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Design and Implementation of Controllers for a CSTR Process

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***Abstract*—Continuous Stirred Tank Reactor (CSTR) is the most important process which plays a significant role in process and chemical industries. Various process variables like temperature, concentration have to be controlled in this Process. The Proportional Integral Derivative (PID) controller has been used in industries for various process control applications. It provides control action to the discrepant values from the desired values in process output. Hence appropriate control action is needed to maintain this process in the desired condition. The PI controller yields an overshoot and long settling time, which exacerbate the process. Hence it is not well suited for many complex processes in industries. Model Predictive Control (MPC) is found to be very accurate and reliable in controlling the process variable. MPC has the ability to anticipate the future events and takes action accordingly. In this research work comparison of PI controller with MPC is made and the best controller for this CSTR temperature control process is to be selected**.

Index Terms— Continuous Stirred Tank Reactor, Proportional Integral Derivative, Overshoot, Long settling time, Model Predictive Control

I. Introduction

In any manufacturing process, where a chemical change is taking place, a chemical reactor is the heart of the plant. Depending on the mode of operation, reactors are classified as batch-wise or continuous. In batch-wise mode, reactants are charged at the beginning of the reaction and products are removed at the end of the reaction. In continuous stirred tank reactor (CSTR), reactants are continuously charged and products are continuously removed.

Chemical reaction systems are usually nonlinear dynamical systems.

Process control has become an integral part of process plants. An automatic controller must be able to facilitate the plant operation over a wide range of operating conditions. The proportional-integral (PI) or proportional-integral-derivative (PID) controllers are commonly used in many industrial control systems. These controllers are tuned with different tuning techniques to deliver satisfactory plant performance. However, specific control problems associated with the plant operations severely limit the performance of conventional controllers. The increasing complexity of plant operations together with tougher environmental regulations, rigorous safety codes and rapidly changing economic situations demand the need for more sophisticated process controllers.

Model Predictive Control (MPC) is an important advanced control technique which can be used for difficult multivariable control problems. The term MPC describes a class of computer control algorithms that control the future behaviour of the plant through the use of an explicit process model. At each control interval the MPC algorithm computes an open loop sequence of manipulated variable adjustments in order to optimize future plant behaviour. The first input in the optimal sequence is injected into the plant, and the plant entire optimization is repeated at subsequent control intervals.

The various MPC algorithms only differ amongst themselves in the model used to represent the process and the noises and the cost function to be minimized. This type of control is of an open nature within many works have been developed, being widely received by the academic world and by industry.

II. Description of CSTR process

The first principles model of the continuous stirred tank reactor and the operating data as specified in the Pottman and Seborg [1] has been used in the simulation studies. Highly nonlinear CSTR is common in chemical and petrochemical plants. The process considered for the simulation study is shown in Figure 2.1. Here an irreversible, exothermic chemical reaction A→ B occurs in constant volume reactor that is cooled by a single coolant stream. A feed material of composition CA0 enters the reactor at temperature T0, at a constant volumetric flow rate ‘q’. Product is withdrawn from the reactor at the same volumetric flow rate ‘q’. The mixing is assumed to be efficient enough to guarantee homogeneity of the liquid content within the reactor. In a jacketed CSTR the heat is added or removed by virtue of the difference between the jacket fluid and the reactor fluid. Often, the heat transfer fluid is pumped through the agitation nozzles that circulate the fluid through the jacket at a high velocity. The coolant flows at a flow rate of ‘qc’ and at a feed temperature Tc0. The exit temperature of the coolant fluid is Tc.

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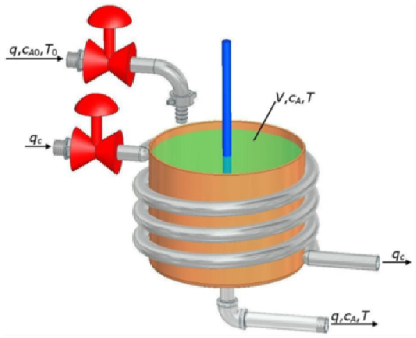

Figure 1. Schematic diagram of a continuous stirred tank reactor.

MATHEMATICAL MODELLING

The following assumptions are made to obtain the simplified modelling equations of an ideal CSTR:

2.2.1 Reactor Mass Balance

$$V\frac{dC_A}{dt} = q(C_{A0} - C_A) - Vr_A$$

Where, C_A is the product (effluent) concentration of component A in the reactor and r_A is the rate of reaction per unit volume. The Arrhenius expression is normally used for the rate of reaction. A first order reaction results in the following expression.

$$r_A = C_A K_0 e^{\left(-\frac{E}{RT}\right)}$$

Where, k_o is the reaction rate constant, E is the activation energy, R is the ideal gas constant and T is the reactor temperature on an absolute scale (Kelvin).

