Application of LQR and MPC on Distillation and Batch Crystallization Process

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By

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CERTIFICATE

This is to certified that the thesis entitled **"Application of LQR and MPC on Distillation and Batch Crystallization Process"** submitted by **Mr. Sagar C. Bandpatte (211CH1256)** to National Institute of Technology, Rourkela, India for the award of degree of **Master of Technology** in engineering, is a bonafide record of investigation carried out by him in Department of Chemical Engineering, under the guidance of **Dr. M. Kundu**. The thesis is up to the standard of fulfillment of M. Tech degree as prescribed by regulation of this institute.

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NOMENCLATURES

A   Total heat transfer surface area (μm^2)

b   Nucleation rate exponent

B   Nucleation rate

C   Solution concentration (g solute g solvent^{-1})

C_m Metastable concentration (g solute g solvent^{-1})

C_p Heat capacity of the solution (J kg^{-1} K^{-1})

C_{pi} Heat capacity of cooling water (J kg^{-1} K^{-1})

Cs Saturation concentration (g solute g solvent^{-1})

E   Activation energy

f   Population density of crystals (no. of crystals μm^{-1} gsolvent^{-1})

F_j Cooling water flow rate (μm^3 s^{-1})

g   Growth rate exponent

G   Growth rate (μm s^{-1})

ΔH_c Heat of crystallization (J kg^{-1})

k_b Birth rate coefficient (s^{-1} μm^{-3})

k_g Growth rate coefficient (μm s^{-1})

k_v Volumetric shape factor

L   Characteristic crystal length (μm)

R   Gas constant

M   Mass of solvent in the crystallizer (kg)

t   Time (sec)

T	Reactor temperature (K)
T_j	Cooling jacket temperature (K)
T_{jsp}	Set point of the jacket temperature (K)
U	Overall heat transfer coefficient (J μm^{-2} s^{-1} K^{-1})
V_j	Jacket volume (µm3)

GREEK SYMBOLS

ρ	Density of crystals (g μm^{-3})
ρ_j	Density of cooling water (kg μm^{-3})
μ_0	Zeroth moment of the CSD (no. of crystals g $solvent^{-1}$)
μ_1	First moment of the CSD (µm g $solvent^{-1}$)
μ_2	Second moment of the CSD (μm^2 g $solvent^{-1}$)
μ_3	Third moment of the CSD (μm^3 g $solvent^{-1}$)

Superscript

n	Nucleation
s	Seeded crystal

ABSTRACT

As the widespread use of a batch crystallization process in many industries, finding an optimal operating condition and effective control strategy are significant for improving product quality and downstream processing. To achieve these, an accurate model is required to predict the process behavior and to design controller. However, due to unknown disturbances and batch-to batch variations, the kinetic parameters obtained from experimental study may not represent the real process resulting in poor control and estimation performances. In this work, improvement of batch crystallization control under uncertain kinetic parameters has been proposed. Model predictive controller (MPC) is used for optimal control of distillation and batch crystallization process. Feedback control strategy is found out using LQR technique. A Kalman filter has been designed to estimate uncertain parameters and immeasurable states. A MPC TOOLBOX in MATLAB software is used to obtain desired crystal size distribution (CSD).

Keywords: Batch Crystallization, Linear Quadratic Regulator, Model Predictive Control, Kalman Filter

CONTENTS

CHAPTER 1

INTRODUCTION

CHAPTER 1

INTRODUCTION

Batch crystallization is widely used process in chemical, food and pharmaceutical industries for separation and purification of product. The driving force for the process is supersaturation. Supersaturation can be achieved either by cooling the solution below its saturation temperature, evaporation of solution or salting of solute to change the solute solubility. Out of these, cooling technology is most commonly use due to its ease of operation and dependence of solute solubility on temperature. Once the supersaturation is achieved, nucleation and subsequent crystal growth takes place. The growth of crystal is effectively controlled by maintaining crystal size distribution (CSD).

To control CSD, model predictive controller (MPC) is most widely used with crystallizer process. Traditional control work on principle of change in output target of system i.e. control action takes place after the disturbances in system whereas MPC set the control action before change in output target. This ability of controller helps in achieving smoother and easier control on process. Figure 1.1 shows the basic structure of MPC.
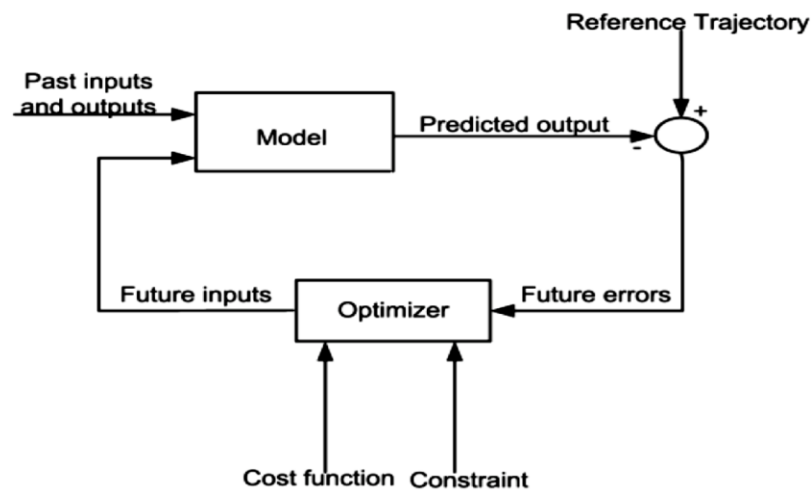
Figure 1.1: Basic Structure of MPC

For the batch crystallizer, all the state variables are not measurable. Only temperature and concentration of process can be measured. To measure un-measured state variables, Kalman

filter is associated with MPC to control crystallizer in term of crystal moments. The Kalman filter also called as a linear quadratic estimation (LQE). It is an algorithm based on two stages which takes series of observed measurement containing noise and other inaccuracies to estimate unmeasured state variables. In the first step, it estimates current state variables containing inaccuracies and updates takes place in second steps. It is found that estimated state variables of Kalman Filter are more precise than those based on a single measurement alone. In this present work, Kalman Filter is used to estimate unmeasured crystal moment to control desired crystal size distribution.

The optimal control of a process generally refers to operating a process at minimum cost. The case where linear differential equations represent system dynamics and a quadratic functional represents cost function then the problem of controlling system at optimal control is solved by linear quadratic regulator (LQR) technique. It is just finding a proper way of feedback control strategy which reduces a tedious work of system engineer.

1.1 Objective of Thesis

The aim of this thesis is to control the CSD of industrial batch crystallizer using nonlinear model based control approach.

The scope of the present work includes

- Modeling and dynamic simulation of batch crystallization process.
- Design of optimal control for CSD of industrial batch crystallizer.
- Design of model predictive controller (MPC) for CSD of industrial batch crystallizer.

1.2 Organization of Thesis

Chapter 1: Present chapter of the thesis provides the brief introduction of batch crystallization process, overview on Linear Quadratic Control (LQR) and MPC. The objective of the thesis with chapter layout is also presented in this chapter.

Chapter 2: Theory of batch crystallization process, its modeling and open loop simulations are the traits of the present chapter.

Chapter 3: This very chapter renders theoretical postulations about state feedback control with a special mention to LQR scheme and its implementation in batch crystallization process. This chapter also provides a brief theory on state estimator, specifically the Kalman filter.

Chapter 4: It deals with model predictive controller, its complete algorithm and implementation of MPC for SISO and MIMO model.

Chapter 5: This chapter presents the closed loop simulation of batch crystallization process using MPC and Kalman filter and ensures perfect CSD.

Chapter 6: In an ending note this chapter concludes the thesis with future recommendation.

CHAPTER 2

BATCH CRYSTALLIZATION

CHAPTER 2

BATCH CRYSTALLIZATION

Crystallization is nothing but separation of solute from solvent in solid state where molecules are essentially arranged in regular pattern. The major advantages of crystallizer process are that it is a single stage separation process giving high purity, operated at relatively mild condition and requires low level of energy consumption. Batch crystallization is mostly used when frequent change in process parameter is required, volume of production is very low or requirement of isolated system e.g. Safety and sterility. [1]

2.1 Principles of Crystallization

Solute can be separated from vapors, solution or melt. For removal of solute from solution, mostly crystallization is used. The key variable for the process is supersaturation which largely affects the product quality. The product quality is determined in terms of its crystal shape, CSD, its purity and polymorphic state.

In crystallization, supersaturation is defined as the difference between solubility of solute at normal condition to saturation state. Solubility is the equilibrium concentration of the solute in the solvent at the given process conditions.

$$\Delta C = C\,(T) - C^*(T) \tag{2.1}$$

Where C is the solute concentration; T is the temperature; C^* is the saturation concentration of solute, namely the solubility. Greater the difference, higher is the degree of supersaturation.
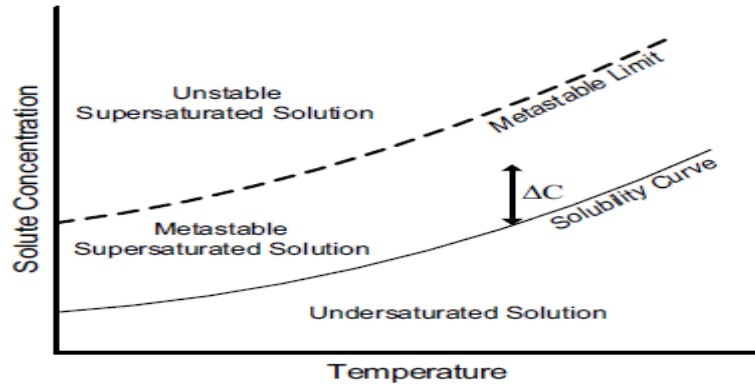
Figure 2.1: The Phase Diagram

A systematic representation of control mechanism of crystallizer is shown in figure 2.1. It is divided in three zones namely Undersaturated, Metastable supersaturated and unstable supersaturated zone.

    1. Undersaturated zone: - regions where solute are completely soluble making the crystallization process impossible.

    2. Metastable supersaturated zone: - a region of supersaturation containing growth of crystal in absence of spontaneous nucleation of solution.

    3. Unstable supersaturated zone: - spontaneous nucleation zone.

Crystallization process is operated by controlling desired supersaturation state. Process is governed by kinetics of crystal growth, nucleation and agglomeration. Agglomeration and spontaneous nucleation are undesirable conditions for crystallization. In most of the practice, a known amount of crystals are injected in crystallizer along with feed to startup initial kinetics of crystallization but done only at a starting of process. The process is then called as seeded batch crystallization. Supersaturation can be achieved by lowering the solubility of solute through evaporation of solvent, addition of antisolvent or cooling the solution. [1]

2.2 State of Art in Control of Batch Crystallizers

Because of industrial competitions and increasing demand of high quality product, various interesting technologies are developed in this field. Depending on these technologies, number of

controlling approaches has been proposed which are broadly classified in to 'model based controlled approach' and 'direct design approach'. [1]

2.2.1 The Direct Design Approach

In most of the practice, the solute concentration window lies in region of metastable zone. This operating policy is maintained by feedback control on solute concentration. The main aim is to follow the concentration-temperature mechanism in between metastable zone. The principle idea of direct design approach is given in figure 2.2.
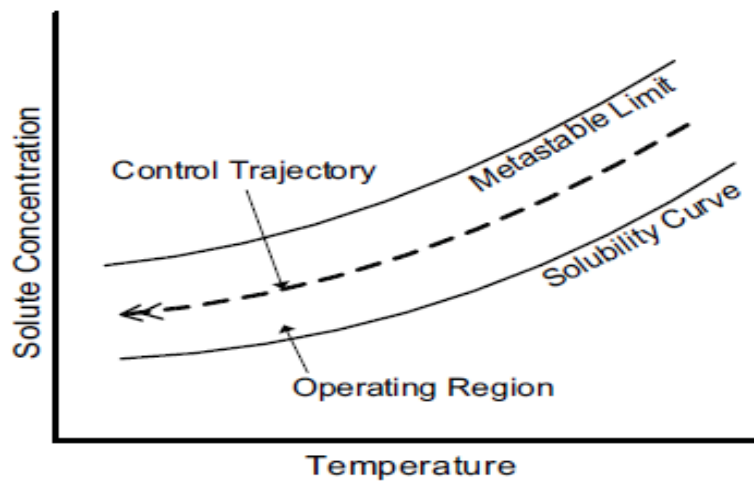
Figure 2.2: The Direct Design Approach

This approach avoids the spontaneous nucleation and processing time in crystallization. The solute concentration is measured by spectroscopic instruments with respect to temperature. The knowledge of thermodynamics is also essential to maintain desired trajectory of solute concentration.

The feedback strategy of solute solubility curve is given by mathematical equation

$$C^*(T) \; = \; C - \Delta C \tag{2.2}$$

Where ΔC is a predefined supersaturation profile within the metastable zone is, C is the solute concentration; T is the temperature.

The temperature setpoint of process is calculated by solving above mathematical expression. Predefined supersaturation profile is depending on required product quality and not a function of time. [2]

2.2.2 The Model Based Control Approach

The initial framework of model is prepared from material and energy balance. Solid balance is given by probability balance equation (PBE). PBE gives an effect of crystallization kinetics on CSD. Model based control is difficult to handle due to distributed nature of PBE. To solve this problem, PBE is approximated by considering different moments of crystal. Crystal moments normally consider various physical properties of crystal growth such as number, length, area and volume. But moment model does not give complete knowledge of CSD. Production of crystal having a large mean crystal size and a narrow size distribution is the prime objective of model based control approach.

Initially open loop control was used for model based control approach but it is highly sensitive to batch to batch variation and enables to handle process uncertainty. This is mainly due to uncertainty associated with crystallization kinetics. So an effective control strategy is online control of optimum control policy during batch run. The systematic representation of optimum operating policy is given in figure 2.3. An observer is combined with MPC to measure the unmeasured parameters of process. [2]
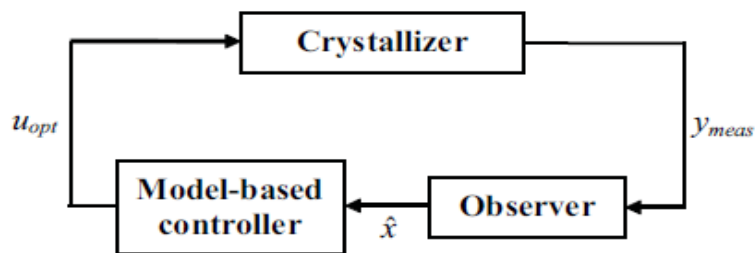
Figure 2.3: The Output Feedback Model Based Control Approach

2.3 Literature Review on Batch Crystallization Process

Producing a crystalline product with a large mean crystal size and a narrow size distribution is traditionally the prime objective in model-based control of batch crystallizers (Rawlings et al. 1993).[3]Matthews and Rawlings (1998) identified a model for batch cooling crystallization of an organic photochemical heptanes system; model parameter uncertainties were minimized by applying different optimal experiment design techniques.[4]Chung et al. (1999) performed a comprehensive study on dynamic optimization of the seed distribution in a batch cooling crystallizer.[5]Nowee et al. (2007) presented a model for a seeded batch cooling crystallization process, in which crystal dissolution took place. The nonlinear process model was utilized to optimize the temperature profile and the initial seed size distribution. Experimental implementation of the off-line optimized profiles resulted in the desired crystal mean size. [6]

Among the numerous attempts to perform output feedback control of batch crystallizers, the work of Chang and Epstein (1987) can be recognized as a pioneering study.[7] They incorporated a feedback mechanism into the optimal control scheme presented in their earlier work (Chang and Epstein 1982). The application of the feedback control strategy for a batch crystallizer was then demonstrated by simulation studies.[8]Eaton and Rawlings (1990) investigated feedback control of several constrained nonlinear multivariable chemical processes, including a batch cooling crystallizer, using nonlinear estimation and optimal control strategies.[9]Zhang and Rohani(2003) developed an online control strategy for optimal control of a seeded batch cooling crystallizer. An extended Kalman filter was employed to estimate the unmeasurable state variables and to account for plant model mismatch as well as process uncertainties. The simulation results showed notable improvements in the product CSD in comparison with that obtained by open-loop implementation of the optimal cooling policy.[10]

2.4 Model Development

Model-based control approach depends on dynamic relations between inputs and outputs of physical system. These dynamics relations of batch crystallizer depend not only on process variables such as concentration and temperature, but also are a function of certain physical properties of crystals. This makes the system distributed in nature which is dependent on crystal

growth, nucleation, breakage, agglomeration and dissolution. The present work depends on first-principle modeling approach having material and energy balances with empirical equations of crystallization kinetics. Distributed nature of PBE is converted to ordinary set of differential equations by considering method of moment.[1]

2.4.1 Population Balance

Properties of crystalline products are depending on internal crystal states, e.g. size and shape. To avoid the high computational effort of detailed mechanistic models, one internal coordinate system, namely the crystal size is used to describe the characteristics of a crystalline material.

PBE provides distributed nature of crystal formed by calculating the number of crystals in a crystallizer. PBE is a well developed mathematical frame work for dynamic modeling of particle size distribution in numerous particulate systems such as polymerization, precipitation, etc.

In well-mixed batch crystallizer, PBE can be expressed in terms of the internal coordinates and crystallization kinetics containing nucleation and crystal growth. The one-dimensional PBE for a crystallization process undergoing nucleation and crystal growth can be written as

$$\frac{\partial(V(t)n(L,t))}{\partial t} + V(t)\frac{\partial(G(L,t)n(L,t))}{\partial L} =$$
$$V(t)B(L,t) + \left[\sum_{k=1}^{N_i}\varphi v_{,in,k}(t)_{in,k}(L,t) - \sum_{l=1}^{N_0}\varphi v_{,out,l}(t)h_{cf}(L)\,n(L,t)\right] \tag{2.3}$$

where $n(L,t)$ is the number density function $(1/m^4)$; t is the time (s); L is the internal coordinate, via the crystal characteristic size (m); $G(L,t)$ is the crystal growth rate (m/s); $B(L,t)$ is the nucleation rate $(1/m^4 s)$; $V(t)$ is the crystallizer volume (m^3); N_i and N_0 are the number of inlet and outlet streams, respectively; $\varphi v(t)$ is the volumetric flow rate (m^3/s); $h_{cf}(L)$ is the crystal classification function. The initial condition of the PBE is

$$n(L,t_0) = n_0(L) \tag{2.4}$$

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Equation (2.4) represents either a clear solution with no crystal population or the size distribution of seed crystals. In addition, the boundary condition of the PBE is expressed as

$$n\,(L_0, t) = 0 \quad if\ G(L, t) \geq 0, \quad \forall L. \tag{2.5}$$

Equation (2.5) implies that there exist no crystals with size L_0.

