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**Research Article** 

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## Simulation of temperature control methodologies for chemical reactor

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## ABSTRACT

A Continuous Stirred Tank Reactor (CSTR) is a highly non linear process particularly when chemical reaction takes place. The heat energy will be either liberate or absorbed by the reactor due to the reaction. The control of temperature for this process is a real challenge due to non linear temperature changes during reaction. This paper compares the performances of the Proportional Integral Derivative Controller (PID) controller, Fuzzy PID Controller, Model Predictive Controller (MPC) and MPC based PID Controller. The mathematical model of CSTR is obtained and the state space model is derived. The various controllers have been designed and performances were compared for the CSTR process. The proposed MPC-Based PID controller shows better control of temperature than the other controllers like PID and MPC.

Keywords: CSTR, PID, MPC, FUZZY-PID, MPC-PID

## INTRODUCTION

Chemical reactors are often the most difficult units to control in a chemical plant, particularly if the reactions are rapid and exothermic. A continuous stirred reactor with a constant feed rate, feed concentration, and holdup time, with irreversible exothermic reaction is considered. The heat generated by chemical reaction, the heat removed by the jacket and the product stream are plotted against reactor temperature shows three possible operating regions [1]. The amount of heat released by exothermic reaction is sigmoid function of temperature in the reactor. The heat removed by the coolant is linear function of temperature. The intersection of these two curves yields three states [2]. A CSTR at steady state will have the heat generated by reaction is equal to heat removed by the coolant. A controller that ensures the stability of the operation at the middle steady state is desirable. The control of non isothermal CSTR using PID, IMC controller given [3] provides the basic control strategies. The implementation of neural control [4] of CSTR is also detailed. Figure 1. Shows a CSTR in which an irreversible exothermic reaction is removed by a coolant medium that flows through a jacket around the reactor.

## **Model Description**

The assumptions made for developing the mathematical model is that there is perfect mixing inside reactor and the jacket, Volume of reactor and jacket is constant and the parameter values are fixed. The dynamic model of the reactor is obtained by writing material and energy balance equation. The change in concentration of the reactant and temperature of the reactor is mathematically written as [5] given below.

$$\frac{dCa}{dt} = \frac{F}{V} * (Caf - Ca) - Ko * exp\left(-\frac{Ea}{R*T}\right) * C$$
(1)

$$\frac{\mathrm{dT}}{\mathrm{dt}} = \frac{F}{V} * \left( \mathrm{Tf} - \mathrm{T} \right) + \left( \frac{-\Delta H}{\rho * Cp} \right) * Ko * exp \left( -\frac{Ea}{R * T} \right) * Ca - \left( \frac{U * A}{V * \rho * Cp} \right) * \left( \mathrm{T} - \mathrm{Tj} \right)$$
(2)

The steady state solution is obtained when the two state derivatives are set equal to zero.



Figure1. CSTR with cooling jacket

The CSTR is modeled with parameters [6] given in Table 1

Variables	Description	Values
Ea	Activation Energy	32400 Btu/lb.Mol
Ко	Arrhenius factor or Pre Exponential Factor	15e12 per Hr
$-\Delta H$	Heat of Reaction	-45000 Btu/lb.Mol
U	Heat Transfer Coefficient	75 Btu/Hr.Ft <sup>2</sup> .°F
$\rho * Cp$	Density* Specific Heat Capacity	53.25 Btu/ft <sup>3</sup>
R	Gas Constant	1.987 Btu/lb.Mol. °F
V	Volume of Reactor	750 Ft <sup>3</sup>
F	Flow Rate of Coolant	3000 Ft <sup>3</sup> /Hr
Caf	Concentration of Component A in feed	0.132 lb.Mol/ Ft3
Tf	Temperature of the feed	60 °F
A	Heat Exchange Surface Area	1221 Ft <sup>2</sup>

Table 1.Parameters of CSTR

The generic state space model is of the form.

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

$$\dot{y} = Cx + Du$$

(4)

The state space model obtained [7] for the reactor with operating point concentration and temperature of 0.08 lb.Mol/  $Ft^3$  and 80  $^{O}F$  is given below.

$$A = \begin{bmatrix} -4.0060 & 0\\ 5.10704 & -6.2615 \end{bmatrix} \\ B = \begin{bmatrix} 0\\ 2.2930 \end{bmatrix} \\ C = \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix} \\ D = \begin{bmatrix} 0\\ 0 \end{bmatrix}$$

The initial reactor concentration and temperature are 0.1 lb. Mol/ft3 and 40  $^{\rm O}$ F respectively.

#### **EXPERIMENTAL SECTION**

#### **Proportional Integral Derivative (PID) Controller**

The PID controller has been used for the Temperature and Concentration control for CSTR over past two decades. The time domain representation of PID control is

$$u(t) = K_c \left\{ e(t) + \frac{1}{\tau_i} \int_0^t e(t) dt + \tau_d \, \frac{de(t)}{dt} \right\}$$
(5)

The initial  $K_p$ ,  $K_i$ ,  $K_d$  values of the parameter are chosen as 10,100, 0.001 respectively. The PID parameters are found using Zeigler –Nichols method. The block diagram used for the simulation of the closed loop response of state space model of the plant with and without PID Controller is shown in Figure 2.