2.2.1 Reactor Energy Balance

$$\frac{dT}{dt} = \frac{q}{V}(T_0 - T) - \left(\frac{-\Delta H}{\rho C_p}\right) C_A K_0 e^{\left(-\frac{E}{RT}\right)} + \frac{\rho_c C_{pc}}{\rho C_p V}(q_c)\left[1 - \exp\left(\frac{-hA}{\rho_c C_{pc} q_c}\right)\right](T_{c0} - T)$$

Where, $(-\Delta H)$ is the heat of reaction, hA is the heat transfer coefficient, T_0 is the feed temperature and T_{c0} is the inlet coolant temperature.

2.2.1 Linearization

The nonlinear equations are linearized and cast into the state variable form as follows:

$$\dot{X} = AX + B\tilde{U}$$

$$Y = CX$$

Where matrices A and B represent the Jacobian matrices corresponding to the nominal values of the state variables and input variables, x̃, ũ and ỹ represent the deviation variables.

The output matrix is represented as C.

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

The Jacobian matrix A is given as,

The Jacobian matrix B is given by

The output matrix C is given by

TABLE I. STEADY STATE OPERATING DATA

Parameters	Symbols	Values
Product concentration	CA	0.0882 mol/l
Reactor temperature	T	441.2 K
Coolant flow rate	q c	100 l/min
Feed flow rate	q	100 l/min
Feed concentration	CA0	1 mol/l
Feed temperature	T0	350 K
Inlet coolant temperature	Tc0	350 K
CSTR volume	V	100 l
Heat transfer term	hA	7×10^5cal/(min K)
Reaction rate constant	k o	7.2×10^{10} min^{-1}
Activation energy term	E/R	1×10^4 K
Heat of reaction	$-\Delta H$	-2×10^5cal/mol
Liquid densities	ρ, ρ_c	1×10^3 g/l
Specific heat	C_p, C_{pc}	1 cal/(g K)

2.2.1 Steady State Analysis

The steady-state analysis shows the behaviour of the system in the steady-state and results in optimal working point in the sense of maximal effectiveness and concentration yield. Mathematical meaning of the steady-state is that derivatives with respect to time variable are equal to zero. (d(.)/dt = 0). The reactant and cooling heat must be equal in the steady-state, Hence, $Q_r = Q_c$, The equations (2.4) and (2.5) can be rewritten as,

$$a_1(T_0 - T) + a_2.k_1.c_A + a_3.q_c\left(1 - e^{\frac{a_4}{q_c}}\right)(T_{c0} - T) = 0$$

and results in relations for these heats Q_r and Q_c:

$$Q_r = a_2.k_1.c_A^s$$

$$Q_c = \left[a_1 + a_3.q_c\left(1 - e^{\frac{a_4}{q_c}}\right)\right]T^s - \left[a_1.T_0 + a_3.q_c\left(1 - e^{\frac{a_4}{q_c}}\right)\right]$$

If Q_r and Q_c are computed for various values of the temperature from 300K to 500K for operating point q = 100 l/min and q_c = 100 l/min, three steady-states are obtained as given in

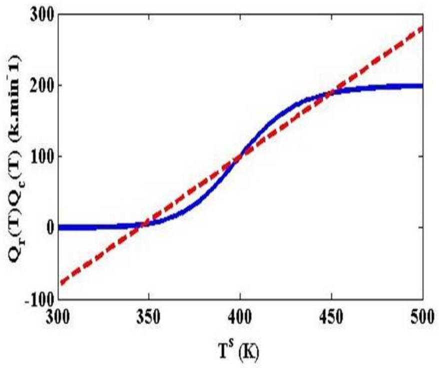


Figure 2. Heat balance inside the reactor

It can be clearly seen that, this system has two stable steady states (S_1 and S_2) and one unstable steady state (N_1). The steady-state values of the state variables in these points are:

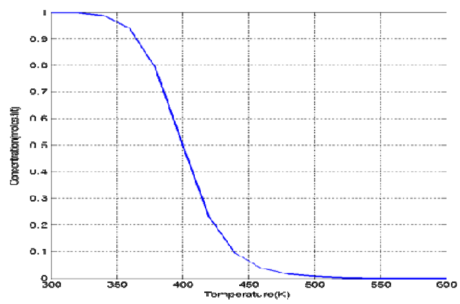
The steady-state model is described by the set of nonlinear functions

$$T^s = \frac{a_1.T_0 + a_2.k_1.c_A^s + a_3.q_c.T_0\left(1 - e^{\frac{a_4}{q_c}}\right)}{a_1 + a_3.q_c\left(1 - e^{\frac{a_4}{q_c}}\right)}$$

$$C_A^s = \frac{a_1.C_{A0}}{a_1 + k_1}$$

The graph between temperature vs. concentration is given in

Fig.2.3. From the Fig. 2 and Fig. 3



The nonlinear CSTR has been linearized at three stable operating points using the data given in Table 2.1. The operating points selected for the linear models are presented in Table 2.2. The eigen values, damping factor obtained at the respective operating points are presented in Table 2.3.