To avoid the occurrence of undesirable phenomena such as primary nucleation and agglomeration, mostly a seeded batch crystallizer is used. For seeded batch crystallizer, PBE is written in form of partial differential equation,

$$\frac{\partial\big(V\,(t)n(L, t)\big)}{\partial t} + V\,(t)\frac{\partial\big(G(L, t)n(L, t)\big)}{\partial L} =$$
$$\left[\sum_{k=1}^{Ni} \varphi v_{,in,k}(t)_{in,k}(L, t) - \sum_{l=1}^{No} \varphi v_{,out,l}(t)h_{cf}(L)\,n(L, t)\right] \tag{2.6}$$

With the left boundary condition,

$$n(L_0, t) = \frac{B_0(t)}{G(t)_{L0}} \tag{2.7}$$

Where $B_0(t)$ denotes the total nucleation rate of crystals of infinitesimal size ($1/m^3s$).[1]

2.4.2 Mass and Energy Balances

PBE indicates that crystal size distribution (CSD) is depend mainly upon rates of crystal growth and nucleation which in turn depend upon chemical potential. The chemical potential difference is expressed as

$$\Delta\mu_c = kT\ln(\frac{C(T)}{C*(T)}) \tag{2.8}$$

Where $\Delta\mu$ is the change in chemical potential; C is the solute concentration (*wt.%*); C^* is the saturation concentration (*wt.%*); T is the solution temperature (*K*); k is the Boltzmann constant (*J/K*). supersaturation is normally used as a chemical potential for crystallization process. It is defined as

$$\Delta C = C(T) - C^*(T) \tag{2.9}$$

Supersaturation is depending on solute concentration and temperature, thus mass and energy balances must always be coupled with PBE. [1]

2.4.2.1 Energy Balance

For energy balance, it is assumed that potential energy, kinetic energy and shaft work are assumed to be negligible. The energy balance in form of enthalpy balance is given as

$$\frac{dH(t)}{dt} = \sum_{k=1}^{Ni} \emptyset H_{,in,k}(t) - \sum_{l=1}^{No} \emptyset H_{,in,l}(t) - \emptyset H, v_{,out}(t) + Q(t) \tag{2.10}$$

With the initial condition

$$H(t_0) = H_0. \tag{2.11}$$

In the energy balance, $H(t)$ is the enthalpy (*J*); $\emptyset H(t)$ and $\emptyset H_v(t)$ are the enthalpies of solution and vapor streams, respectively (*J/s*); $Q(t)$ is the net rate of heat addition to the system (*J/s*).

2.4.2.2 Mass Balance

The component mass balance in liquid phase for the solvent is

$$\frac{dm_{L,solvent}(t)}{dt} = \sum_{k=1}^{N_t} \emptyset_{m,L,solvent,in,k}(t) - \sum_{l=1}^{N_0} \emptyset_{m,L,solvent,out,k}(t)$$

$$-\emptyset_{m,v,solvent,out}(t) + M_{solvent} \sum_{q=1}^{N_s} V_{s,solvent,q}[\emptyset_{mol,grow,q}(t) + \emptyset_{mol,necl,q}(t)] \tag{2.12}$$

With the initial condition

$$m_{L,solvent}(t_0) = m_{L,solvent,0} \tag{2.13}$$

In equation (2.12), $m_{L,solvent}(t)$ is the mass of solvent (kg); $\emptyset_{m,L,solvent}(t)$ and $\emptyset_{m,v,solvent}(t)$ are the solvent mass flow rates in liquid and vapor phases, respectively (kg/s); $M_{solvent}$ is the solvent molecular weight ($kg/mole$); $V_{s,solvent}$ is the solvent stoichiometric coefficients in the solid phase; N_s is the number of solid phases; $\emptyset_{mol,grow}(t)$ and $\emptyset_{mol,necl}(t)$ are the molar flows of crystal growth and nucleation ($mole/s$), respectively.

It is assumed that vapor stream is free of crystalline material and solute, and then liquid phase component mass balance for the solute is given as

$$\frac{dm_{L,solute}(t)}{dt} =$$

$$\sum_{k=1}^{N_t} \emptyset_{m,L,solute,in,k}(t) - \sum_{l=1}^{N_0} \emptyset_{m,L,solute,out,l}(t) + M_{solute} \sum_{q=1}^{N_s} V_{s,solute,q}[\emptyset_{mol,grow,q}(t) +$$

$$\emptyset_{mol,necl,q}(t)] \tag{2.14}$$

With the initial condition,

$$m_{L,solute}(t_0) = m_{L,solute,0} \tag{2.15}$$

In equation (2.14), $m_{L,solute}(t)$ is the mass of solute (kg); $\emptyset_{m,L,solute}(t)$ is the solute mass flow rate in the liquid phase (kg/s); M_{solute} is the solute molecular weight ($kg/mole$); $V_{s,solute}$ is the solute stoichiometric coefficient in the solid phase.

The component mass balances and population balance are coupled by the molar flows of crystal growth and nucleation,

$$\emptyset_{mol,grow}(t) = -\frac{k_v \rho_s}{M_{solute}} V(t) \int_{L=0}^{\infty} \frac{\partial(G(L,t)n(L,t))}{\partial L} L^3 dL \tag{2.16}$$

$$\emptyset_{mol,nucl}(t) = \frac{k_v \rho_s}{M_{solute}} V(t) \int_{L=0}^{\infty} B(L,t) L^3 dL \tag{2.17}$$

Where k_v is the volume shape factor of the crystalline material; ρ_s is the density of the crystalline material (kg/m^3). Expressions for the rates of crystal growth and nucleation follow from the kinetic models. [1]

2.4.3 Crystallization Kinetics

Dynamic evolution of crystals population under the condition supersaturation is given by Crystallization kinetics. Growth and nucleation are two important parameters for favorable transition of the solute to the requisite quality solid.

2.4.3.1 Nucleation

Process of formation of nuclei through clusters of solute molecules is called as nucleation. It is broadly categorized into primary nucleation and secondary nucleation. Figure 2.4 shows the complete nucleation phenomenon.
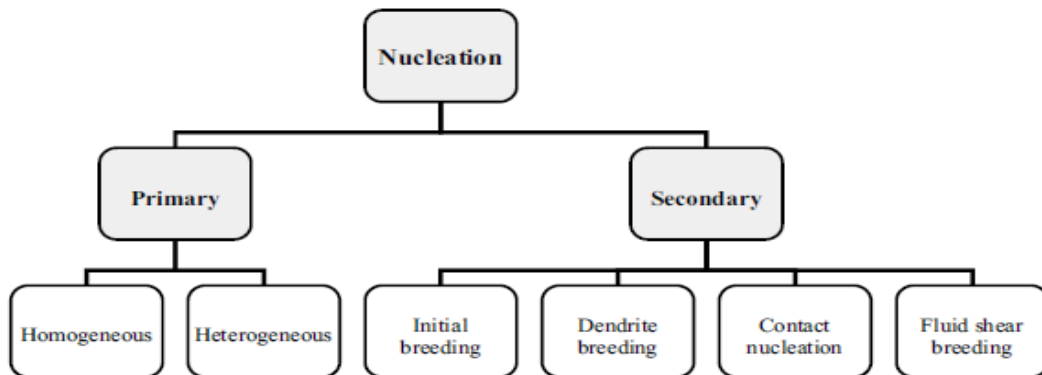

Figure 2.4: Mechanisms of Crystal Nucleation

Primary nucleation mechanisms are again of two type's homogeneous and heterogeneous nucleation. Homogeneous nucleation occurs in pure solution in absence of surface through the formation of clusters of solute whereas heterogeneous nucleation is the result of present

impurity. Primary nucleation requires high levels of supersaturation than secondary nucleation. There is variety of secondary nucleation mechanisms like Initial breeding, dendrite breeding, and fluid shear breeding and contact nucleation. Initial breeding occurs due to adherence of crystalline dust fragments to the surface of dry seed crystals. Breakage of growing crystal phase due to hydrodynamic shear forces and breakage of dendrites from the parent crystals lead to fluid shear breeding and dendrite breeding respectively. Mechanical forces like crystal-crystal, crystal-impeller, and crystal-hardware collisions result in contact nucleation. Contact nucleation generally dominates among the various secondary nucleation mechanisms.[2]

2.4.3.2 Crystal Growth

Growth of stable crystal nuclei in to visible size is called as crystal growth. Crystal growth comprises of mainly two steps, solute molecules diffusion towards the crystal surface and crystal lattice formation due to integration of these growth units. The diffusion step contains transfer of mass towards stagnant layer of crystal surface. This is followed by surface diffusion, spatial orientation, and the subsequent surface integration reaction that constitute the integration step. Crystal growth depend on rate of diffusive transport and surface integration as well as degree of supersaturation and can be diffusion controlled, surface integration-controlled or a combination of both.[2]

2.5 Modeling of Batch Crystallization Process

Crystallization is a heterogeneous dispersed phase having high nonlinear modeling. A mathematical framework for modeling a batch crystallization process consists of the population balance equation (PBE) describing a conservation equation for a number of crystals in a population, mass balance and energy balance. A typical batch crystallizer is as follows:
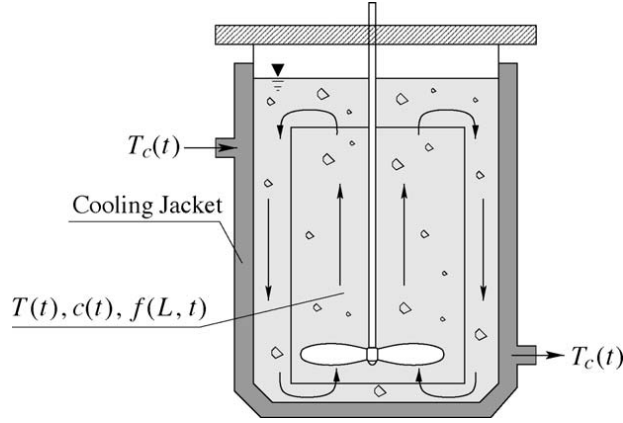
Figure 2.5: Typical Batch Crystallizer

Few assumptions are considered to develop PBE like well mixed condition, neglecting the suspension volume change in the system, size independent crystal growth and the agglomeration and breakage of crystals. With these assumptions, the PBE for the CSD of the process can be written as:

$$\frac{\partial f(L,t)}{\partial t} + G(t)\frac{\partial f(L,t)}{\partial L} = 0 \tag{2.18}$$

With initial and boundary conditions for the evolution of the CSD:

$$f(0,t) = \frac{B(t)}{G(t)} \tag{2.19}$$

$$f(0,L) = f_{seed}(L) \tag{2.20}$$

The mass balance describing the change of solute concentration in continuous phase is as follows:

$$\frac{dC}{dt} = -3A\rho_c k_v G(t) \int_0^\infty f(L,t)L^2 dL \tag{2.21}$$

The energy balances for the batch crystallizer and the jacket are

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$$\frac{dT(t)}{dt} = -3\frac{\Delta H_c}{C_p}\rho_c k_v G(t)\int_0^\infty f(L,t)L^2 dL - \frac{UA}{MC_p}\left(T(t) - T_j(t)\right) \tag{2.22}$$

$$\frac{dT_j(t)}{dt} = \frac{F_j}{V_j}\left(T_{jsp}(t) - T_j(t)\right) + \frac{UA}{\rho_j V_j C_{p_j}}\left(T(t) - T_j(t)\right) \tag{2.23}$$

Nucleation and growth rates are the kinetic phenomena influencing the formation of crystals. The measurement of driving force of super saturation (S) is given in Eq. (2.22):

$$S = \frac{C - C_s(T)}{C_s(T)} \tag{2.24}$$

The rate of nucleation and growth are developed by assuming an empirical functional form as given in Eqs. (2.25) and (2.26):

$$B(t) = K_b e^{\frac{-E_b}{RT}} S^b \int_0^\infty f(L,t)L^3(t)dL \tag{2.25}$$

$$G(t) = K_g e^{\frac{-E_b}{RT}} S^g \tag{2.26}$$

A set of algebraic equations are formed from PBE (Eq. (2.18))by a finite difference method. Then mass and energy balance equations (Eqs. (2.21) – (2.23)) with set of algebraic equations are solved to determine conservation of a numbers of crystals.

In this study, the seeded batch crystallizer of potassium sulfate production is considered. The physical properties and initial conditions of the crystallizer are given in Table 2.1. [11]

Table 2.1: The Physical Parameters and Initial Conditions of the Seeded Batch Crystallizer

Parameters	Value	Parameters	Value
B	2	g	2
K_b	285.0 1/(sμm^3)	K_g	1.44*10^8(μms^{-1})
E_b/R	7517.0	E_g/R	4859.0

U	$5 * 10^{-10} \text{J}\mu\text{m}^{-2}\text{s}^{-1}\text{K}^{-1}$	A	$0.25 * 10^{12}\mu\text{m}^2$
ΔH_c	44500 J kg^{-1}	C_p	3800 J kg^{-1}K^{-1}
M	27.0 kg	ρ_c	$2.66*10^{-15}$ g/μm^3
K_v	1.5	t_r	1800 s
V_j	$0.015*10^{18}\mu\text{m}^3$	F_j	$0.001*10^{18}\text{m}^3 \text{ s}^{-1}$
ρ_j	10^{-15} kgμm^{-3}	C_{pj}	4184 J kg^{-1}K^{-1}
$C(0)$	0.1743 g solute/g solvent	$T(0)$	323K

The initial distribution of the seeded crystals in the batch crystallizer is assumed to be a parabolic distribution as the function of the crystal characteristic length ranging from 250 to 300 mm.

$$f_{seed}(L,0) = \begin{cases} 0.0032\ (300-L)(L-250) \ for\ 250\ \mu m \le L \le 300\ \mu m \\ 0 \qquad\qquad\qquad\qquad\qquad for L < 250\ \mu m\ and\ L > 300\ \mu m \end{cases} \qquad (2.27)$$

Solution concentration (C) for the process in metastable zone indicate default region of process to be operated. The region is bounded by metastable limit, $C_s < C < C_m$ between solubility curves. The equations given below are used to calculate saturation and metastable concentrations.

$$C_s(t) = 6.29 \times 10^{-2} + 2.46 \times 10^{-3}T - 7.16 \times 10^{-6}T^2 \qquad (2.28)$$

$$C_m(t) = 7.76 \times 10^{-2} + 2.26 \times 10^{-3}T - 8.10 \times 10^{-6}T^2 \qquad (2.29)$$

To avoid high computational time required in solving of the PBE for an optimization problem, its direct use in the design of a MPC controller is always avoided. So PBE is transformed to a set of ordinary differential equations (ODEs) by the method of moments. In principle, the method of moments defines the ith moment in terms of the population density function by:

$$\mu_i = \int_0^\infty f(L,t)L^i(t)dL \quad i = 0,1,2,3 \tag{2.30}$$

Where μ_i is the ith moments representing total number of crystals (μ_0), total length of crystals (μ_1), overall surface area of crystals (μ_2), and overall volume of crystals (μ_3).

