10].

3.1.2 Adaptive Control Design

For implementing the basic adaptive controller using MATLAB Simulink, the plant transfer function is to be defined which is to be controlled. The continuous time transfer function of the system is given as:

$$g_p(s) = \frac{1.458s + 11.65}{s^2 + 3.434s + 3.342}$$

Secondly, a model should be defined that will match with the given plant. To determine the model, the characteristics should be defined. In order to define the characteristics, an arbitrary second-order model will be selected [12] as:

$$g_m(s) = \frac{\omega_n^2}{s^2 + 2\xi\omega_n s + \omega_n^2}$$

The damping factor ξ and the natural frequency ω_n should be determined in order to get the required performance.

For the concentration control, a maximum overshoot of 5% and the settling time less than 3 is selected [8]. The following mentioned condition is used to determine the damping factor ξ and the natural frequency ω_n [12].

$$\xi = \frac{\ln M_p / 100}{-\pi} \sqrt{\frac{1}{1 + \left(\frac{\ln M_p / 100}{-\pi}\right)^2}}$$

$$\omega_n = \frac{3}{\xi T_s}$$

Based on the above formula, the damping factor and the natural frequency are determined as: $\xi = 0.713, \omega_n = 2.134$

Therefore, the transfer function for the model is defined as

$$g_m(s) = \frac{4.76}{s^2 + 3.1s + 4.76}$$

3.1.3 MIT Rule

To present the MIT rule, we can consider a closed loop system in which the controller has one adjustable parameter. The desired closed loop response is specified by a model output Y_m . The error (e) is the difference between the output of the system (Y) and the output of the reference model (Y_m) [11,12,14].

The Modeling error e is given by equation [12] :

$$e = Y - Y_m$$

One possibility is to adjust parameters in such a way that the loss function $J(\theta)$ is minimized.

$$J(\theta) = \frac{1}{2}e^2$$

To make J small, it is reasonable to change the parameters in the direction of the negative gradient of J [14].

$$\frac{d\theta}{dt} = -\gamma \frac{\delta J}{\delta \theta} = -\gamma e \frac{\delta e}{\delta \theta}$$

This is the celebrated MIT rule. The partial derivative $\frac{\delta e}{\delta \theta}$ is called the sensitivity derivative of the system, tells how the error is influenced by the adjustable parameter. Here, γ is called adaptation gain.

3.2 Internal Model Control System configuration

The IMC configuration is designed for setting up a comparison between the process and model output

to form a standard feedback structure. Figure 4 shows the basic IMC implementation in the process transfer function [6].

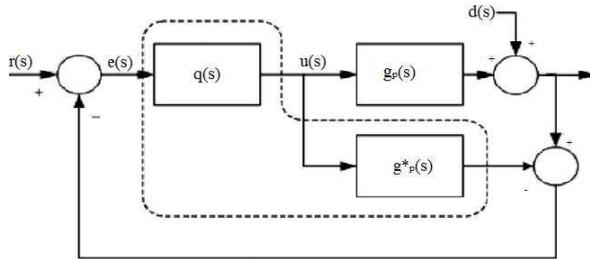


Figure 4: IMC configuration

Considering the IMC based PID design procedure for a second order system of CSTR process model of type:

$$\tilde{g}_p(s) = \frac{(\beta s + 1)}{(\tau^2 s^2 + 2\xi\tau s + 1)}$$

$$\tilde{g}_p(s) = \tilde{g}_{p+}(s) \tilde{g}_{p-}(s) = \frac{(\beta s + 1)}{(\tau^2 s^2 + 2\xi\tau s + 1)}$$

$$\tilde{q}(s) = \tilde{g}_{p-}^{-1}(s) = \frac{\tau^2 s^2 + 2\xi\tau s + 1}{(\beta s + 1)}$$

$$q(s) = \tilde{q}(s) f(s) = \tilde{g}_{p-}^{-1}(s) f(s) = \frac{\tau^2 s^2 + 2\xi\tau s + 1}{(\beta s + 1)} \frac{1}{\lambda s + 1}$$