TABLE II. STEADY STATE OPERATING POINTS FOR THE IDEAL CSTR

Operating Point	Feed Flow (l/min)	Coolant Flow (l/m)	Concentration (mol/l)	Temperature (K)
1	103	97	0.0748	445.3
2	100	100	0.0882	441.2
3	97	103	0.1055	436.8

TABLE III. EIGEN VALUES AT THE THREE OPERATING POINTS OF THE IDEAL CSTR

Operating point	Eigen value
1	-3.0764±2.8533j
2	-1.9837±3.0573j
3	-1.0493±2.9064j

TABLE IV. RGA MATRICES AT THE THREE OPERATING POINTS

Operating Point	RGA
1	$\begin{bmatrix} -2.07638 & 3.076380 \\ 3.076380 & -2.07638 \end{bmatrix}$
2	$\begin{bmatrix} -2.269567 & 3.2695670 \\ 3.2695670 & -2.269567 \end{bmatrix}$
3	$\begin{bmatrix} -2.58955 & 3.58955 \\ 3.589550 & -2.58955 \end{bmatrix}$

From the above table, it can be inferred that the process is stable at all the operating points as the eigen values have negative real parts.

III. DESIGN OF GAIN SCHEDULING IMC BASED PID CONTROLLER

PID controllers have been used widely in the industry due to the fact that they have simple structures and they assure acceptable performance for the majority of the industrial processes. Because of their simple structures, PID controllers are easy to design, operate and maintain. Consequently, PID controllers earn their popularity among practitioners in the industry. Beginning with Zeigler and Nichols work, various parameter tuning methods for conventional PID controllers have been proposed. On the other hand, controlling MIMO systems is not straight forward due to the interactions between the channels. The interactive multivariable systems can be controlled by either of the following:

1. a multivariable or centralized MIMO controller or
2. a set of SISO controllers

2.2.1 Design of Decentralized Controllers

The decentralized controllers are designed for the local linear models at the three chosen operating points. Figure 3.1 shows the block diagram representation of decentralized control of an ideal CSTR. The manipulated variables are the feed flow rate (u_1) and coolant flow rate (u_2). The outputs are the effluent concentration (y_1) and reactor temperature (y_2).

The controller parameters of the two loops such as gc_1 and gc_2 are obtained using IMC based design procedure.

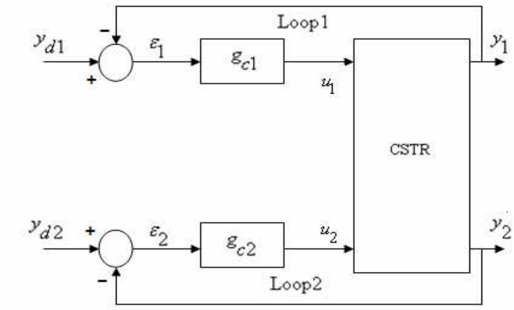


Figure 2. Block diagram representation of decentralized control scheme for the ideal CSTR

IMC Based tuning procedure for tuning the PI controller parameters IMC based tuning approach is taken up and the procedure proposed by Bequette (2003) yields the following controller parameters. The PI controller parameters at the three operating points are presented in Tables 3.2 and 3.3. It should be noted that the controller gain has been found to be a function of the filter parameter λ. The filter parameter values are chosen by trial and error method and the selection of the appropriate filter parameter value is decided by the performance index measured in the closed loop.