The rate equation of the moments is derived by determining separately the moments of the nuclei and seed classes for the CSD as in Eqs. (2.31-2.34),

$$\frac{d\mu_0}{dt} = B(t) \tag{2.31}$$

$$\frac{d\mu_i^n}{dx} = i\, G(t)\mu_{i-1}^n(t) \qquad i = 1,2,3 \tag{2.32}$$

$$\mu_0^s = 0 \tag{2.33}$$

$$\frac{d\mu_i^s}{dx} = i\, G(t)\mu_{i-1}^s(t) \qquad i = 1,2,3 \tag{2.34}$$

The overall i^{th} moments are defined as $\mu_i = \mu_i^n + \mu_i^s$. It shouldbe noted that since the crystal breakage and agglomeration phenomena are not considered in the proposed crystallizer model, a total number of crystals growing from seeds μ_0^s is constant and determined by the initial seed size distribution (Eq.2.31).[11]

2.6 Dynamic Simulation of Batch Crystallization Process

The following are the input and output of the system.
Inputs:
➤ Tj,in = Jacket inlet Temperature
Outputs:
➤ μ_0= zeroth moment of the CSD
➤ μ_1= first moment of the CSD
➤ μ_2 = second moment of the CSD

- ➤ μ_3 = third moment of the CSD
- ➤ C = concentration
- ➤ T = temperature of system
- ➤ Tj= jacket outlet temperature

Dynamic simulation is obtained by using ODE 45 solver in MATLAB software. Dynamic responses of state variables are shown in figure 2.6.
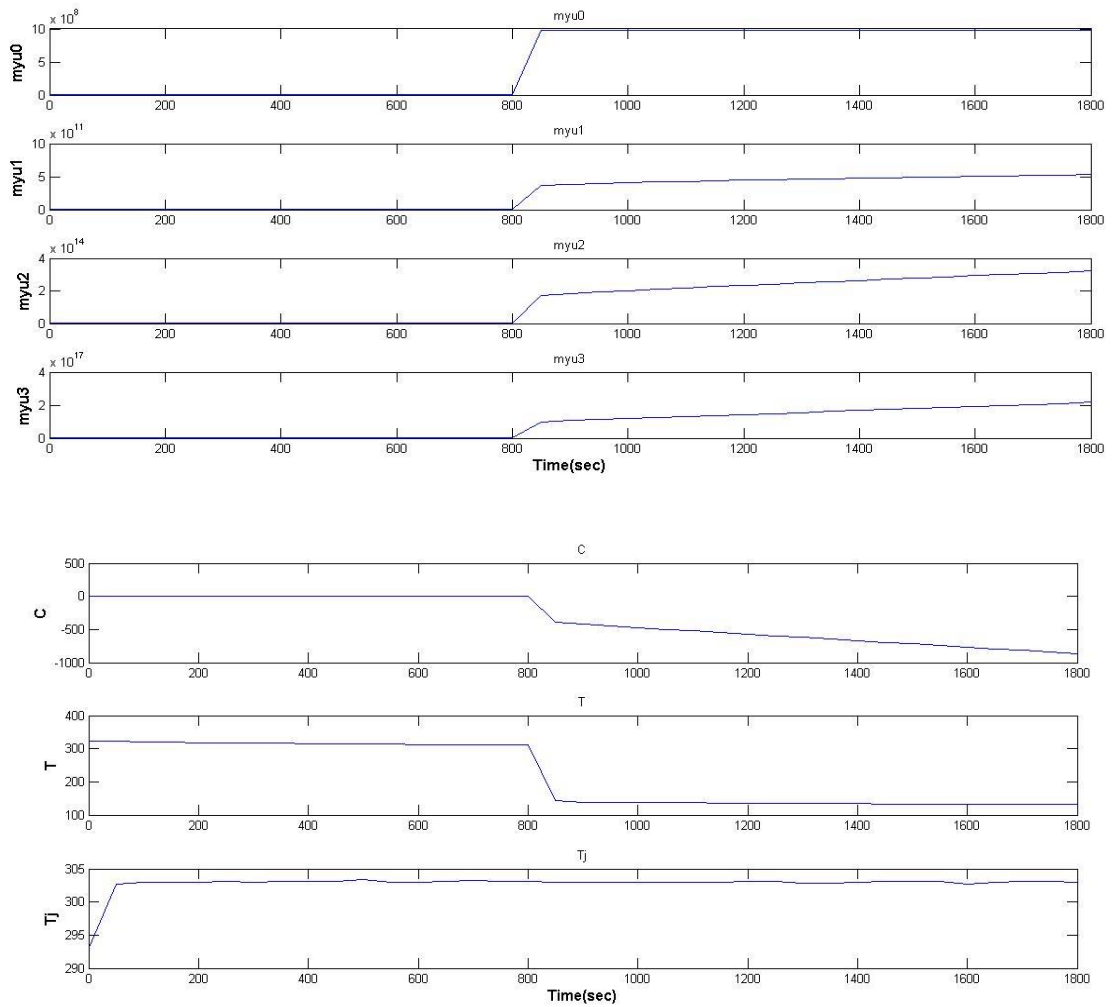

Figure 2.6: Dynamic Simulation of Batch Crystallization Process

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CHAPTER 3

OPTIMAL CONTROL: THEORETICAL POSTULATIONS

CHAPTER 3

OPTIMAL CONTROL: THEORETICAL POSTULATIONS

The designing of a set of state equations describing the dynamic behavior of plant to be controlled is the starting point of optimal control. Optimum control of plant is made possible by feedback controllers. Feedback controllers require the complete measurement of state variables. States need to measure completely using some techniques like observer, if not measurable. Here Linear Quadratic Regulator (LQR) is used for optimal control of batch crystallization process. [1]

3.1 Linear Quadratic Regulator (LQR)

The system where a set of linear differential equations describes the plant and a quadratic function describes the cost is called LQ problem and its solution is provided by linear quadratic regulator (LQR), a feedback controller. LQR problem with feedback configuration is shown in figure 3.1.
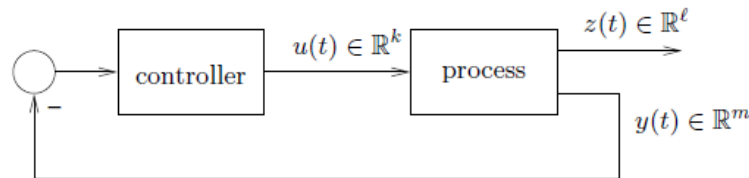
Figure 3.1: Linear Quadratic Regulation (LQR) Feedback Configuration with Negative Feed Back and the Absence of a Reference Signal

In this configuration, the state-space model of the process has two distinct outputs:

I.   The measured output is $y(t) \in R^k$ which is available for control. It is given as $y = -C(s)U(s)$ if $C(s)$ is controller transfer-matrix. $U(s)$ and $Y(s)$ are Laplace transforms of the process input $u(t)$ and the measured output $y(t)$, respectively.

II. $z(t) \in R^l$ Corresponds to The controlled output signal that should be as small as possible. To make it very small, sometimes $z(t) = y(t)$ is used.

The controlled output $z(t) \in R^l$ corresponds to signal that one would like to make as small as possible in the shortest possible amount of time. One simply needs to make one of the measured outputs $y(t)$ small if output $y(t)$ is a vector. [1]

3.1.1 Optimal Regulation

The LQR problem is defined as follows: Finding the control input $u(t)$, that makes the following criterion as small as possible

$$J_{LQR} = \int_0^\infty \|z(t)\|^2 + \rho \|u(t)\|^2 dt \tag{3.1}$$

Where ρ is a positive constant.
The term,

$$\int_0^\infty \|z(t)\|^2 dt$$

Corresponds to the energy of the controlled output and the term

$$\int_0^\infty \|u(t)\|^2 dt$$

to the energy of the control signal. In LQR, one seeks a controller that minimizes both energies. However, decreasing the energy of the controlled output will require a large control signal and a small control signal will lead to large controlled outputs. The role of the constant ρ is to establish a trade-off between these goals:

I.   When we chose ρ very large, the most effective way to decrease J_{LQR} is to use little control, at the expense of a large controlled output.

II.   When we chose ρ very small, the most effective way to decrease J_{LQR} is to obtain a very small controlled output, even if this is achieved at the expense of a large controlled output.

Often the optimal LQR problem is defined more generally and consists of finding the controller transfer-matrix $C(s)$ that minimizes

$$J_{LQR} = \int_0^\infty (x'Qx + \rho\, u'Ru)dt \tag{3.2}$$

Where Q is an $l \times l$ symmetric positive-definite matrix and, R an $m \times m$ symmetric positive definite matrix, and ρ a positive constant.[1]

3.2 State Feedback Controller

The main objective of controller is bringing the system to zero states from none zero state and control system is given by $u = r - kx$. In state feedback control, whole state x should be measurable so that it is easily available for control. It is state regulatory system since desired output is set to be zero. The LQR controller has the following form

$$u(t) = -R^{-1}B^T Px(t) \tag{3.3}$$

Where $P \in R^{n \times n}$ is given by the positive (symmetric) semi definite solution of

$$PA + A^T P - Q + PBR^{-1}B^T P = 0 \tag{3.4}$$

This equation is called Ricatti equation. It is solvable if pair (A, B) is controllable and (C, A) is observable. A process is said to be completely controllable if it can be transferred from its initial state $x(t_0)$ to any other state in a limited time interval t_0 and observable if every state $x(t_0)$ can be determined from the observation of $y(t)$ over a limited time interval. [1]

3.3 LQR Design with Observers

To find an observer gain with desirable characteristics using LQR techniques, simply replacing (A, B) by (A^T, C^T) and $L = \frac{u(t)}{x(t)}$ in the LQR design equations (3.3) and (3.4). This works for any number of outputs p. To find specific matrix equations for observer design, one may formally manipulate these into their dual forms using matrix transposition to obtain,

$$AP_0 + P_0 A^T + Q_0 - P_0 C^T R_0^{-1} C P_0 = 0 \tag{3.5}$$

$$L = P_0 C^T R_0^{-1} \tag{3.6}$$

Observer design matrices Q_0, R_0 and the observer auxiliary matrix P_o are written with subscripts. The first of these equations is a matrix quadratic equation known as the observer Algebraic Riccati Equation (ARE).

3.4 Implementation of LQR Controller for Batch Crystallization Process

LQR technique is implemented on Batch Crystallization process using MATLAB software. State space matrices are found out using model design equations 2.18- 2.34 from chapter 2. State space matrices obtained are,

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 32 & 65 & 3377 & 29 & 5069 \end{bmatrix} \tag{3.7}$$

$$B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.067 \end{bmatrix} \qquad (3.8)$$

$$C = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad (3.9)$$

$$D = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (3.10)$$

The gain matrix obtained is

$$K = [64.015 \quad 210.64 \quad 231.25 \quad 490.37 \quad 409.94 \quad 280.44 \quad 141.96] \qquad (3.11)$$

Using algorithm of LQR controller, State variables of batch crystallization process are controlled to zero states shown in figure 3.2.
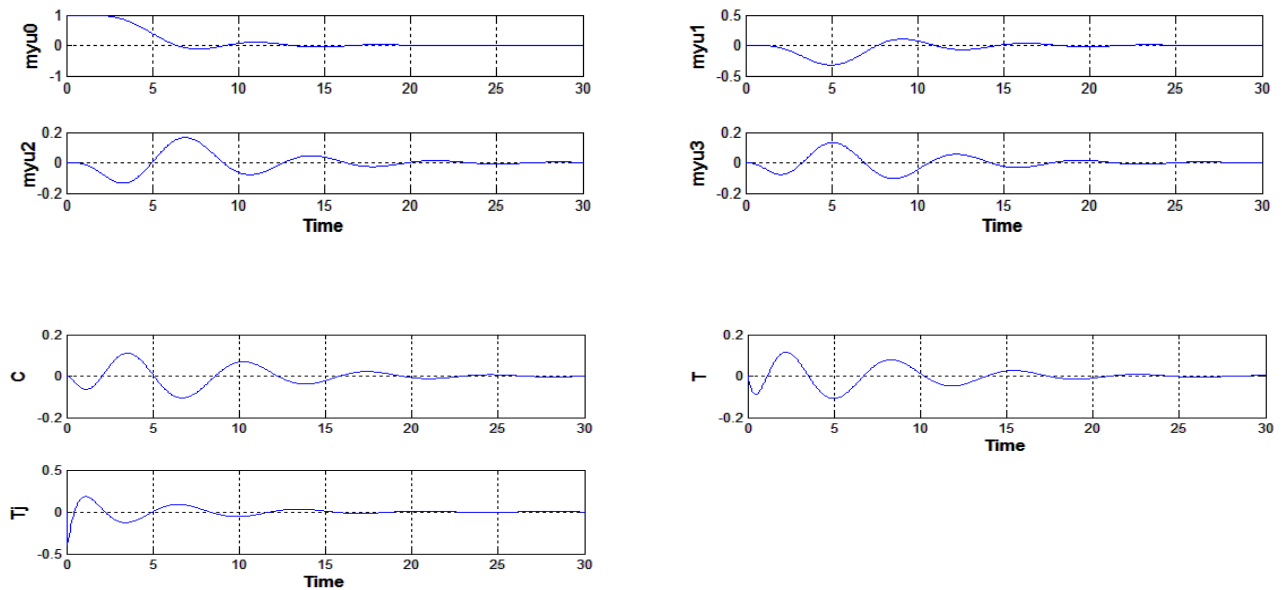

Figure 3.2: Closed Loop Performance of Batch Crystallizer Using LQR Controller

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3.5 Observer Design (Kalman Filter)

Kalman filter called as linear quadratic estimation (LQE), utilizes series of measurements containing noise and inaccuracies and estimates the unmeasured state variables. The name of filter was given on the honors of Rudolf Kalman , one of the primary developers of its theory. Kalman filter has number of application in guidance and control of vehicles, particularly aircraft and spacecraft. It is also used in time series analysis like signal processing and econometrics.

Kalman Filter algorithm initially produces current state variables along with uncertainties. Then, estimated state variables are again updated after observation of next measurement using a weighted average, with more weight being given to estimates with higher certainty. The algorithm is recursive in nature with real time using only the present input measurements and the previously. [1]

The Kalman filter estimate state variables by following steps:

Initial State Estimate: The first step is assumption of initial guess of state variables x_{init}.
Initially predicted state estimate x_p is equal to initial value.

$$x_p(0) = x_{init} \tag{3.12}$$

Predicted Measurement Estimate: Calculating the predicted measurement estimate using the predicted state estimate at any instant of time K,

$$y_p(K) = g[x_p(k)] \tag{3.13}$$

Innovation Variable: This step deals with calculation of error from difference between the measurement $y(k)$ and the predicted measurement $y_p(k)$:

$$e(k) = y(k) - y_p(k) \tag{3.14}$$

Corrected State Estimate: Calculation of corrected state estimate $x_c(k)$ is done by adding the corrective term $ke(k)$ to the predicted state estimate $x_p(k)$. K is a Kalman Filter gain.

$$x_c(k) = x_p(k) + Ke(k) \tag{3.15}$$

Predicted State Estimate: Calculation of predicted state estimate for next time step $(k + 1)$ from known input $u(k)$ of process and present state estimate $x_c(k)$.[1]

$$x_p(k + 1) = f[x_c(k), u(k)] \tag{3.16}$$

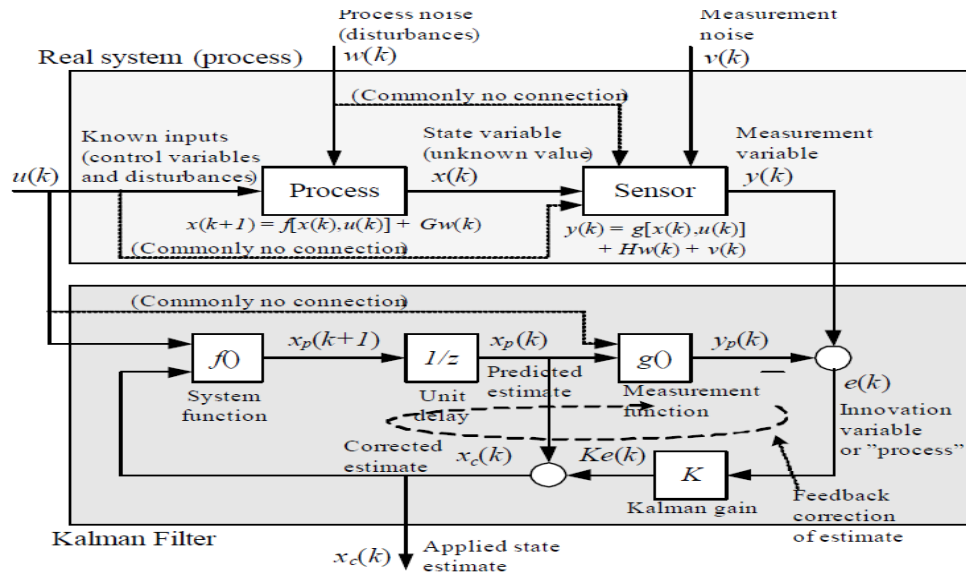The above steps are represented in figure 3.3.

Fig 3.3: Real System Process with Observer

The estimation $x_p(k)$ is done by integrating in real time the following ODE,

$$\dot{x}_p(k) = Ax_p + Bu + L(y - C\hat{x}) \tag{3.17}$$

With the following matrices calculated

$$L = PC^TR^{-1} \tag{3.18}$$

$$0 = AP + PA^T - PC^TR^{-1}CP + Q^Y, \quad P \geq 0, \tag{3.19}$$

$$Q = E(ww^T), R = E(vv^T) \tag{3.20}$$

The Riccati equation above has its origin in the minimization of the cost function

$$J[x_p(k)] = \int_{-\infty}^{0}[(x_p - x)(x_p - x)^T]dt \tag{3.21}$$

Output feedback controller can be obtained by using the estimated state $\hat{x}$ leads to the following output-feedback controller.

$$\dot{x}_p = (A - LC)x_p + Bu + Ly = (A - LC - BK)x_p Ly \tag{3.22}$$

$$u = -Kx_p \tag{3.23}$$

With negative feedback transfer matrix given by

$$C(s) = K(sI - A + LC + BK)^{-1}L \tag{3.24}$$

This is usually known as an LQG output-feedback controller and the resulting closed loop is shown in fig. 3.4. [1]
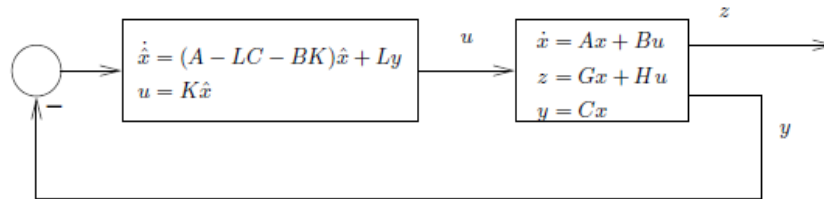

Figure 3.4: LQR Output Feedback

3.6 Implementation of Kalman Filter for State Space Model

Considering general example of state space matrixes having 2 input and 7 state variables,

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -0.91 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0.22 & 0 & -0.5 & 0 & 0 \\ -4.14 & 0 & 1.35 & 0 & 0 & -0.880 \\ 0 & 0 & 0 & -4.5 & -50 & -5 & 0 \end{bmatrix} \tag{3.25}$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & .8 \\ -.35 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{3.26}$$

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{3.27}$$

Since all the state variables are not measurable, so Kalman filter is designed to find unmeasured output using above algorithm (eq. 3.10-3.17). The Kalman gain matrix obtain is

$$K = \begin{bmatrix} -1.0412 & 0.0534 & 0 & 0 & 0 & 1 & 0 \\ 0.0534 & -7.1475 & 0 & 0 & 0 & 0 & 1 \\ -0.1080 & 0.0946 & -0.9091 & 0 & 0 & 0 & 0 \\ -0.0047 & -0.0375 & 0 & -1 & 0 & 0 & 0 \\ 0.0839 & 0.7523 & 0.2182 & 0 & -0.5 & 0 & 0 \\ -4.1846 & 0.6881 & 1.3588 & 0 & 0 & -0.08820 \\ -0.2505 & -25.0448 & 0 & 4.50 & -50.00 & -5 & 0 \end{bmatrix} \tag{3.28}$$