$$g_c(s) = \frac{q(s)}{1 - q(s) \tilde{g}_p(s)} = \frac{\frac{\tau^2 s^2 + 2\xi\tau s + 1}{(\beta s + 1)(\lambda s + 1)}}{1 - \frac{\tau^2 s^2 + 2\xi\tau s + 1}{(\beta s + 1)(\lambda s + 1)} \frac{(\beta s + 1)}{(\tau^2 s^2 + 2\xi\tau s + 1)}}$$

$$g_c(s) = \frac{\tau^2 s^2 + 2\xi\tau s + 1}{\lambda s (\beta s + 1)}$$

Comparing with the transfer function of the PID controller,

$$g_c(s) = k_c \left[\frac{\tau_i \tau_d s^2 + \tau_i s + 1}{\tau_i s} \right]$$

Then from the second order model parameters, the following IMC PID controller tuning formula is used as shown in Table 3.

Table 3: IMC PID controller tuning

$\tilde{g}_p(s)$	$f(s)$	k_c	τ_i	τ_d
$\frac{(\beta s + 1)}{(\tau^2 s^2 + 2\xi\tau s + 1)}$	$\frac{1}{\lambda s + 1}$	$\frac{2\xi\tau}{\lambda}$	$2\xi\tau$	$\frac{\tau}{2\xi}$

4. Results

In this section, the proposed controller design is implemented to the continuous time transfer function of CSTR models to show the efficiency of the proposed controllers.

Firstly, the step response of the open loop CSTR model is shown (Figure 5); secondly the step responses of CSTR model based on conventional PID and IMC based PID controls are shown (Figure 6) and lastly, the Adaptive control step response of the CSTR model is demonstrated (Figures - 7,8,9,10).

4.1 Open-loop response of a Jacketed CSTR

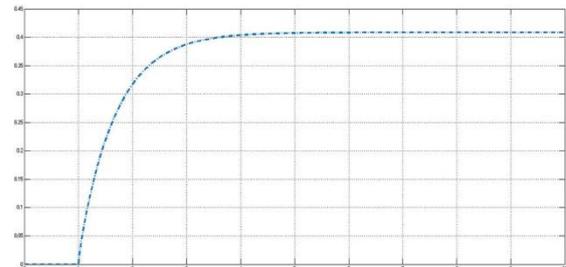


Figure 5: Step response of the open loop CSTR model

Figure 5 shows the open loop response of the non-ideal CSTR where x-axis defines the time and y-axis defines the effluent concentration.

4.2 Response based on Internal Model Control (IMC)

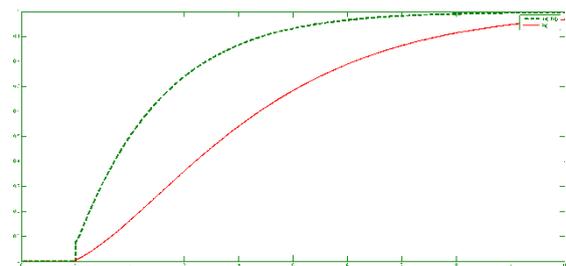


Figure 6: Step responses of conventional PID and IMC based PID controller

The simulation results show that the IMC based PID controller has no overshoot and fast response compared to the conventional PID.

4.3 Response based on Adaptive control

After obtaining the transfer function of process and the transfer function of the reference model, a MATLAB Simulink model is developed by applying the MIT rule [12].

The following parameters are plotted on the graph: plant output using adaptive control for different values of γ .