TABLE V. IMC BASED PI CONTROLLER SETTINGS FOR EFFLUENT CONCENTRATION CONTROL USING DECENTRALIZED CONTROL SCHEME

Operating point	K_c	K_i
q=103,q_c=97, C_A=0.0748,T=445.3	67.6114	193.9954
q=100,q_c=100, C_A=0.0882, T=441.2	17.8919	81.73940
q=97,q_c=103, C_A=0.1055, T=436.8	31.1897	104.75157

TABLE VI. IMC BASED PI CONTROLLER SETTINGS FOR REACTOR TEMPERATURE CONTROL USING DECENTRALIZED CONTROL SCHEME

Operating point	K_c	K_i
q=103,q_c=97, C_A=0.0748,T=445.3	0.0380	0.4148
q=100,q_c=100, C_A=0.0882,T=441.2	0.1136	0.3807
q=97,q_c=103, C_A=0.1055,T=436.8	0.0304	0.1385

2.2.2 Design of Decoupling Controllers

The Block diagram representation of decoupled control scheme for the multivariable control of CSTR is given in Fig. 3.2. The manipulated variables are the feed flow rate (u_1) and coolant flow rate (u_2). The outputs are the effluent concentration (y1) and reactor temperature (y2). In this work, the decouplers are designed using static decoupling method, to reduce the interaction brought in
by cross coupling. It consists of two steps: first, to design
the decouplers and second, to design the controllers for decoupled systems.

Operating point	g_{I1}	g_{I2}
q=103,q_c=97,C_A=0.0748, T=445.3	1.8496	0.8010
q=100,q_c=100,C_A=0.0882, T=441.2	1.7377	0.8290
q=97,q_c=103,C_A=0.1055, T=436.8	1.6291	0.8508

The static decouplers are designed as follows:

$$g_{I1} = \frac{-g_{12}(0)}{g_{11}(0)}$$

$$g_{I2} = \frac{-g_{21}(0)}{g_{22}(0)}$$

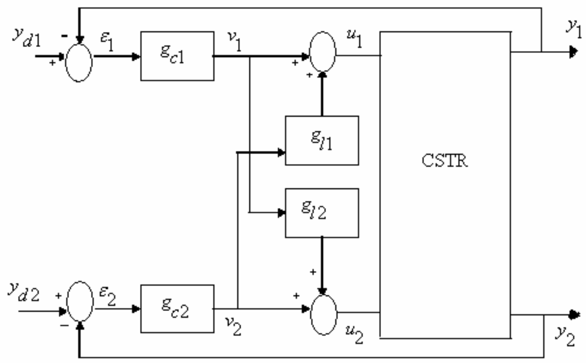


Figure 3. Block diagram representation of decoupled control scheme for the ideal CSTR

In the presence of decouplers, the multivariable system behaves like two independent loops, for which the controllers can be designed independently. The static decouplers at the three operating points are given in Table 3.4.

TABLE VII. STSTIC DECOUPLERS AT THE THREE OPERATING POINTS

Operating point	g_{I1}	g_{I2}
q=103,q_c=97, C_A=0.0748,T=445.3	1.8496	0.8010
q=100,q_c=100, C_A=0.0882,T=441.2	1.7377	0.8290
q=97,q_c=103, C_A=0.1055,T=436.8	1.6291	0.8508

The equations for the two loops of a 2 x 2 multivariable system including the decouplers are given by

$$y_1 = \left(g_{11} - \frac{g_{12}g_{21}}{g_{22}} \right) v_1$$

$$y_2 = \left(g_{22} - \frac{g_{12}g_{21}}{g_{11}} \right) v_2$$

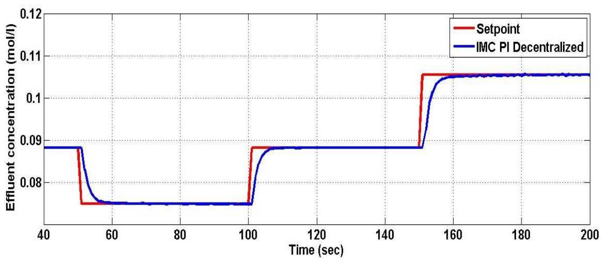
Substituting the values of gij in equations (3.12) and (3.13), the controllers are designed using IMC based tuning method. The PI controller parameters obtained at different operating points are given in Tables 3.5 and 3.6.

TABLE VIII. IMC BASED PI CONTROLLER SETTINGS FOR EFFLUENT CONCENTARATION CONTROL USING DECENTRALIZED CONTROL SCHEME

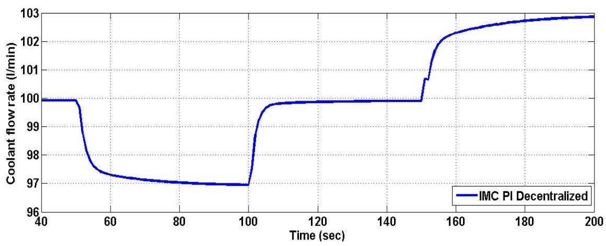
Operating point	K_c	K_i
q=103,q_c=97, C_A=0.0748,T=445.3	56.3117	161.3464
q=100,q_c=100, C_A=0.0882,T=441.2	35.7523	120.0243
q=97,q_c=103, C_A=0.1055,T=436.8	20.8270	95.0907