By using MATLAB simulation, the state variables obtain from Kalman filter is given below:
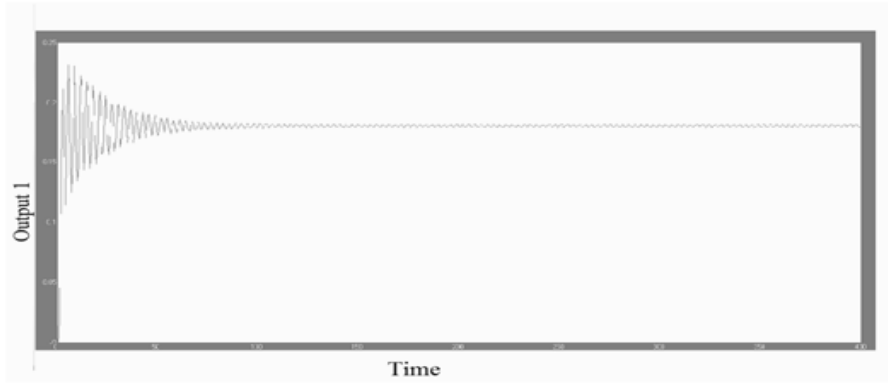
Figure 3.5: Output 1 Vs Time

Figure 3.6: Output 2 Vs Time

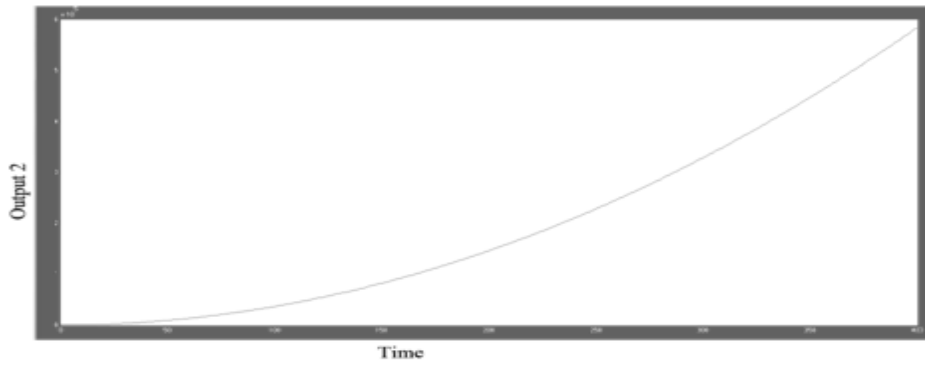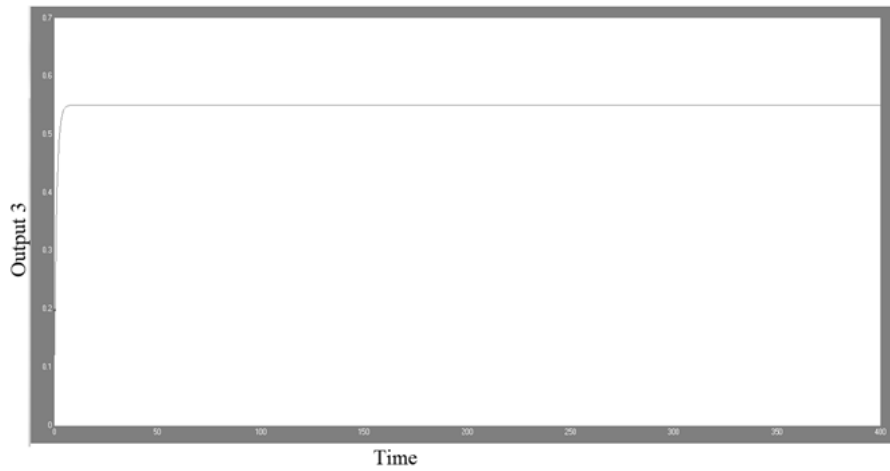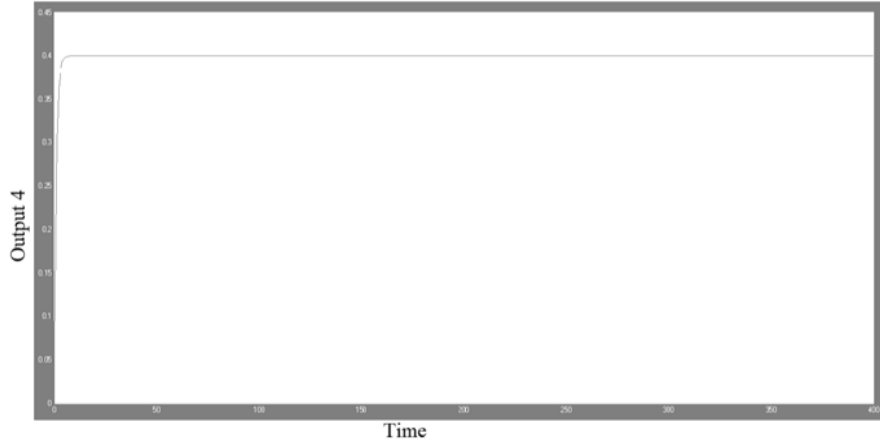**Figure 3.7**: Output 3 Vs Time
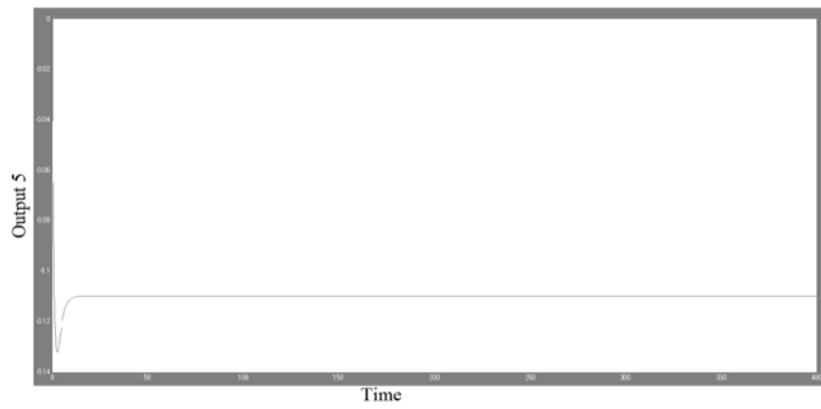
Figure 3.8: Output 4 Vs Time

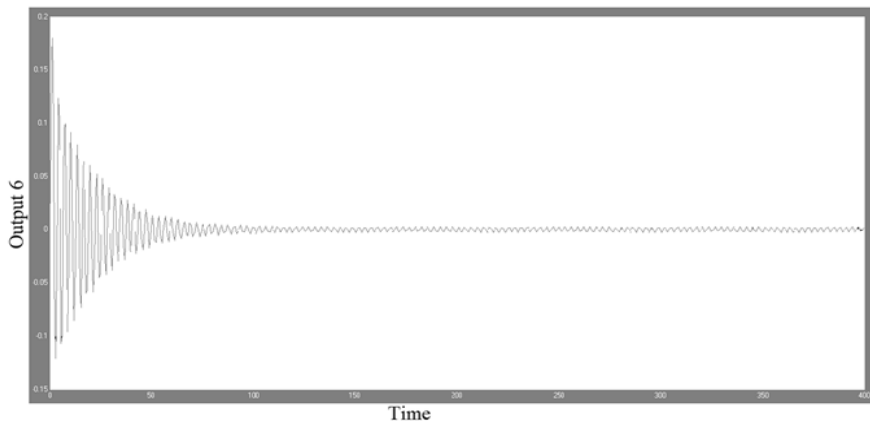**Figure 3.9**: Output 5 Vs Time

Figure 3.10: Output 6 Vs Time
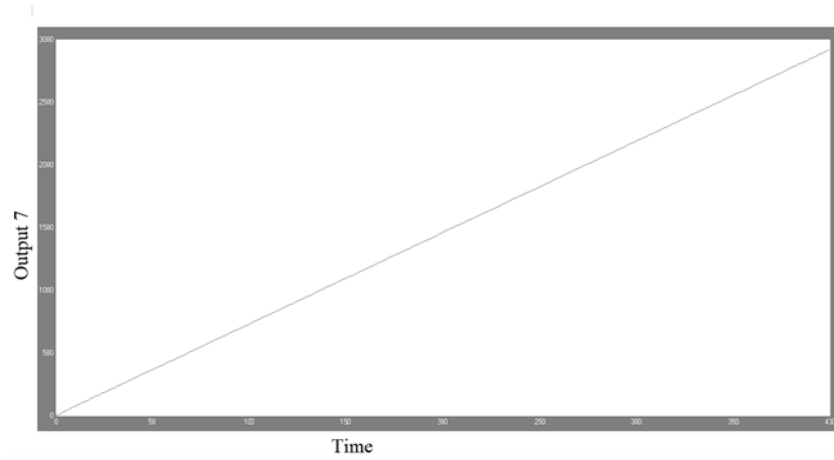
Figure 3.11: Output 7 Vs Time

References:

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CHAPTER 4

MODEL PREDICTIVE CONTROL

CHAPTER 4

MODEL PREDICTIVE CONTROL

4.1 Introduction

Model predictive control (MPC) is often used to control multiple input output processes with satisfying inequality constraints on the input output variables. It predict the future output if reasonably accurate dynamic model of process is available and then depending on predicted and measured output, appropriate change in measured input can be calculated. Output variables are called as controlled variables (CV) while input variables are manipulated variables (MV). Measured disturbances are also called as feed forward variables. Major advantages of Model predictive control are:

1) Provides dynamic and static interaction between input, output, and disturbance variables.
2) Systematic control on constraints on input and outputs.
3) Controlled calculations are synchronized with set points provided.
4) Prediction of future output gives early warning of possible problems. [1]

Basic block diagram model predictive control is given by

Figure 4.1: Block Diagram Model Predictive Control

Basic structure of MPC is given above. Current values of the output variables are calculated using a process model and then difference between predicted and actual outputs are used as a feedback signal to a prediction block. The predicted outputs are used in controlled

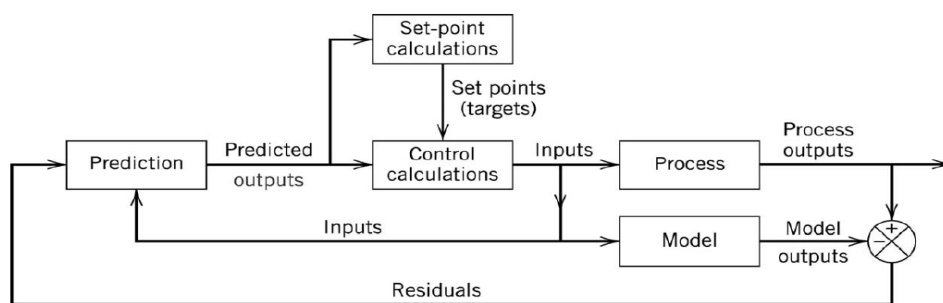calculation and setpoint calculation after considering constraints on the input and output variable. MPC configuration is analogues to both internal model control configuration and smith predictor configuration because model and process are parallel acted and difference act as feedback control signal. But coordination of the control and set point calculations makes MPC superior than others. Moreover, MPC is largely used in MIMO control problems than IMC or Smith predictor.

Traditionally economic optimization setpoint for the control calculation, called as target, is calculated from a steady-state model of the process. Economic optimization is depending on maximizing a cost function, or maximizing a production rate. The optimum values of set points are distorted continuously which in turn functions of variations in process conditions, equipment, and instrumentation, as well as economic data such as prices and costs. In MPC, Set points are calculated in each sampling time. Control action is determined based on current measurements and predictions of the future output. For linear model prediction, a multivariable version of the step response or differential equations model are used while nonlinear process uses nonlinear dynamic models and empirical models, such as neural networks. [2]
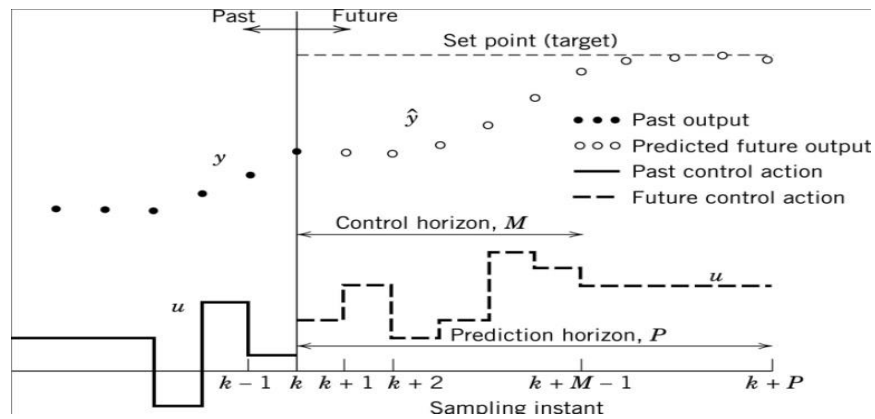

Figure 4.2: Basic Concept of MPC

$y, \hat{y}$ and u shown in figure above are actual output, predictive output and manipulated input respectively. The main objective of the MPC is to determine the set of control moves so that predicted reaches the desired set point. At any sampling time, MPC decides a set of M input

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values containing a present input $u(k)$ and future $M-1$ inputs $\{u(k+i-1), i=1,2,3....M\}$. Set of inputs are calculated in such a way that a set of $'P'$ predicted output $\{\hat{y}(k+i), i=1,2,..P\}$ should reach the optimum setpoint. Objective function is optimized to find out control moves. Number of control moves M is called the control horizon while number of prediction p is referred to as the prediction horizon.

Receding horizon approach makes MPC a unique control approach. Although for each sampling time, MPC gives sequence of M control moves, only first moves is actually implanted. Then again for next sampling instant, a new set of control moves are determined and only the first input move is implemented and process is repeated for each sampling instant. [3]

4.1.1 Limitation of MPC

Traditional MPC has many of performance limitations which are summarized below:

Model Structure

Applications of MPC are limited by finite step and impulse response models and need numerous model coefficients to explain the response of system. Integrating systems are handled after taking derivative of an integrating output as controlled output.

Disturbance Assumption

Output disturbances are generally assumed to be constant which may give some misleading performance if real disturbance occurs at the plant input.

Finite Horizons

MPC gives deteriorating performance if prediction or control horizons are not calculated correctly, even if the model is perfect.

4.2 Control Objective Function of MPC

Various objective functions are available but mostly standard least-squares or quadratic programming (QP) objective function which provides smoother control action to MPC and MPC will have more sensitive tuning parameters. The QP formulation based MPC is used in this thesis.The objective function is nothing but sum of square of the predicted errors and control

moves. Predicted error is difference between the set points and the model-predicted outputs whereas changes in the control action from step to step are called control moves. [1]

A quadratic objective function for a control horizon of 2 and a predictive horizon of 3 is given as

$$\varphi = Q(r_{k+1} - \hat{y}_{k+1})^2 + Q(r_{k+2} - \hat{y}_{k+2})^2 + Q(r_{k+3} - \hat{y}_{k+3})^2 + R\Delta u^2_k + R\Delta u^2_{k+1} \qquad (4.1)$$

Where $\hat{y}$ denotes the model predicted outputs, r is the set point, Δu is the change in manipulated input from one sample time to the next, Q and R is a weight for the change in the output and manipulated input respectively.

The least square objective function for a prediction horizon of P and a control horizon M is written as.

$$\varphi = Q\sum_{i=1}^{P}(r_{k+i} - \hat{y}_{k+i})^2 + R\sum_{i=0}^{M-1}\Delta u^2_{k+i} \qquad (4.2)$$

The optimization problem deals with a minimization of the objective function by manipulating M control moves. [1]

4.2.1 Dynamic Matrix Control (DMC)

DMC is a step response model developed by shell Oil Company in 1960s and 1970s. the silent features of DMC control are

1. A finite prediction horizon for quadratic performance objective.
2. Linear step response model for the plant.
3. Predicted future responses are calculated after considering set point so that it should follow setpoint as closely as possible.

Predicted output is given as

$$\hat{y}_k = S_1\Delta u_{k-1} + S_2\Delta u_{k-2} + \cdots\cdots\cdots\cdots\cdots + S_{N-1}\Delta u_{k-N+1} + S_N u_{k-N} \qquad (4.3)$$

Its generalized form written as

$$\hat{y}_k = \sum_{i=1}^{N-1} S_i \Delta u_{k-i} + S_N u_{k-N} \qquad (4.4)$$

Where $\hat{y}_k$ the model prediction at time is step$k$, and u_{k-N} is the manipulated input of N steps in the past$\Delta u(k - i + 1) = u(k - i + 1) - u(k - i)$ .The predicted output should be equal to the actual measured output at any time instant.