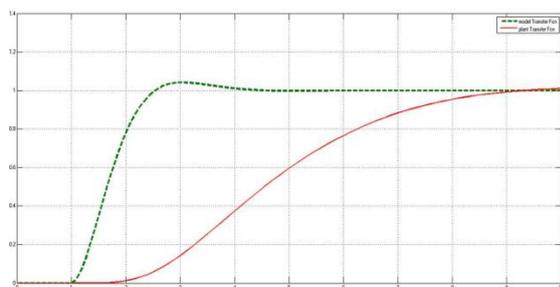


Figure 7: Step response of CSTR based on Adaptive controller when $\gamma = 0.5$

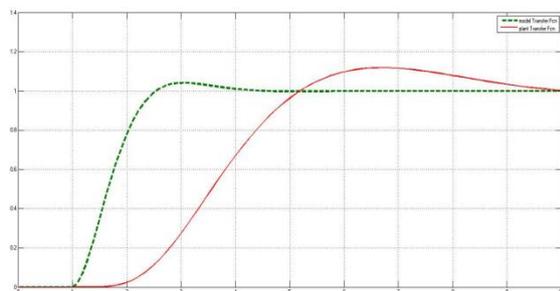


Figure 8: Step response of CSTR based on the adaptive controller when $\gamma = 1$

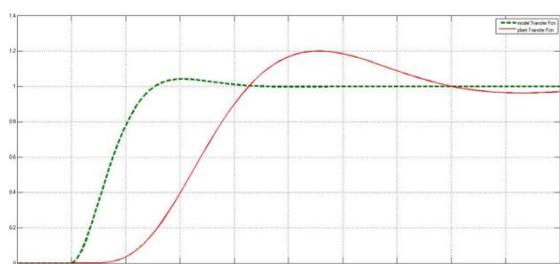


Figure 9: Step response of CSTR based on adaptive controller when $\gamma = 1.5$

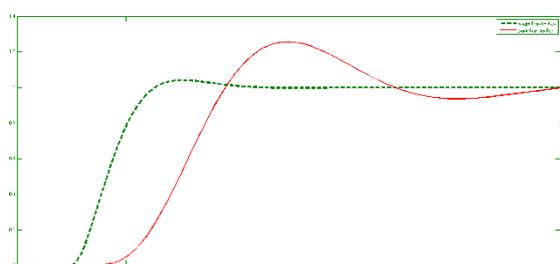


Figure 10: Step response of CSTR based on adaptive controller when $\gamma = 2$

The effect of adaptive control is analyzed on the time response characteristic of the system. It is observed that with a smaller value of adaption gain the response is very slow. The transient parameters such as settling time, rise time, peak time can be decreased by increasing the value of adaption gain.

Unit step responses of the IMC based PID controller, the conventional PID controller and adaptive controller have been listed in Table 4, which shows that adaptive control requires less

settling time to reach desired steady state and gives less overshoot as compared to the IMC based PID controller and conventional PID controller.

Table 4: Unit step responses of the IMC based PID controller, the conventional PID controller and the adaptive controller

	Settling Time (T_s)	Rise Time (T_r)	Peak Time (T_p)
Conventional PID	2.8×10^3	2.6×10^3	2948
IMC based PID	513.5	1.59×10^3	1742
MRAC with adaptive gain = 0.5	75.94	37.60	85

5. Conclusion and Future Scope

The behaviour of the Jacketed CSTR based on adaptive control using MIT rule has been analyzed in this paper. The time response characteristics are observed based on the various adaption gain values. The transient characteristics such as settling time, rise time can be decreased by increasing the adaption gain value. Simulation results of the non-linear model equation of Jacketed CSTR for a first-order irreversible exothermic chemical reaction show that the controller based on adaptive control will give a better response as compared to the IMC based PID controller and conventional PID controller.

The analyzed results and issues during the course of the work give rise to a number of possible directions for future work. Some of them are briefly summarized below:

- (i) Modelling and control of a non-ideal reactor with second-order reaction can be carried out.
- (ii) Tuning of PID can be done using different tuning methodologies such as Cohen-Coon and Artificial Bee-colony based tuning methods, and comparison can be made between the new tuning methods with the proposed control schemes.
- (iii) Modelling can be done by considering Dead space to be a function of time.

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