TABLE IX. IMC BASED PI CONTROLLER SETTINGS FOR REACTOR TEMPERATURE CONTROL USING DECENTRALIZED CONTROL SCHEME

Operating point	K_c	K_i
q=103,q_c=97, C_A=0.0748,T=445.3	0.01730	0.64660
q=100,q_c=100, C_A=0.0882,T=441.2	0.01509	0.18498
q=97,q_c=103, C_A=0.1055,T=436.8	0.01010	0.31190



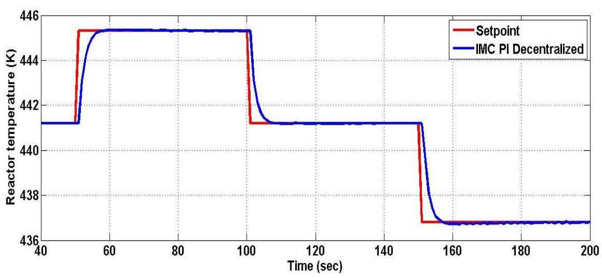
(a) Variations in effluent concentration



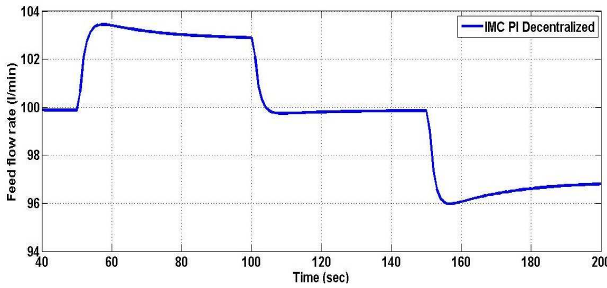
(b) Variations in coolant flow rate

(c)

Figure 3.1 Servo response for effluent concentration control using decentralized control scheme

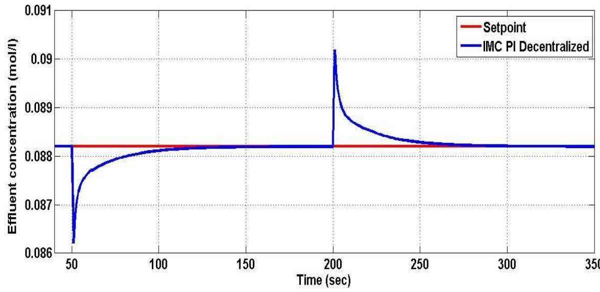


(a) Variations in reactor temperature

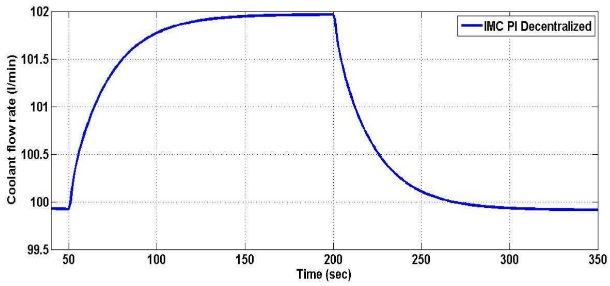


(b) Variations in feed flow rate

Figure 3.2 Servo response for reactor temperature control using decentralized control scheme

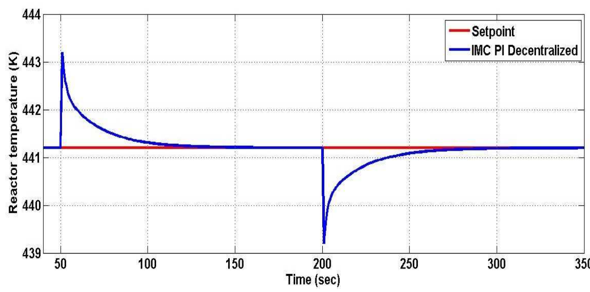


(a) Variations in effluent concentration

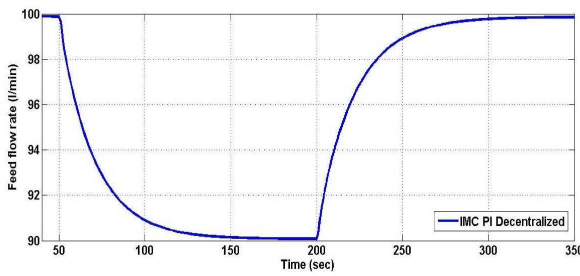


(b) Variations in coolant flow rate

Figure 3.3 Regulatory response for effluent concentration control using decentralized control scheme