The model-predicted output is unlikely to be equal to the actual measured output at time step. The difference between the measured output (y_k) and model prediction$\hat{y}_k$ is called the additive disturbance given as

$$d_k = y_k - \hat{y}_k \tag{4.5}$$

Consider corrected prediction is then equal to the actual measured output at step k

$$\hat{y}^c_{k} = \hat{y}_k + d_k \tag{4.6}$$

Similarly, the corrected predicted output at the first time step in the future can be found from

$$\hat{y}^c_{k+1} = \hat{y}_{k+1} + \hat{d}_k \tag{4.7}$$

From equation (4.4) and (4.7), we can write

$$\hat{y}^c_{k+1} = \sum_{i=1}^{N-1} S_i \Delta u_{k-i+1} + S_N u_{k-N+1} + \hat{d}_{k+1} \tag{4.8}$$

$$\hat{y}^c_{k+1} = S_1 \Delta u_k + \sum_{i=2}^{N-1} S_i \Delta u_{k-i+1} + S_N u_{k-N+1} + \hat{d}_{k+1} \tag{4.9a}$$

$$\hat{y}^c_{k+2} = S_1 \Delta u_{k+1} + S_2 \Delta u_k + \sum_{i=3}^{N-1} S_i \Delta u_{k-i+2} + S_N u_{k-N+2} + \hat{d}_{k+1} \tag{4.9b}$$

So corrected future output for j th step is

$$\hat{y}^c_{k+j} = \sum_{i=1}^{j} S_i \Delta u_{k-i+j} + \sum_{i=j+1}^{N-1} S_i \Delta u_{k-i+j} + S_N u_{k-N+j} + \hat{d}_{k+j} \tag{4.10}$$

$\sum_{i=1}^{j} S_i \Delta u_{k-i+j}$ {Effect of current and future moves}

$\sum_{i=j+1}^{N-1} S_i \Delta u_{k-i+j} + S_N u_{k-N+j}$ {Effect of past moves}

$\hat{d}_{k+j}$ {Correction term}

Correction term is always considered as constant in future

$$\hat{d}_{k+j} = \hat{d}_{k+j-1} = \cdots\cdots = d_k = y_k - \hat{y}_k \tag{4.11}$$

Change in control action is recorded till control horizon of M steps, after that control moves are constant.

$$\Delta u_{k+M} = \Delta u_{k+M+1} = \cdots\cdots = \Delta u_{k+P-1} = 0 \tag{4.12}$$

The corrected predicted future output matrix of P steps and a control horizon of M stepsare

$$
\underbrace{\begin{bmatrix} \hat{y}^c_{k+1} \\ \hat{y}^c_{k+2} \\ \vdots \\ \hat{y}^c_{k+j} \\ \vdots \\ \hat{y}^c_{k+P} \end{bmatrix}}_{\substack{P\times 1 \\ corrected output \\ prediction\,\bar{y}^c}} = \underbrace{\begin{bmatrix} s_1 & 0 & 0 & \cdots & 0 & 0 \\ s_2 & s_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & & & \\ s_j & s_{j-1} & s_{j-2} & \cdots & \cdots & s_{j-M+1} \\ \vdots & \vdots & \vdots & & & \vdots \\ s_P & s_{P-1} & s_{P-2} & \cdots & \cdots & s_{P-M+1} \end{bmatrix}}_{\substack{P\times M \\ dynamic matrix.\,s_f}} \underbrace{\begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \Delta u_{k+M-2} \\ \Delta u_{k+M-1} \end{bmatrix}}_{\substack{M\times 1 \\ current and future \\ control moves,\,\Delta u_f}}
$$

$$
+ \underbrace{\begin{bmatrix} s_2 & s_3 & s_4 & \cdots & s_{N-2} & s_{N-1} \\ s_3 & s_4 & s_5 & \cdots & s_{N-1} & 0 \\ \vdots & \vdots & & & 0 & 0 \\ s_{j+1} & s_{j+2} & \cdots & s_{N-1} & 0 & 0 \\ \vdots & \vdots & \vdots & & & \vdots \\ s_{P+1} & s_{P+2} & \cdots & 0 & \cdots & 0 \end{bmatrix}}_{\substack{P\times(N-2) \\ past control \\ matrix.\,s_{past}}} \underbrace{\begin{bmatrix} \Delta u_{k-1} \\ \Delta u_{k-2} \\ \vdots \\ \Delta u_{k-N+3} \\ \Delta u_{k-N+2} \end{bmatrix}}_{\substack{(N-2)\times 1 \\ past control \\ moves,\,\Delta u_{past}}} + s_N \underbrace{\begin{bmatrix} u_{k-N+1} \\ u_{k-N+2} \\ \vdots \\ u_{k-N+P} \end{bmatrix}}_{\substack{P\times 1 \\ past inputs,\,u_p}} + \underbrace{\begin{bmatrix} d_{k+1} \\ d_{k+2} \\ \vdots \\ d_{k+P} \end{bmatrix}}_{\substack{predicted disturbanes,\,\bar{d}}}
\tag{4.13}
$$

Equation (4.13) can be written in matrix-vector notation

$$\hat{y}^c = S_f \Delta u_f + S_{past} \Delta u_{past} + S_N u_p + \hat{d} \tag{4.14}$$

Equation (4.14) is composed from a free response (the output changes that are predicted if there is no future control moves) and forced response (contribution of the current and future control moves). The difference between the set point trajectory, r, and the future prediction is

$$r - \hat{y}^c = r - \left[S_{past} \Delta u_{past} + S_N u_p + \hat{d} \right] - S_f \Delta u_f \tag{4.15}$$

$r - \hat{y}^c = E^c$Is corrected predicted error

$r - [S_{past}\Delta u_{past} + S_N u_p + \hat{d}] = E$ is unforced error (if no current and future control moves)

Above equation (4.15) can be given as

$$E^c = E - S_f \Delta u_f \tag{4.16}$$

Where the future predicted errors are composed of free response (E) and forced response $(-S_f \Delta u_f)$ contributions.

The least square objective function equation (4.2) can be written as

$$\varphi = Q \sum_{i=1}^{P} (e^c{}_{k+i})^2 + R \sum_{i=0}^{M-1} (\Delta u_{k+i})^2 \tag{4.17}$$

The quadratic terms are written in matrix-vector as

$$Q \sum_{i=1}^{P} (e^c{}_{k+i})^2 = Q[e^c{}_{k+1} e^c{}_{k+2} \cdots\cdots e^c{}_{k+P}] \begin{bmatrix} e^c{}_{k+1} \\ e^c{}_{k+2} \\ \vdots \\ \vdots \\ e^c{}_{k+P} \end{bmatrix} \tag{4.18}$$

$$Q \sum_{i=1}^{P} (e^c{}_{k+i})^2 = (E^c)^T Q E^c \tag{4.19}$$

$$R \sum_{i=0}^{M-1} (\Delta u_{k+i})^2 = R[\Delta u_k \Delta u_{k+1} \cdots \Delta u_{k+M-1}] \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \vdots \\ \Delta u_{k+M+1} \end{bmatrix} \tag{4.20}$$

$$R \sum_{i=0}^{M-1} (\Delta u_{k+i})^2 = \Delta u^T{}_f R \Delta u_f \tag{4.21}$$

Therefore objective function can be written with equation (4.19) and (4.21)

$$\varphi = (E^c)^T Q E^c + \Delta u^T{}_f R \Delta u_f \tag{4.22}$$

From equation (4.16) and (4.22) one can write

$$\varphi = (E - S_f \Delta u_f)^T Q (E - S_f \Delta u_f) + \Delta u^T{}_f R \Delta u_f \tag{4.23}$$

Optimization problem deals with minimization of objective function differentiate equation (4.23) with respect to control move and are written as

$$\frac{\partial \varphi}{\partial \Delta u_f} = -2S^T_f QE + 2(S^T_f QS_f + R)\Delta u_f = 0 \tag{4.24}$$

Δu_f from equation (4.24) is

$$\Delta u_f = (S^T_f QS_f + R)^{-1} S^T_f QE \tag{4.25}$$

$$K_c = (S^T_f QS_f + R)^{-1} S^T_f Q \tag{4.26}$$

Kc is called controller gain matrix having dimension rM × mP where r and m are number of output and input respectively.

The current and future control move vector (Δu_f) is proportional to the unforced error vector (E). That is, a controller gain matrix, K_c multiplies the unforced error vector (the future errors that would occur if there were no control move changes implemented)

Since only current control move is actually implemented, only first row of the K_c matrix is useful

$$\Delta u_k = K_{c1} E \tag{4.27}$$

K_{c1} Having dimension r × mP

In case of SISO dimension of Kc matrix is M × P and K_{c1} matrix is 1 × P.[1]

4.2.2 MPC with Inequality Constraints

Inequality constraints were a primary motivation for MPC design in early development of MPC. Inequality constraints on input and output variables on MPC make the MPC unique in nature. Physical limitations on plant equipments such as the pump, control valve, and piping characteristics are responsible for input constraints.

Plant operating strategy is mainly depending on constraints on output variables. For instance, production rate with satisfaction of constraints on product quality and avoiding undesirable operating condition like conning is prime objective of distillation column control.

Inequality constraints help in easy distinction between hard constraints and soft constraints which are also included in control calculations in many ways. Key features of the QDMC algorithm is

1. A finite prediction horizon for quadratic performance.
2. Linear step response for the plant.
3. Predicted response is trying to follow set point as closely as possible.
4. Optimal inputs computed as the solution to a quadratic program.

The input constraints can be of the following form

$$u_{min} \leq u_{k+i} \leq u_{max} \tag{4.28}$$

Similarly velocity constraints limits for the control moves at each sample time is in form

$$\Delta u_{min} \leq \Delta u_{k+i} \leq \Delta u_{max} \tag{4.29}$$

Where $\Delta u_{min} = -\Delta u_{max}$. In order to use a standard quadratic program (QP), the constraints in (4.27) should be written in terms of the control moves, Δu_{k+i} since the previously implemented control action Δu_{k-1} is known. So we can write,

$$u_k = u_{k-1} + \Delta u_k$$

$$u_{k+1} = u_{k-1} + \Delta u_k + \Delta u_{k+1} \tag{4.30}$$

The manipulated input constraints are enforced over the control horizon of M steps, (4.27) and (4.29) yield

$$\begin{bmatrix} u_{min} \\ u_{min} \\ \vdots \\ \vdots \\ u_{min} \end{bmatrix} \leq \begin{bmatrix} u_{k-1} \\ u_{k-1} \\ \vdots \\ \vdots \\ u_{k-1} \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix} \leq \begin{bmatrix} u_{max} \\ u_{max} \\ \vdots \\ \vdots \\ u_{max} \end{bmatrix} \tag{4.31}$$

Most standard QP codes use a "one-sided" form

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix} \geq \begin{bmatrix} u_{min} - u_{k-1} \\ u_{min} - u_{k-1} \\ \vdots \\ \vdots \\ u_{min} - u_{k-1} \end{bmatrix} \tag{4.32a}$$

And

$$-\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix} \geq \begin{bmatrix} u_{k-1} - u_{max} \\ u_{k-1} - u_{max} \\ \vdots \\ \vdots \\ u_{k-1} - u_{max} \end{bmatrix} \tag{4.32b}$$

This has the form $A\Delta u_f \geq b$

The velocity constraints are implemented as bounds on the control moves

$$\begin{bmatrix} \Delta u_{min} \\ \Delta u_{min} \\ \vdots \\ \vdots \\ \Delta u_{min} \end{bmatrix} \leq \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix} \leq \begin{bmatrix} \Delta u_{max} \\ \Delta u_{max} \\ \vdots \\ \vdots \\ \Delta u_{max} \end{bmatrix} \tag{4.33}$$

Most of the time, only input constraints are considered to solve MPC. For wholeness sometimes process outputs constraints are also used. The predicted output should be in the range of minimum and maximum limits.

$$y_{min} \leq \hat{y}^c_{k+i} \leq y_{max} \tag{4.34}$$

Above equation (4.34) can be written in the following form

$$\hat{y}^c = S_f \Delta u_f + f \tag{4.35}$$

Wheref, the free response of the corrected-predicted output (if no current and future control moves are made) is

$$f = S_{past}\Delta u_{past} + S_N u_P + \widehat{d} \tag{4.36}$$

So that equation (4.33) can be written as

$$y_{min} - f \leq \hat{y}^c_{k+i} \leq y_{max} - f \tag{4.37}$$

In term of one side inequalities

$$S_f \Delta u_f \geq y_{min} - f$$

$$-S_f \Delta u_f \geq -y_{max} + f \tag{4.38}$$

Expanding equation (4.38) we get objective function

$$\varphi = -2\Delta u^T_f S^T_f QE + \Delta u^T_f (S^T_f QS_f + R)\Delta u_f \tag{4.39}$$

Equation (4.39) writes in this form

$$\varphi = \frac{1}{2}\Delta u^T_f H \Delta u_f + c^T \Delta u_f \tag{4.40}$$

Where

$$H = S^T_f QS_f + R \quad \text{And } c^T = \Delta u^T_f S^T_f E = E^T \Delta u_f S_f$$

$$A\Delta u_f \geq b \tag{4.41}$$

Inequality matrices A and b in equation (4.41) incorporate the matrices in equation (4.31) and (4.35). [2]

4.2.3 Extensions of the Basic MPC Model Formulation

Extensions of the basic MPC problem formulation are required for convenient application.

Integrating Process

Step response model generated above is not suitable for an integrating process due to its bounded response. Since the output rate $\Delta y(k) = y(k + 1) - y(k)$ is bounded, simple alteration removes this problem. $\hat{y}_k$ of equation $\Delta \hat{y}_k = \hat{y}_k - \hat{y}_0$ is replaced for integrating process.

$$\Delta \hat{y}_k = \sum_{i=1}^{N-1} S_i \Delta u_{k-i} + S_N u_{k-N} \tag{4.42}$$

Or equivalently,

$$\hat{y}_k = \hat{y}_0 \sum_{i=1}^{N-1} S_i \, \Delta u_{k-i} + S_N u_{k-N} \tag{4.43}$$

Known Disturbance

If the disturbances can be calculated, it is also added in step-response model. Let s_i^d and d denote step-response coefficients of known disturbance and a measured disturbance respectively.

Then the standard step-response model can be written by adding a disturbance term,

$$\hat{y}_k = \sum_{i=1}^{N-1} S_i \, \Delta u_{k-i} + S_N u_{k-N} + \sum_{i=1}^{N_d-1} S^d_i \Delta d_{k-i} + S^d_N d_{k-N_d} \tag{4.44}$$

Where N_d is the number of step-response coefficient for the disturbance variables.

Impulse Response Model

MPC model is based either on step response or impulse-response since these two inputs are closely associated. The derived model for step response is analogous to impulse response.[2]

4.2.4 Predictions for MIMO Models

Principle of superposition is used to convert SISO model to MIMO model. For simplicity, a process with two outputs, y_1 and y_2, and two inputs, u_1 and u_2 is considered. Four individual step responses will be formed one for each input-output pairs.

$$\hat{y}_{1k} = \sum_{i=1}^{N-1} S_{11,i} \, \Delta u_{1k-i} + S_{11,N} u_{1k-N} + \sum_{i=1}^{N-1} S_{12,i} \, \Delta u_{2k-i} + S_{12,N} u_{2k-N} \tag{4.45}$$

$$\hat{y}_{2k} = \sum_{i=1}^{N-1} S_{21,i} \, \Delta u_{1k-i} + S_{21,N} u_{1k-N} + \sum_{i=1}^{N-1} S_{22,i} \, \Delta u_{2k-i} + S_{22,N} u_{2k-N} \tag{4.46}$$

Where $S_{12,i}$ denotes the *ith* step-response coefficient for the model that relates y_1 and u_2. Other step responses are written in same manner. Vector-matrix notations are convenient to express MIMO step-response models. Let the output transpose vector be $y = [y_1, y_2, ..., y_m]^T$ and the input transpose vector is $u = [u_1, u_2, ..., u_r]^T$. Then dynamic matrix form of MIMO model is

$$\tilde{y}(k+1) = S\Delta U(k) + \hat{Y}^0(k+1) + \delta[y(k) - \hat{y}(k)] \tag{4.47}$$

Where $\tilde{y}(k+1)$ is the dimensional vector of corrected predictions over the prediction horizon P.

$$\tilde{y}(k+1)\overset{\Delta}{=}col[\tilde{y}(k+1),\,\tilde{y}(k+2),\ldots\ldots\ldots,\tilde{y}(k+p)]$$ (4.48)

$\hat{y}^o(k+1)$ is the dimensional vector of the predicted unforced responses,

$$\hat{y}^o(k+1)\overset{\Delta}{=}col[\hat{y}^o(k+1),\,\hat{y}^o(k+2),\ldots\ldots\ldots,\hat{y}^o(k+p)]$$ (4.49)

And $\Delta U(k)$ is the dimensional vector of the next M control moves,

$$\Delta U(k)\overset{\Delta}{=}col[\Delta u(k),\Delta u(k+1),\ldots\ldots,\Delta u(k+M-1)]$$ (4.50)

The $mP \times m$ matrix δ in equation (4.46) is defined as

$$\delta \overset{\Delta}{=} [I_m I_m \ldots\ldots\ldots I_m]^T \, p \text{ Times}$$ (4.51)

Where I_m denotes the $m \times m$ identity matrix.

The dynamic matrix S is defined as

$$S \overset{\Delta}{=} \begin{bmatrix} S_1 & 0 & \ldots\ldots & 0 \\ S_2 & S_1 & \ldots\ldots & 0 \\ \vdots & \vdots & \vdots\cdots\cdots & \vdots \\ S_M & S_{M-1} & \ldots\ldots & S_1 \\ S_{M+1} & S_M & \ldots\ldots & S_2 \\ \vdots & \vdots & \cdots\cdots\cdots & \vdots \\ S_P & S_{P-1} & \ldots\ldots & S_{P-M+1} \end{bmatrix}$$ (4.52)

$$S_i \overset{\Delta}{=} \begin{bmatrix} S_{11,i} & S_{12,i} & \ldots\ldots & S_{1r,i} \\ S_{21,i} & S_{22,i} & \ldots\ldots & S_{2r,i} \\ \vdots & \vdots & \cdots\cdots\cdots & \vdots \\ S_{m1,i} & S_{m2,i} & \ldots\ldots & S_{mr,i} \end{bmatrix}$$ (4.53)

Equation (4.52) represents dynamic matrix for MIMO systems which has same structure as for SISO system. [1]

4.3 Design Parameters

Straight way of reaching an optimum performance is Tuning a controller before application. An MPC controller has certain parameters setting to achieve its optimum performance. Those parameters are sampling time (Δt), prediction horizon (P), control horizon (M), model horizon (N), controlled variable weights. [1]

4.3.1 Default Setting

I.   Sampling time period and model horizon:

Selection of sampling period Δt and mode horizon N should be in such a way that it should satisfy $N\Delta t = t_s$ where t_s denotes settling time for the open-loop response. Typically,30<N<120.

II.   Control M and prediction P horizons:

Typically $5 \leq M \leq 20$ and $N/3 \leq M \leq N/2$. A different value of M is selected for each input. The prediction horizon P is calculated from $P = N + M$.