Figure 2. CSTR Simulink Block with and without PID Controller



Figure 3. Closed loop response with and without PID Controller

There is a initial temperature of 40  $^{0}$ F in the reactor. The closed loop response of plant model with and without PID controller is given in Figure 3. A set point of 80  $^{\circ}$ F is given as step input at 1Sec. The difference between set point and the measured temperature i.e., the error is given as a input to the PID controller. For the system with PID Controller the delay time, rise time, settling time is around 0.0392 Sec, 0.0738 Sec and 0.0918 Sec respectively. There is a little over shoot of 4.522 % in the response. The steady state error is negligible for the plant with PID controller. For a plant without controller the temperature settles at a lower stable value.

#### **Model Predictive Controller (MPC)**

A plethora of Model Predictive Controller for control of temperature, concentration, Ph without neural strategy for CSTR is given in [8, 9, 10]. The control literature [11, 12, 13, 14] has proposed neural network based model predictive control for non linear CSTR process. The simulink block diagram of CSTR with MPC is shown in Figure

4. The control interval is chosen to be 0.1 time unit. The Prediction horizon and Control Horizon are chosen as 5 and 1 interval respectively.



#### Figure 4. CSTR Simulink Block with MPC

A set point of 80 °F is given as step input at 1 Sec. For the system with MPC the delay time, rise time, settling time is around 0.0976 Sec, 0.3109 Sec and 0.4782 Sec respectively. There is a no over shoot in the response. The response of the plant model with Model Predictive Controller is shown in Figure 5.



Figure 5. Closed loop response with MPC





### **Fuzzy PID Controller**

The Fuzzy PID Controller takes error and rate of change of error as its input variable and provides the controller output. The  $K_p$ ,  $K_i$ ,  $K_d$  values are tuned using fuzzy logic. These three values are then given to the PID controller present at next stage. In the fuzzy control the membership functions are applied to the input variables.ie, fuzzufication is done during preliminary stage. It uses rule base to obtain the fuzzy output. The defuzzification is done to convert them to crisp values. The Fuzzy logic with engineering applications [15] and Neuro-fuzzy soft computing techniques [16] are studied for the implementation of the simulation work. The Figure 6. Shown below is the simulink block for Fuzzy PID Controller.

The Fuzzy logic controller for level control [17] and temperature control [18] of CSTR Process shows good performance. The fuzzy PID controller is compared with ZN PID for temperature control for different operating states shows reasonable set point tracking [19]. The PI controller for temperature control of CSTR process using fixed gain, optimized gain, adaptive gain and fuzzy PI is detailed [20]. The fuzzy PI controller [21] and fuzzy predictive model [22] control for stability of CSTR process is also detailed. The Fuzzy Inference System (FIS) for Fuzzy PID controller is shown in Figure 7.



Figure 7. Fuzzy Inference System



#### Figure 8. Response with Fuzzy PID Controller

The Error and change in error are chosen in the range between -80 to 80 and -1 to +1 respectively. The  $K_p$ ,  $K_i$ ,  $K_d$  values are choose in the range between 0.5 to 23, 30 to 105 and 0.0001 to 0.1 respectively. Five Triangular membership functions labeled Negative Big, Negative Medium, Zero, Positive Medium and Positive Big are chosen for each of the inputs and outputs respectively. Five rules are applied for the Fuzzy Inference System. The fuzzy PID

controller also shows better response than conventional PID Controller. The fuzzy controller has quick delay time. With higher delay time and settling time. They have no steady state error and overshoot. The  $K_p$ ,  $K_i$ ,  $K_d$  parameter range are specified in the fuzzy PID controller. The response of plant with Fuzzy PID controller response is shown in Figure 8.

For the CSTR plant with Fuzzy PID Controller the delay time, rise time and settling time are 0.0274 sec, 0.0929 sec and 0.1253 sec respectively.

## **MPC-PID** Controller



Figure 9. CSTR Simulink Block with MPC-PID Controller

The Proposed MPC-PID controller block diagram is given in Figure 9.The initial  $K_p$ ,  $K_i$ ,  $K_d$  values of the MPC based PID parameter are chosen as 350, 10, 0.1 respectively. The PID tuning parameters are found using Zeigler – Nichols method. For the CSTR plant with MPC-PID Controller the delay time, rise time and settling time are 0.0011 sec, 0.0035 sec and 0.0048 sec respectively. The response of the MPC-PID Controller is shown in the Figure 10.



Figure 10. Response with MPC-PID Controller

## **RESULTS & DISCUSSION**

The comparative responses of the CSTR model for different controllers are shown in Figure 11. The response of the CSTR model without controller is also given.



Figure 11. Comparative Response with various Controller

The inference obtained from the response is shown in Table 1

Types of Controller	Delay Time (t <sub>d</sub> ) in Sec.	Rise Time (t <sub>r</sub> ) in Sec.	Settling Time (t <sub>s</sub> ) in Sec.	Peak Overshoot (Mp) %
Conventional PID	0.0392	0.0738	0.0918	4.52
Model Predictive Controller	0.0976	0.3109	0.4782	0
Fuzzy PID	0.0274	0.0929	0.1253	0
Proposed MPC- PID	0.0011	0.0035	0.0048	0

## CONCLUSION

In this paper the performance of Proportional Integral Derivative (PID) Controller, Model Predictive Controller (MPC), Fuzzy-PID Controller and MPC based PID Controller performances are compared. It is found that both the settling time and rise time of MPC is higher compared to conventional PID and Fuzzy PID controller. There is peak overshoot in the response with Conventional PID controller. The MPC based PID has no overshoot with least rise time, delay time and settling time. Extensive simulation study on control strategies is carried out using MATLAB / Simulink software [23]. It is found that for the Non liner systems such as CSTR process the MPC based PID Controller's performance is better than PID and Fuzzy PID controllers.

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