(a) Variations in reactor temperature



(b) Variations in feed flow rate

Figure 3.4 Regulatory response for reactor temperature control using decentralized control scheme

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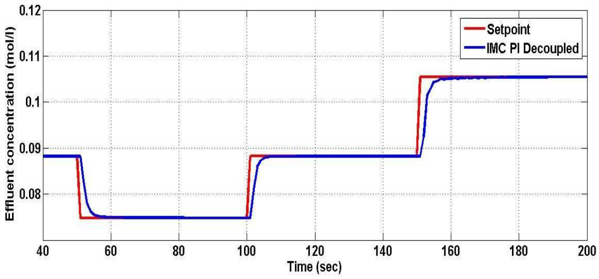
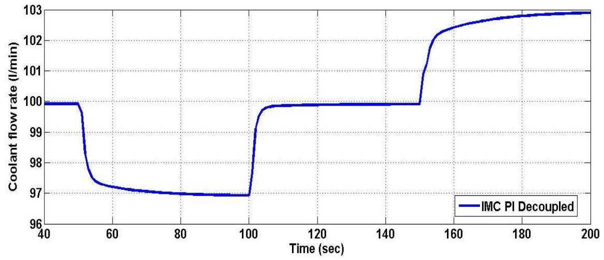
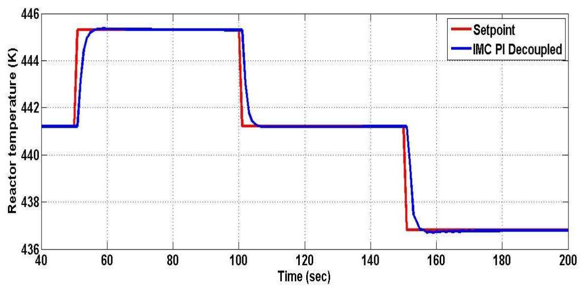


(a) Variations in effluent concentration

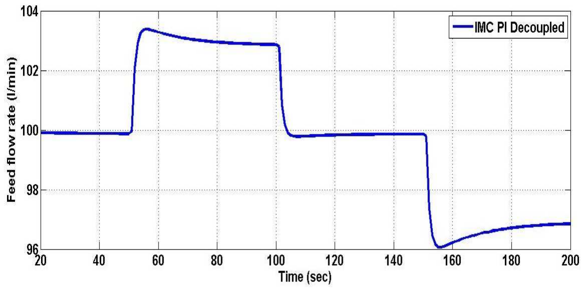


(b) Variations in coolant flow rate

Figure 3.5 Servo response for effluent concentration control using decoupled control scheme

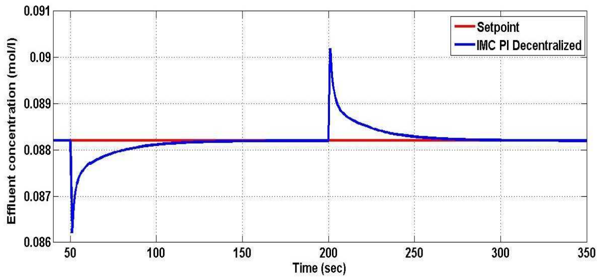


(a)Variations in reactor temperature

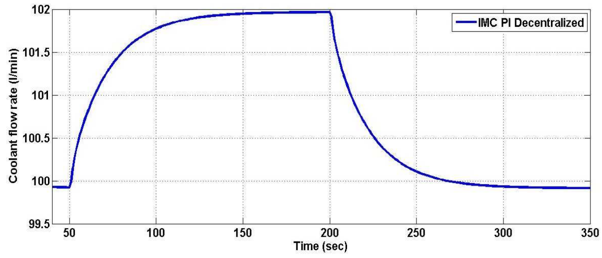


(c) Variations in feed flow rate

Figure 3.6 Servo response for reactor temperature control using decoupled control scheme

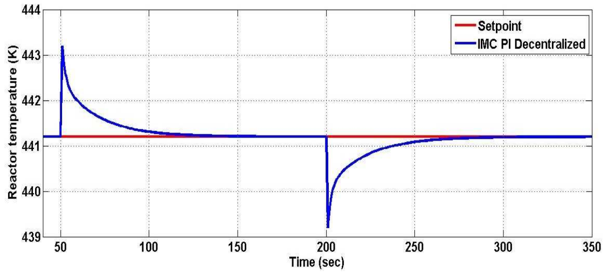


(a) Variations in effluent concentration

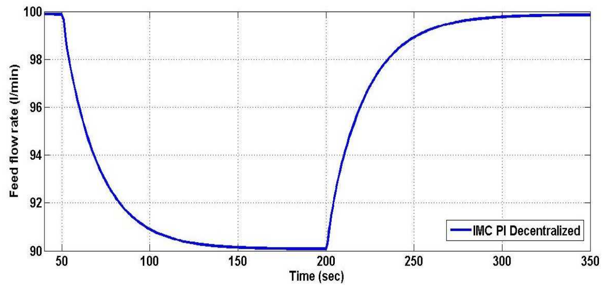


(b) Variations in coolant flow rate

Figure 3.7 Regulatory response for effluent concentration control using decoupled control scheme