III.   Weighting matrices,Q and R:

A $mP \times mP$ diagonal Q matrix allows to the output variableto weight according to their relative importance. Similarly, an $rM \times rM$ input weighting matrix allows input variables to be weighted according to their relative importance.[1]

4.3.2 Non Adaptive DMC Tuning Strategy [4][5]

Table 4.1: Non Adaptive DMC Tuning

S.N.	SISO model	MIMO model
1.	FOPDT model $\frac{Y(S)}{U(S)} = \frac{k_p e^{-\theta_p s}}{\tau_p s+1}$	FOPDT model $\frac{Y(S)}{U(S)} = \frac{k_{rs} e^{-\theta_{rs} s}}{\tau_{rs} s+1}$(r=1,2…R;s=1,2..S)

2.	$T=\max(T\leq 0.1\tau_p \text{ and } T\leq 0.5\theta_p)$	$T=\text{Min}(\text{Max}(0.1\tau_{rs}, 0.5\theta_{rs}))(r=1,2..R,s=1,2..S)$
3.	$P=N=(5\frac{\tau_p}{T}+\frac{\theta_p}{T}+1)$	$P=N=\text{Max}(5\frac{\tau_{rs}}{T}+\frac{\theta_{rs}}{T}+1)(r=1,2..R,s=1,2..S)$
4.	$M=(\frac{\tau_p}{T}+\frac{\theta_p}{T}+1)$	$M=\text{Max}(\frac{\tau_{rs}}{T}+\frac{\theta_{rs}}{T}+1)(r=1,2..R,s=1,2..S)$
5.	$R=\quad 0, M=1: M/500(\frac{3.5\tau_p}{T}+2-(M-1)/2):M>1$	$R=M/500\sum_{r=1}^{R}[Q^2_r(\frac{\theta_{rs}}{T}+1)^2\{P-(\frac{\theta_{rs}}{T}+1)-\frac{3}{2}(\frac{\tau_{rs}}{T})+2-(M-1)/2\}],s=123,\ldots S$

4.3.3 DMC Tuning Strategy Review

A table for DMC tuning, different- authors gave different-2 approach to find tuning parameter which is shown below table 4.2, 4.3 and 4.4.

Prediction Horizon [6]

Table 4.2: Prediction Horizon

PREDICTION HORIZON	AUTHOR
$P=[(t_{80}+t_{90})/2]/T_s$	MaurathP.R.;laub
$P>M+t_d/T_s$	MaurathP.R.,Mellichamp
$P=M+N$	CutlerC.R.
$P=\frac{t_{60}}{T_s}+\frac{t_{95}}{T_s}-1$	Georgiou A.; Georgakis C.;Lubyen W.L.
$P=(5\tau_p+t_d)/T_s$	HindeR.F.;Cooper
$P=\max(\frac{5\tau_{rs}}{T_s}+k_{rs})$ $k_{rs}=\frac{\theta_{rs}}{T_s}+1$	ShridharR.;Cooper

Control Horizon[6]

Table 4.3: Control Horizon

CONTROL HORIZON	AUTHOR
$M = t_{60}/T_s$	Georgiou A.; Georgakis C.;LubyenW.L.
$M = \tau_p/T_s$	HindeR.F.;Cooper
$M = \max\left(\dfrac{\tau_{rs}}{T_s} + k_{rs}\right)$ $k_{rs} = \dfrac{\theta_{rs}}{T_s} + 1$	ShridharR.;Cooper

Model Horizon and Sample Time[6]

Table 4.4: Model Horizon

MODEL HORIZON	AUTHOR
$N > (\max(t_{95,i})/T_s$	Georgiou A.;Georgakis C.;LubyenW.L.
$N = \max\left(\dfrac{5\tau_{rs}}{T_s} + k_{rs}\right)$ $k_{rs} = \dfrac{\theta_{rs}}{T_s} + 1$	ShridharR.;Cooper

Sample Time[6]

Table 4.5: Sample Time

SAMPLE TIME	AUTHOR
$T_S = \min[\max(0.1\tau_{rs}, 0.5\theta_{rs})]$	ShridharR.;Cooper

Where

K_{rs}=FOPDT Model gain for R outputs and S inputs

M =Control horizon

N = Model horizon

P=Prediction horizon.

T_s=sampling time

τ_p =FOPDT Process time constant

τ_{rs} =FOPDT Process time constant (s) for R outputs and S Inputs

$t_{80}, t_{90}, t_{60}, t_{95}$ =Rise time for 80%, 90%, 60% and 95% respectively

t_d =Process delay time

θ_{rs}=FOPDT Process delay time constant(s) for R outputs and S inputs

4.3.4 Conversion of (SOPDT) to (FOPDT)[7]

All design parameter given for first order plus dead time (FOPDT), if process has second order plus dead time (SOPDT) then that time we have to change (SOPDT) to (FOPDT) blow given the procedure.

First- order plus dead-time (FOPDT) Model

$$G(S) = \frac{Ke^{-t_0 s}}{\tau s + 1} \tag{4.54}$$

Second order plus dead-time (SOPDT) Model

$$G(S) = Ke^{-ts}/(\tau_1 s + 1)(\tau_2 s + 1) \tag{4.55}$$

K = The process steady-state gain

t, t_0 = The effective process dead time

τ_1, τ_2, τ = The effective process time

For $\tau_1 = \tau_2 t_0 = 0.505\tau_1 + t\tau = 1.641\tau_1$

49

For $\tau_1 \ll \tau_2 t_0 = \tau_2 + t\tau = \tau_1$

4.4 Implementation

MPC is implemented on SISO and MIMO model to find out the effect of tuning parameters. By trial and error method I have selected some tuning parameters called as default values.

4.4.1 Single Input Single Output System (SISO)

Considering the Van De Vusse reactor problem, the continuous state space model is given by

A= [-2.4048 0; 0.833 2.2381]
B= [7;-1.117]
C= [0 1]
D= [0]

Where the measured state (output) is the concentration of the second component and the manipulated input is the dilution rate[1]
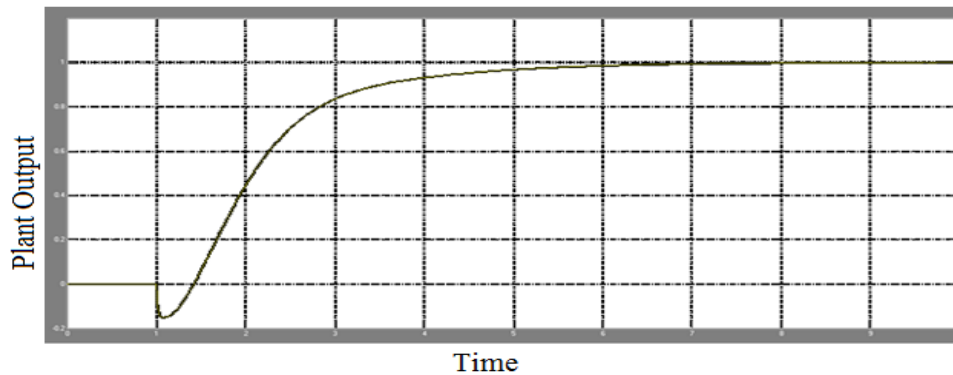
Figure 4.3: Response of Van De Vusse reactor by Using PID Controller
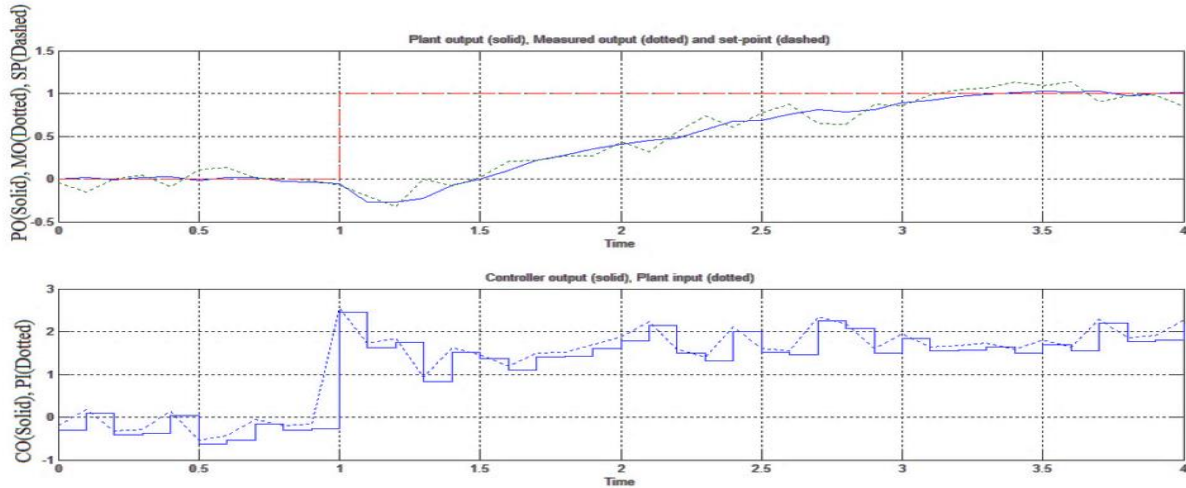
Figure 4.4: Response of Van De Vusse reactor by Using MPC Controller

4.4.2 Multiple Input Multiple Output System (MIMO)

4.4.2.1 2 × 2 Distillation Process

Wood and Berry 2×2 process

$$\begin{bmatrix} X_D(s) \\ X_B(s) \end{bmatrix} = \begin{bmatrix} \frac{12.8e^{-s}}{16.7S+1} & \frac{-18.9e^{-3s}}{21.0S+1} \\ \frac{6.6e^{-7s}}{10.9S+1} & \frac{-19.4e^{-3s}}{14.4S+1} \end{bmatrix} \begin{bmatrix} R(s) \\ S(s) \end{bmatrix} + \begin{bmatrix} \frac{3.8e^{-8.1s}}{14.9s+1} \\ \frac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F(s) \qquad (4.56)$$

Above equation is the model of distillation column it is used to separate methanol and water. Where $X_D(s)$ represents the mole fraction of methanol in distillate, $X_B(s)$ the mole fraction of methanol in bottom are the control variable, manipulated variables $R(s)$ and $S(s)$ are reflux flow rate and steam flow rate respectively and feed flow rate. [7]
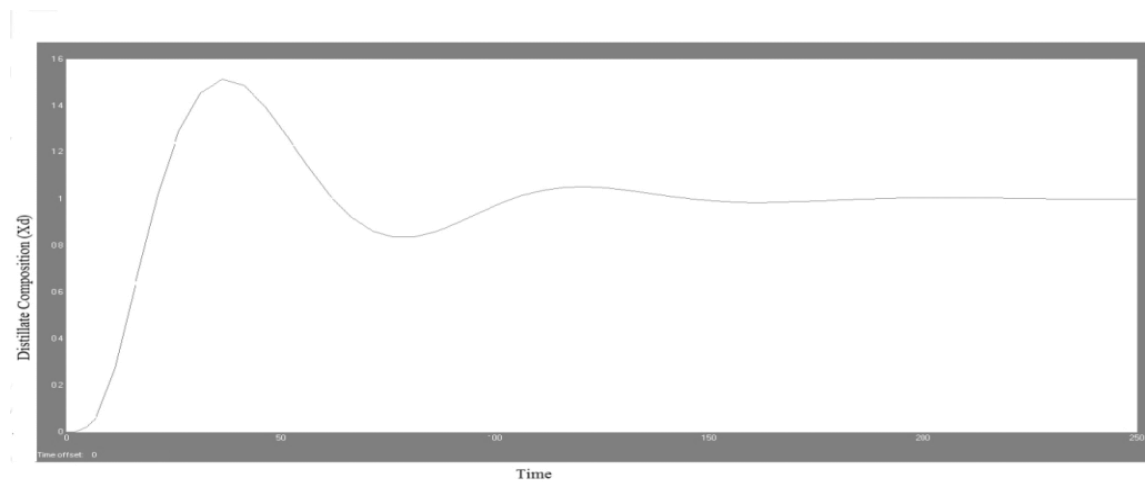
Response of PID Controller:

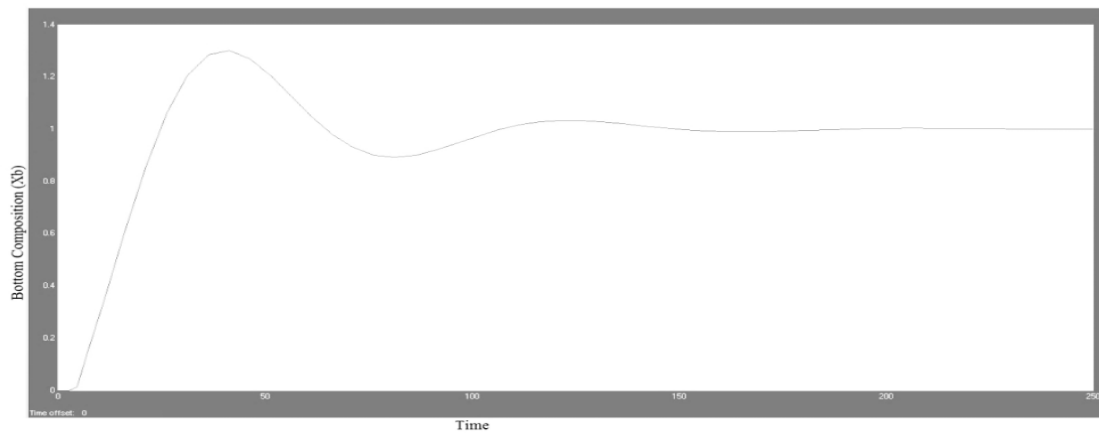**Figure 4.5**: Response of Distillate Composition by Using PID Controller

Figure 4.6: Response of Bottom Composition by Using PID Controller

Response of MPC

Design parameters from table 2.1 found out $M=17$, $P=73$, $T=1.5$ setting other parameters defaults.
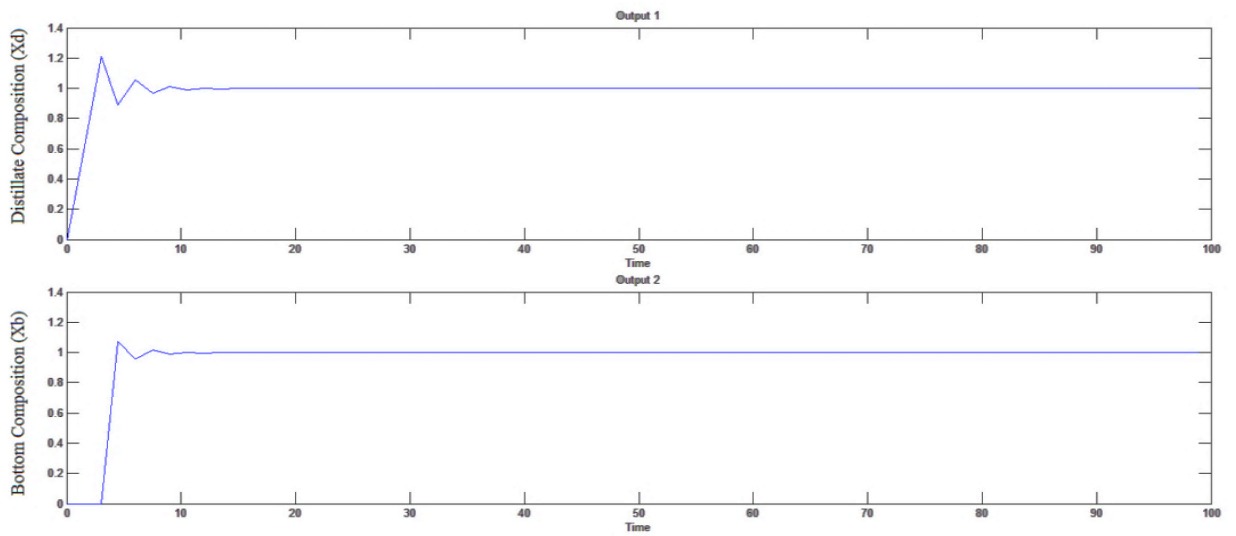
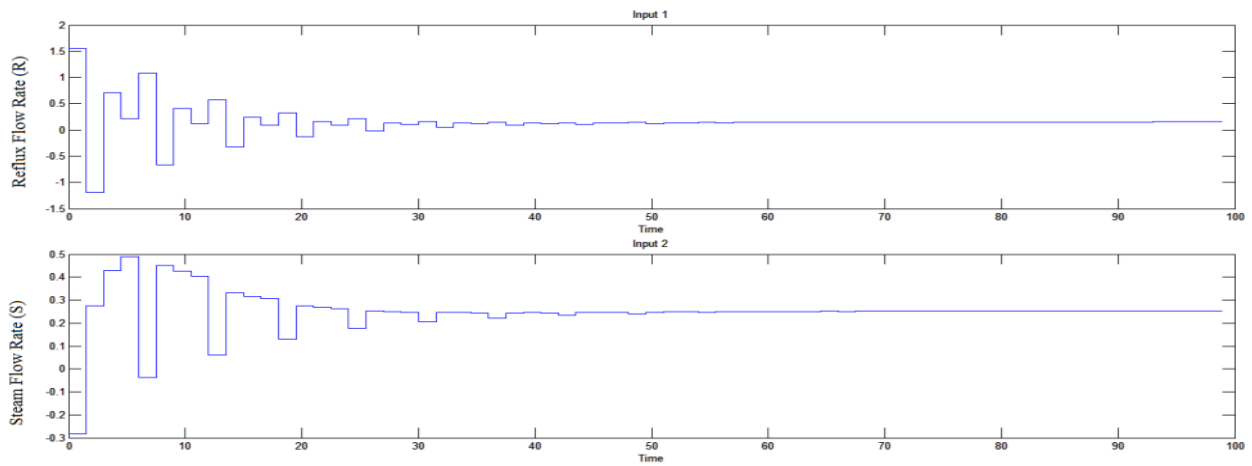**Figure 4.7a:** Response of Wood and Berry without Default