(a) Variations in reactor temperature



(b) Variations in feed flow rate

Figure 3.8 Regulatory response for reactor temperature control using decoupled control scheme

DESIGN OF MODEL PREDICTIVE CONTROLLER

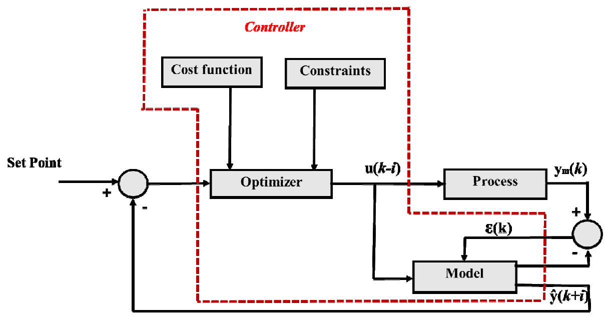


Fig. 4.1. Model Predictive Control block diagram

DESIGN CONTROLLER

This shows how to design a model predictive controller in Simulink. We have built a nonlinear plant model in Simulink. We want to design an MPC controller at a specific equilibrium operating point. This shows that model-based design workflow. We linearized the plant at the desired operating point, design the MPC controller and validate it with nonlinear simulation. It includes steps as per state space model are follows:

1. Define the plant in discrete form.
2. Obtain the state space model of the plant.
3. Define prediction horizon and control horizon.
4. Predict future output and control effort based on previous input, output and control effort.
5. Verify the robustness of the controller in presence of uncertainties in the plant model.
6. Verification of the performance of controller with different weighting functions
7. Verification of the performance of controller with constraints on the control effort.
8. Evaluation of performance of controller with different prediction horizons.

4.4.1 SELECTION OF DESIGN AND TUNING PARAMETERS

A number of design parameters must be specified in order to design an MPC system. In this section, we consider key design issues and recommended values for the parameters. Several design parameters can also be used to tune the MPC controller.

1. N and Δt

These parameters should be selected so that N Δt > open-loop settling time. Typical

Values of N:

$$30 < N < 120 \quad (4.3)$$

2. Prediction Horizon, P

Increasing P results in less aggressive control action

$$\text{Set } P = N + M \quad (4.4)$$

3. Control Horizon, M

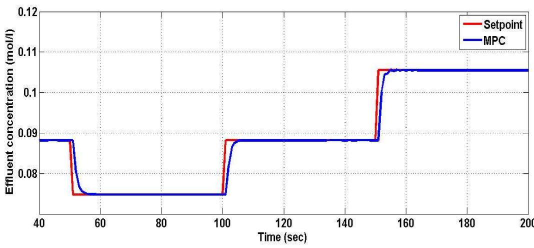
Increasing M makes the controller more aggressive and increases computational

Effort, typically:

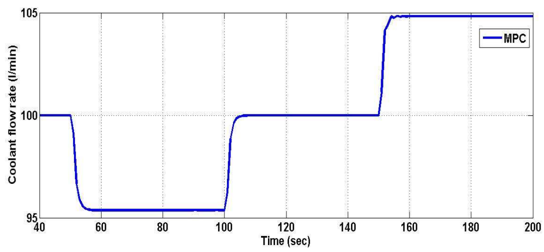
$$1 < M < 20 \quad (4.5)$$

4. Weighting matrices Q and R

Diagonal matrices with largest elements corresponding to most important variables



(a) Variations in effluent concentration



(b) Variations in feed flow rate

Figure 3.6 Servo response for reactor temperature control using decoupled control scheme

The closed loop simulation studies are carried out on the CSTR model with decentralized control, decoupled control using IMC tuned PI and MPC controller settings. In order to assess the tracking capability of the designed controllers, set point variation in effluent concentration is given and the responses are presented in the following Fig. 5.1.The set point variations in the reactor temperature is given and the responses are displayed in Fig. 5.2.

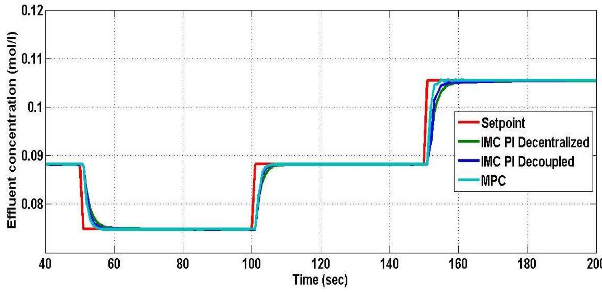


Fig. 5.1 Servo response for Effluent concentration

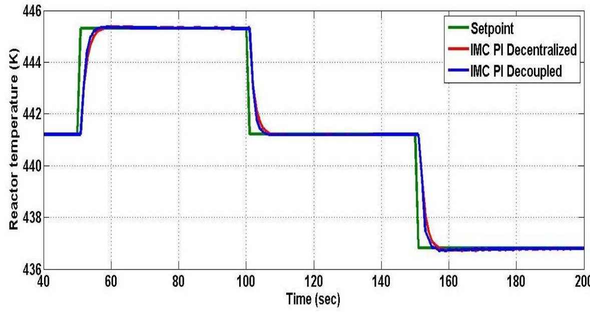


Fig. 4.5 Servo response for Reactor temperature

Table 5.1 provides the performance measures for servoproblem and Table 5.2 provides the performance measures for regulatory problem using decentralized control scheme. Table 5.3 provides the performance measures for servo problem and Table 5.4 provides the performance measures for regulatory problem using decoupled controllers. The comparison of the performance measures such as IAE and ISE values between the decentralized and decoupled control schemes show that the performance is better with the decoupled controllers than with the decentralized controllers.

PERFORMANCE ANALYSIS OF THE CONTROLLERS

Table 5.1 Performance measures for servo problem (Effluent Concentration)

OP	**Decentralized control**		**Decoupled control**		**MPC**	
	IAE	**ISE**	**IAE**	**ISE**	**IAE**	**ISE**
1	**0.009021**	**3.260x 10^{-6}**	**0.004623**	**1.972x 10-6**	**0.0003562**	**2.420x10 -7**
2	**0.008688**	**3.260x 10^{-6}**	**0.004530**	**1.656x 10-6**	**0.0003998**	**2.471x10 -7**
3	**0.010130**	**3.632x 10^{-6}**	**0.005424**	**1.979x 10^{-6}**	**0.0006482**	**2.948x10 -7**

Table 5.2 Performance measures for regulatory problem (Effluent Concentration)

OP	Decentralized control		Decoupled control		MPC	
	IAE	ISE	IAE	ISE	IAE	ISE
1	0.009558	3.262×10^{-6}	0.00462	1.959x 10-6	0.0004422	2.503x10-7
2	0.009097	3.202×10^{-6}	0.00455	1.642x 10-6	0.0005577	3.049x10-7
3	0.010930	3.649×10^{-6}	0.00562	2.009×10^{-6}	0.0006633	4.897x10-7

Table 5.3 Performance measures for servo problem (Reactor Temperature)

OP	Decentralized control		Decoupled control		MPC	
	IAE	ISE	IAE	ISE	IAE	ISE
1	19.88	18.06	5.344	4.500	1.744	1.169
2	21.85	20.72	4.887	4.125	1.408	1.175
3	23.54	22.28	9.096	7.500	2.495	2.065

Table 5.4 Performance measures for regulatory problem (Reactor Temperature)

OP	Decentralized control		Decoupled control		MPC	
	IAE	ISE	IAE	ISE	IAE	ISE
1	4.975	1.129	1.336	0.2813	0.3109	0.0843
2	5.471	1.295	1.222	0.2579	0.3548	0.1169
3	5.898	1.392	2.274	0.4688	0.2279	0.0825

CONCLUSION

An improved MPC (Model Predictive Control) technique is presented and it has been shown to be a simple and efficient algorithm for multivariable control. Simulation results for a continuous fermenter demonstrate the superiority of the MPC compared with the original IMC-PID. MPC maintains a high level of closed-loop performance in both servo and regulatory problems, despite appreciable variations in process dynamics and strong interactions between the manipulated variables. In this work we do not attempt to study the influence of tuning constant sample time on closed-loop performance for the controllers in the multivariable case. In the example, sample time fixed as the inverse of the process gain matrix.

It is clear that to improve the performance of the controller, it is necessary to consider the tuning constant in optimization of the IAE and ISE criterion. The qualitative and quantitative comparison of the closed loop simulation studies conducted on the CSTR using decentralized ,decoupled and MPC control schemes reveal that the MPC control scheme provides better set point tracking and load disturbance rejection than others control scheme.

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