Figure 4.7b: Manipulated Variables Plot Without Default

But in above case, manipulated variables are ringing, so now tried to reduce ringing with the change in design parameters. For reduce ringing, taking design parameter $M=5$, $P=10$, and $T=1.5$.
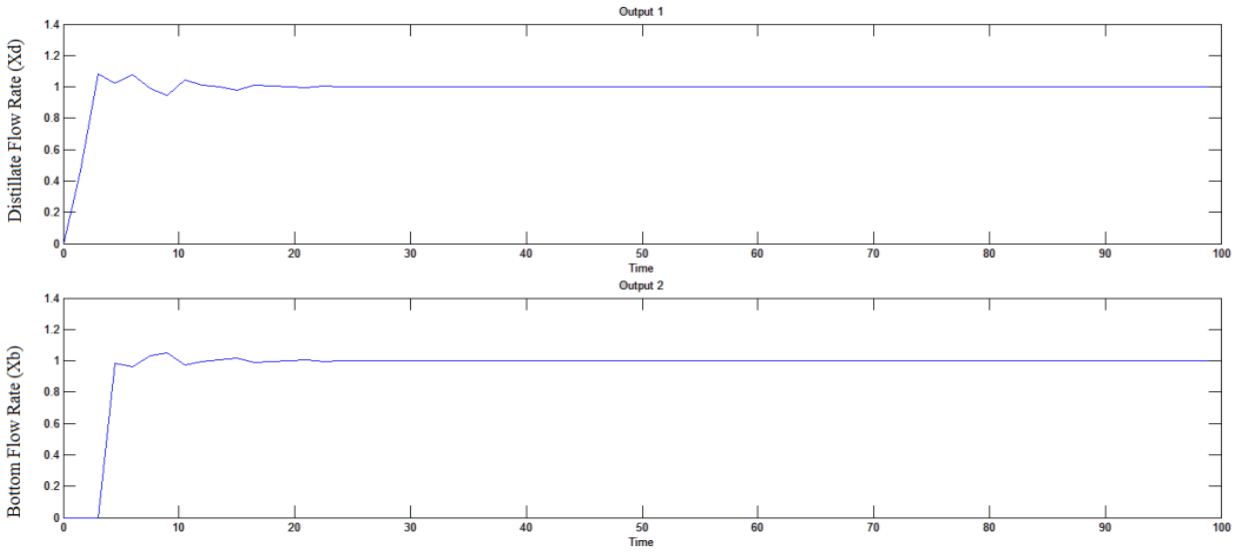
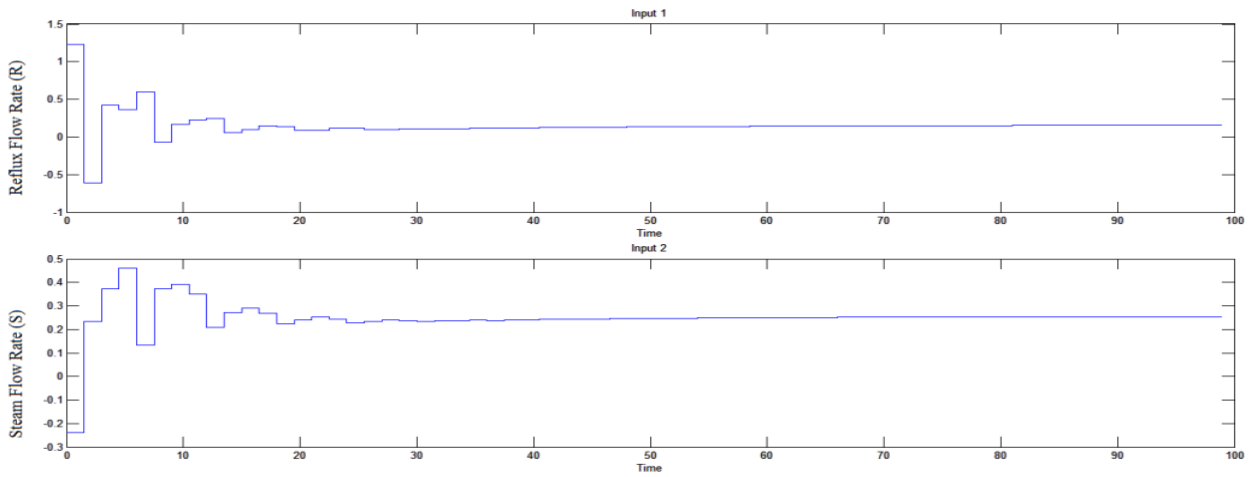**Figure 4.8a:** Response of Wood and Berry with Default

Figure 4.8b: Manipulated Variables Plot with Default
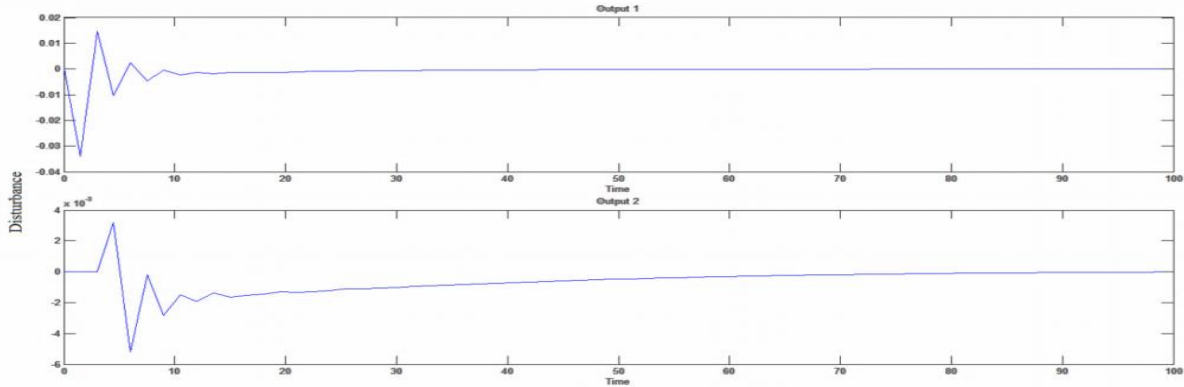
Disturbance Rejection

Figure 4.9: Disturbance Rejection Plot of Wood and Berry Process

In above figure 4.8a and 4.8b manipulated variables ringing less than figure 4.5a and 4.5b. It indicates that with the change of design parameter, ringing of manipulated variable can be reduced.

4.3.2.2 3×3 Distillation Process

$$
\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \dfrac{0.66e^{-2.6s}}{(6.7S+1)} & \dfrac{-0.61e^{-03.5s}}{(8.64S+1)} & \dfrac{-0.0049e^{-s}}{(9.06S+1)} \\ \dfrac{-1.11e^{-6.5s}}{(3.25S+1)} & \dfrac{-2.3e^{-3s}}{(5S+1)} & \dfrac{-0.012e^{-0.5s}}{(7.09S+1)} \\ \dfrac{-34.68e^{-9.2s}}{(8.15S+1)} & \dfrac{46.2e^{-9.4s}}{(10.9S+1)} & \dfrac{-0.0032(19.62s+1)e^{-2.6s}}{(8.94S+1)(7.29S+1)} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} +
$$

$$
\begin{bmatrix} \dfrac{0.1e^{-12s}}{(6.2S+1)} & \dfrac{-0.0011(26.32S+1)e^{-}}{(7.85S+1)(14.63S+1)} \\ \dfrac{0.53e^{-10.5s}}{(6.9S+1)} & \dfrac{-0.0032(19.62S+1)e^{-3.44}}{(7.29S+1)(8.94S+1)} \\ \dfrac{-11.54e^{-0.6s}}{(7.01S+1)} & \dfrac{0.32e^{-2.6s}}{(7.76S+1)} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}
\qquad (4.57)
$$

Above equation given by (Ogunnaike and ray) to separate ethanol and water, where Y_1 is overhead ethanol mole fraction, Y_2 side stream ethanol mole fraction and Y_3 is 19 tray

temperature (^{0}C) (corresponding to bottoms composition). The inputs are u_1 reflux flow rate (m^3/s), u_2 side stream product flow rate (m^3/s), u_3 reboiler stream (kPa). The disturbance is d_1 feed flow rate (m^3/s) and d_2 feed temperature, (^{0}C).[8]

When used DMC tuning strategy from table 2.1 then *M*=30, *P*=90, *T*= 0.71
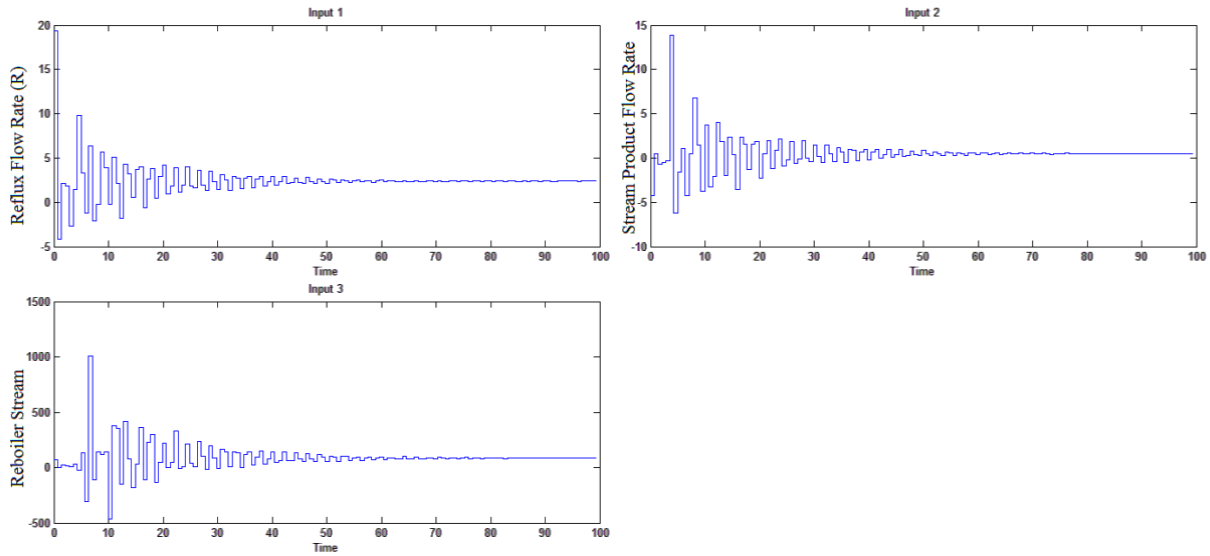

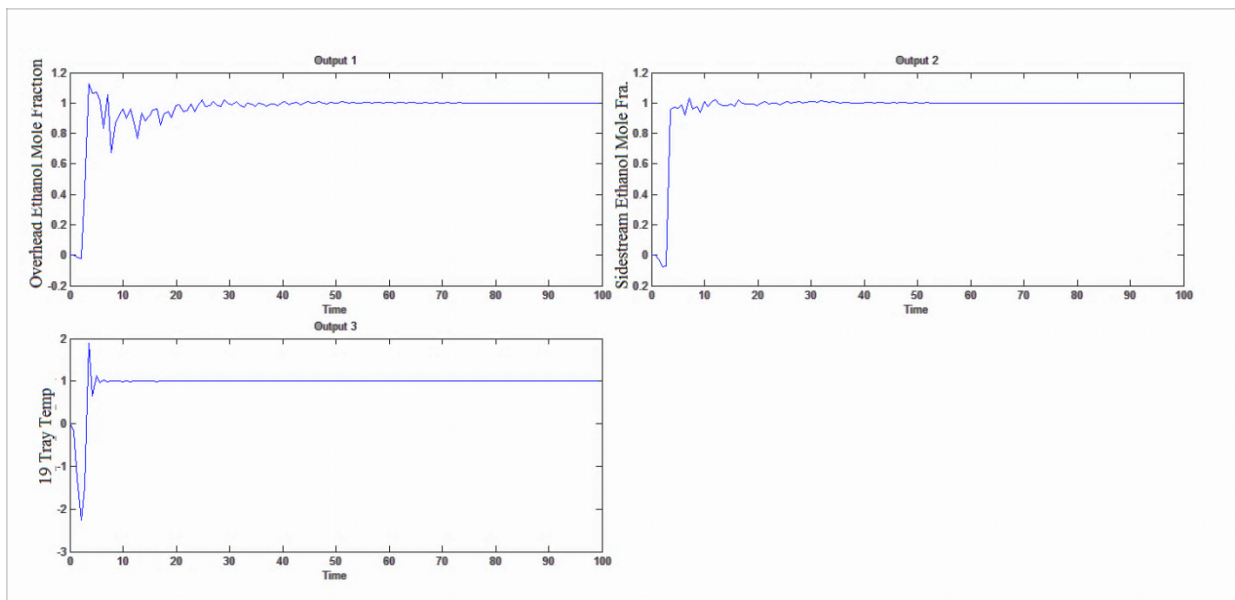**Figure 4.10a:** Manipulated Variables Plot without Default

Figure 4.10b: Response of 3 × 3 Process without Default

But in both of case manipulated variable ringing so now try to reduce ringing with the change of parameter to $T=1.5$, $M=5$, $P=10$, $N=60$.
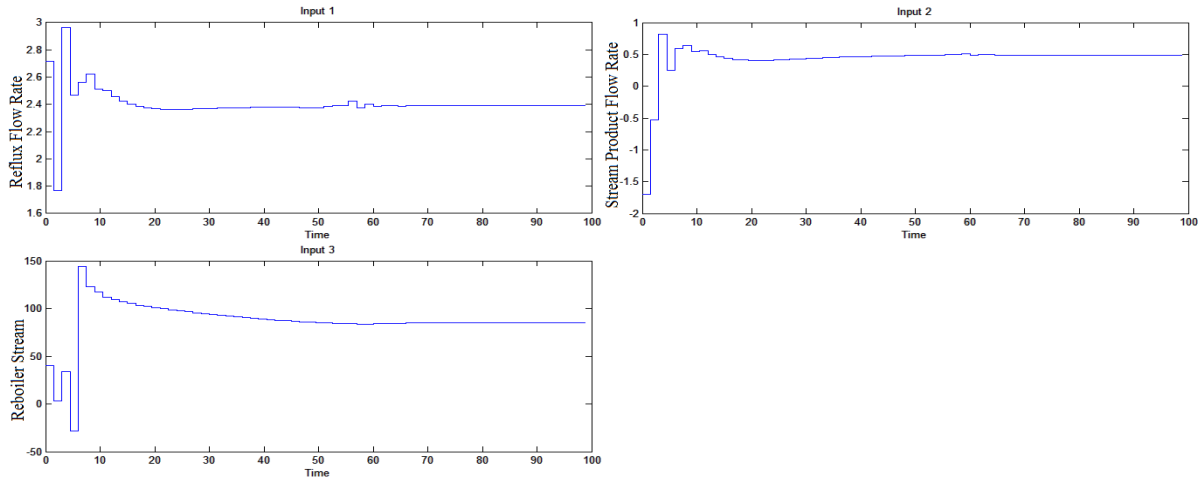

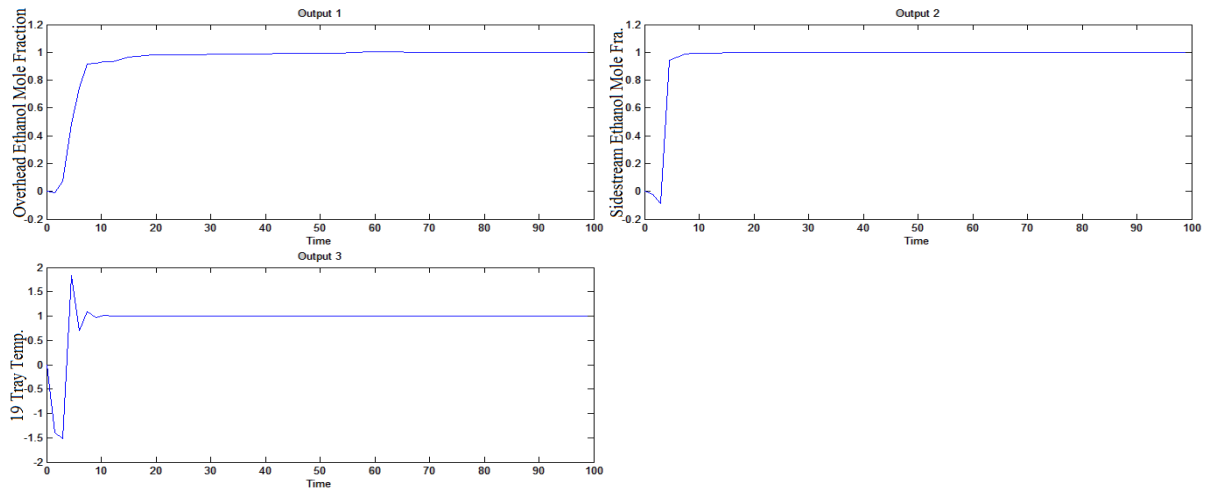
Figure 4.11a: Manipulated Variables Plot with Default

Figure 4.11b: Response of 3×3 Processes with Default
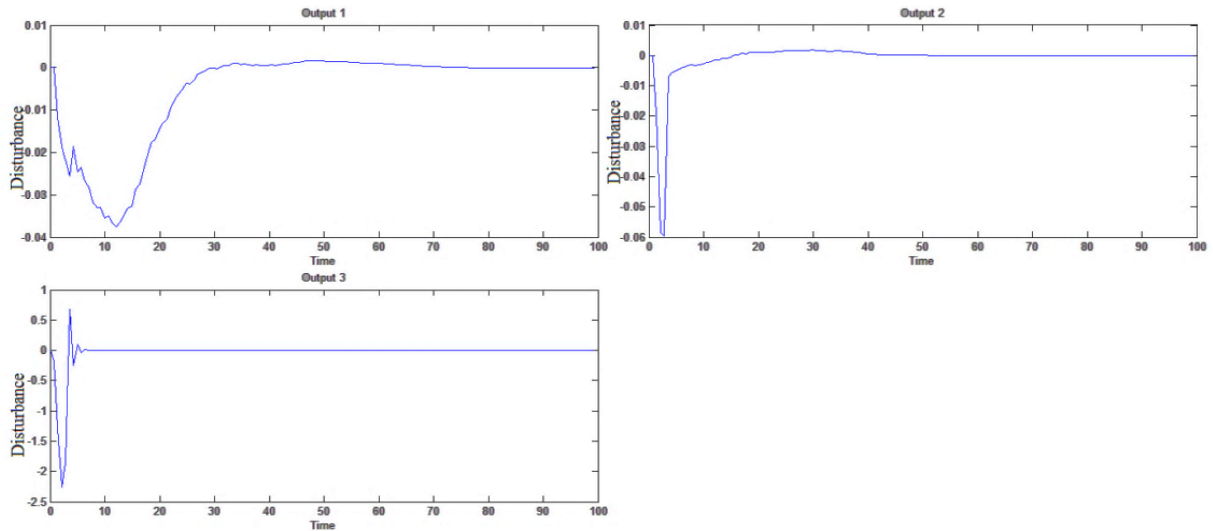
Disturbance Rejection

Figure 4.12: Disturbance Rejection Plot for 3×3 Process

In above figure 4.11a and 4.11b manipulated variables ringing less than figure 4.10a and 4.10b. It indicates that with the change of design parameters, ringing of manipulated variable can be reduced. It rejects the disturbance early compare to without default.

4.3.2.3   4 × 4 Distillation Process:

$$
\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{bmatrix} =
\begin{bmatrix}
\dfrac{-11.3e^{-3.79s}}{(21.74S+1)(21.74S+1)} & \dfrac{0.3746e^{-7.75s}}{(31.6S+1)(22.2s+1)} & \dfrac{-9.811e^{-1.59s}}{(11.36S+1)} & \dfrac{-2.3711e^{-27.33s}}{(33.3S+1)} \\
\dfrac{-5.24e^{-60s}}{(400S+1)} & \dfrac{-1.986e^{-0.71s}}{(66.7S+1)} & \dfrac{-5.984e^{-2.24s}}{(14.29S+1)} & \dfrac{0.422e^{-8.72s}}{(250S+1)^2} \\
\dfrac{-0.33e^{-0.68s}}{(2.38S+1)(2.38S+1)} & \dfrac{0.0204e^{-0.59s}}{(7.14S+1)(7.14S+1)} & \dfrac{2.38e^{-0.42s}}{(1.43S+1)(1.43S+1)} & 0.513e^{-s} \\
\dfrac{-4.488e^{-0.52s}}{(11.11S+1)} & \dfrac{-0.176e^{-0.48s}}{(6.90S+1)(6.90S+1)} & \dfrac{-11.67e^{-1.191s}}{(12.19S+1)} & 15.54e^{-s}
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}
\qquad (4.58)
$$

The above 4 × 4 process is presented by Doukas and Luyben. They studied the dynamic of a distillation column producing a liquid side stream product. The controlled and manipulated variables are Y_1(toluene impurity in the bottom), Y_2(toluene impurity in the distillate),Y_3(benzene

impurity in the side stream), and Y_4(xylene impurity in the side stream); u_1(side stream flow rate), u_2(reflux ration), u_3(reboil duty), and u_4(side draw location).[9]

Above process has eight FOPDTs, six SOPDTs, and two dead times. The six SOPDT models are changed to FOPDTs model in order to apply DMC tuning, DMC tuning find out from table (4.1) is M=1087, T=0.5 and P=4370. The huge DMC parameters are caused by the transfer function g24. MPC controller gives an error statement using DMC tuning from table (4.1).

Below MPC controller output at come at default setting where T=0.1, M=5 P=10, N=60
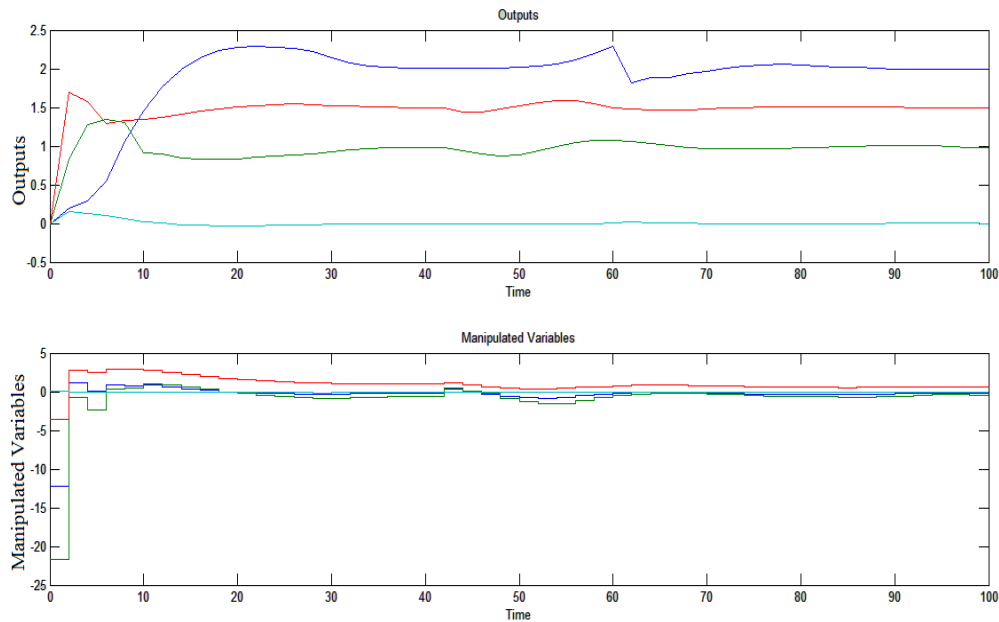

Figure 4.13: Response and Manipulated Variables Plot with Default for 4×4 Process

After studying the response of PID and MPC on SISO and MIMO system, it is seen that MPC gives good performance especially in multivariable process than PID controller. For SISO system, the conventional PID controller is used because SISO system can easily be controlled using PID controller than MPC. So PID is preferred over MPC for SISO system since MPC parameters are difficult in tuning.

References

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9) Doukas, N. And Luyben, W. L., "Control of Sidestream Columns Separating ternary mixtures. Instrumentation Technology", 25, 43-48, 1978.

CHAPTER 5

CLOSED LOOP SIMULATION OF BATCH CRYSTALLIZATION PROCESS USING MPC

CHAPTER 5

CLOSED LOOP SIMULATION OF BATCH CRYSTALLIZATION PROCESS USING MPC

I have considered a batch crystallization process to control its crystal kinetics by controlling crystal size distribution (CSD) using MPC controller. A model equation 2.18-2.34 developed in chapter are used to convert its state space matrices. Since these equations are interrelated to each other in very complicated manner, it is necessary to convert these state space matrices in simplified form for mathematical simplicity. For this, certain canonical forms are used shown in equations 5.2-5.12.

5.1 State Space Representation of Transfer Function System

Transfer function of a process can be converted to state space (SS). The state space representation of a transfer function

$$\frac{y(s)}{U(s)} = \frac{b_0 s^n + b_1 s^{n-1} + \cdots \ldots + b_{n-1} s^1 + b_n}{s^n + a_1 s^{n-1} + \cdots \ldots + a_{n-1} s + a_n} \tag{5.1}$$

can be written in diagonal, controllable, observable and controllable canonical forms.

5.1.1 Controllable Canonical Form

Conversion of transfer function to SS in controllable Canonical form is essential in designing the process trough pole placement method. SS representation in a controllable canonical form is given as: [1]

$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ . \\ . \\ \dot{x}_{n-1} \\ \dot{x}_n \end{bmatrix} =
\begin{bmatrix}
0 & 1 & 0 & . & . & 0 \\
0 & 0 & 1 & . & . & 0 \\
. & . & . & . & : & : \\
. & . & . & : & : & : \\
0 & 0 & 0 & : & : & 1 \\
-a_n & -a_{n-1} & -a_{n-2} & : & : & -a_1
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ x_{n-1} \\ x_n \end{bmatrix} +
\begin{bmatrix} 0 \\ 0 \\ . \\ . \\ 0 \\ 1 \end{bmatrix} u \tag{5.2}
$$

$$y = [b_n - a_n b_0 \quad b_{n-1} - a_{n-1} b_0 \ldots b_1 - a_1 b_o] \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + b_0 u \tag{5.3}$$

5.1.2 Observable Canonical Form.

Equations 5.4 and 5.5 represent a controllable canonical form.

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} 0 & 0 & \cdot & 0 & -a_n \\ 1 & 0 & \cdot & 0 & -a_{n-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \ddots & \cdot & \cdot \\ 0 & 0 & \cdot & 1 & -a_1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} b_n - a_n b_0 \\ b_{n-1} - a_{n-1} b_0 \\ \cdot \\ \cdot \\ \cdot \\ b_1 - a_1 b_0 \end{bmatrix} u \tag{5.4}$$

$$y = [0 \quad 0 \quad \ldots 0 \quad 1] \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + b_0 u \tag{5.5}$$

5.1.3 Diagonal Canonical Form.

Here it is considered than denominator of transfer function represented in equation 5.1consists of distinct roots. So equation (5.1) is given as

$$\frac{y(s)}{U(s)} = \frac{b_0 s^n + b_1 s^{n-1} + \cdots \ldots + b_{n-1} s^1 + b_n}{(s + p_1)(s + p_2) \ldots \ldots (s + p_n)}$$

$$= b_0 + \frac{c_1}{s + p_1} + \cdots \ldots + \frac{c_n}{s + p_n} \tag{5.6}$$

Then representation of SS in diagonal canonical form is

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} -p_1 & 0 & 0 \cdot & \cdot & 0 \\ \cdot & -p_2 & \cdot \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot \cdot & \cdot & \cdot \\ 0 & 0 & 0 \vdots & \vdots & 0 \\ o & 0 & 0 \vdots & \cdot & -p_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix} u \tag{5.7}$$

$$y = [c_1 c_2 \,.... \ c_n]\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ . \\ x_n \end{bmatrix} + b_0 u \tag{5.8}$$

5.1.4 Jordan Canonical Form

Diagonal form should be modified into Jordan Canonical Form when roots of denominator of equation 5.1 are multiple. All the roots are different from one another except first three are $p1 = p2 = p3$. Then equation 5.1 became

$$\frac{Y(s)}{U(s)} = \frac{b_0 s^n + b_1 s^{n-1} + \cdots \ldots \ldots + b_{n-1} s + b_n}{(s + p_1)^3 (s + p_4)(s + p_5) \ldots \ldots (s + p_n)} \tag{5.9}$$

The partial fraction representation of above equation is

$$\frac{Y(s)}{U(s)} = b_0 + \frac{c_1}{(s + p_1)^3} + \frac{c_2}{(s + p_1)} + \cdots \ldots \ldots \ldots + \frac{c_n}{(s + p_n)} \tag{5.10}$$

A SS representation of Jordan canonical form is given as

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ . \\ . \\ . \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} -p_1 & 1 & 0 & 0 & . & 0 \\ 0 & -p_1 & 1 & . & . & . \\ 0 & 0 & -p_1 & 0 & : & 0 \\ 0 & : & 0 & -p_4 & : & 0 \\ 0 & : & : & . & : & : \\ : & : & : & : & : & : \\ 0 & . & 0 & 0 & . & -p_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ . \\ . \\ . \\ x_n \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \\ . \\ . \\ . \\ 1 \end{bmatrix} u \tag{5.11}$$

$$y = [c_1 c_2 \,.... \ c_n]\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ . \\ x_n \end{bmatrix} + b_0 u \tag{5.12}$$

The state-space representation of transfer function in above canonical forms is necessary in designing and controlling of process since modern control system has many inputs and outputs and are interrelated to each other in very complex manner. Canonical forms helps in reducing complexity of mathematical form and helps in restoring this simple form in computers for tedious computations. [1]

5.2 Analysis of Control System in State Space

5.2.1 Controllability

If a process can be transferred from its initial state $x(t_0)$ to any other state in a limited time interval, then process is said to be completely controllable at time t_0.[1]

Conditions of controllability and observability determine the existence of a complete solution of problem while designing a system. It also plays an important role in representing a system in state space. The concept was introduced by a scientist Kalman. The solution of control problem will not exist if a system is not controllable. Then to obtained a control on system, it is essential to find the conditions where system can be controllable and observable. Considering a system having state space representation:

$$\dot{x} = Ax + Bu \tag{5.13}$$

$$y = Cx + Du \tag{5.14}$$

Where, x and y is state and output vector of rank of n and m respectively. u is the control signal (scalar).A, B, C, D are the coefficient matrix of rank $n \times n$, $n \times r$, $m \times n$, $m \times r$.[1]

State Controllability

If a system represented in equations (5.13) and (5.14) can be transferred from an initial state to any final state in a limited time interval $t_0 < t < t_1$ by constructing an unconstrained control signal, then system said to be state controllable at time $t = t_0$. System is called as

completely controllable if all states of a system are controllable. Condition is fulfilled if a $(n \times n)$ represented by $[B \vdots AB \vdots \cdots A^{n-1}B]$ is having a rank n. [1]

Output Controllability

Output controllability of a system is also important since complete state controllability doesn't mean that outputs can also be controlled. A system is called a Output controllable if its initial output $y(t_0)$ can be transferred to any final output $y(t_1)$ in a finite time interval $t_0 < t < t_1$ by constructing an unconstrained control vector $u(t)$. For a system to be a output controllable, its $[CB \vdots CAB \vdots \cdots CA^{n-1}B]$ matrix should have rank n. [1]

5.2.2 Observability

If every state $x(t_0)$ can be determined from the observation of $y(t)$ over a limited time interval, $t_0 < t < t_1$, then a system said to be completely observable. Observability of a system is checked by finding a rank of $n \times n$ matrix $[C^* \vdots A^*C^* \vdots \cdots (A^*)^{n-1}C^*]$, for a process to be completely observable, its rank should be n. [6]

The concept of observability is important when all the states of a system are not completely measurable. The system is not observable is all states are not measurable. [1]

5.3 Closed Loop Simulation on Batch Crystallization Process

State space matrices of batch crystallization process are found out using model equations 2.18-2.34 from chapter 2. For mathematical simplicity, matrices are converted to Controllable Canonical Form discussed in equation 5.2 and 5.3. Controllable Canonical Form of obtained matrices is:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 32 & 65 & 3377 & 29 & 5069 \end{bmatrix} \tag{5.15}$$

$$B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.067 \end{bmatrix} \qquad (5.16)$$

$$C = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad (5.17)$$

$$D = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (5.18)$$

State-space model was used to implement the MPC. The controllability and observability of the processes was checked before the design of the controllers. Closed looped response of MPC on batch crystallizer is obtained using MPC simulation toolbox in MATLAB software.
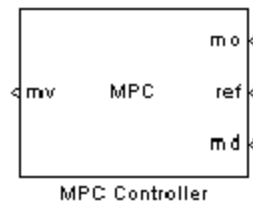
Figure 5.1: MPC Toolbox

The MPC Controller block requires current measured output, reference signal, and measured disturbance signal and optimal manipulated variables after solving a quadratic program. After opening MPC toolbox, a window comes demanding import of plant and controller as shown in figure 5.2.
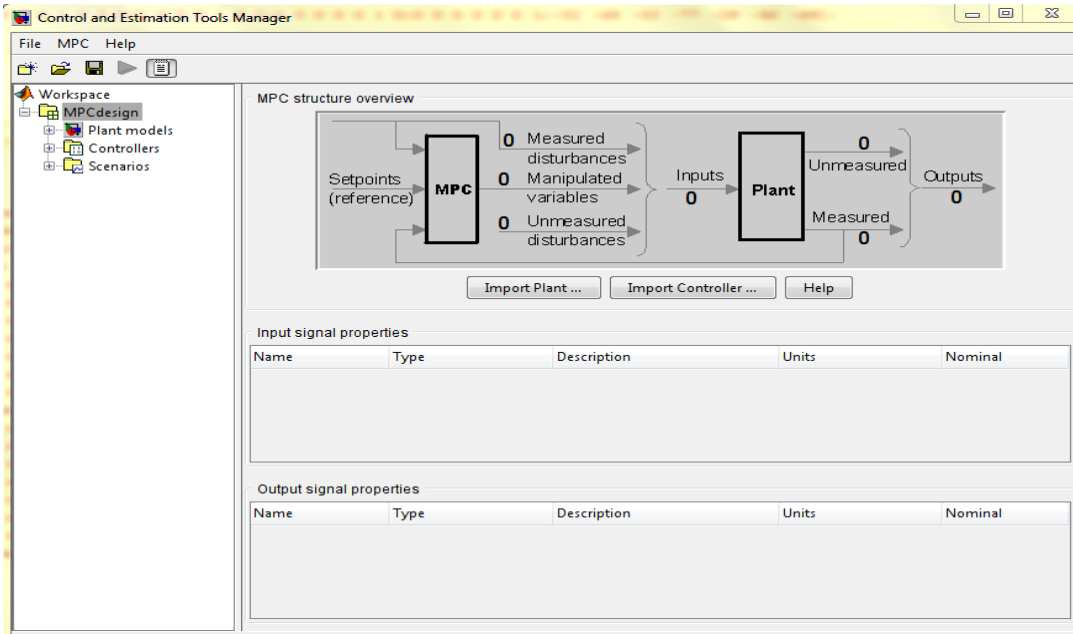
Figure 5.2: Control and Estimation Tools Manager

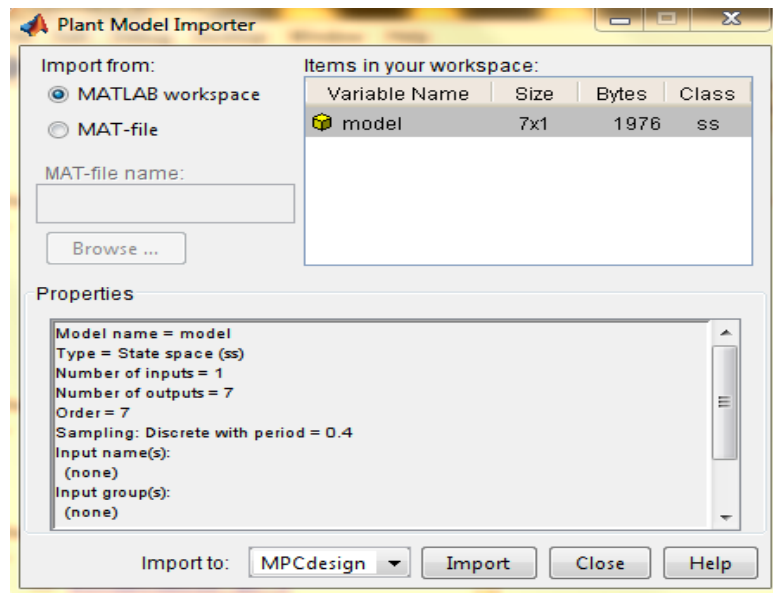Plant can be imported either by specifying it in workspace or by uploading a mat file as shown in figure 5.3.

Figure 5.3: Plant Model Importer

Once a plant gets imported, Control and Estimation Tools Manager represents its complete description. Since our model of batch crystallization process has seven output and one input, it is shown in figure 5.4.
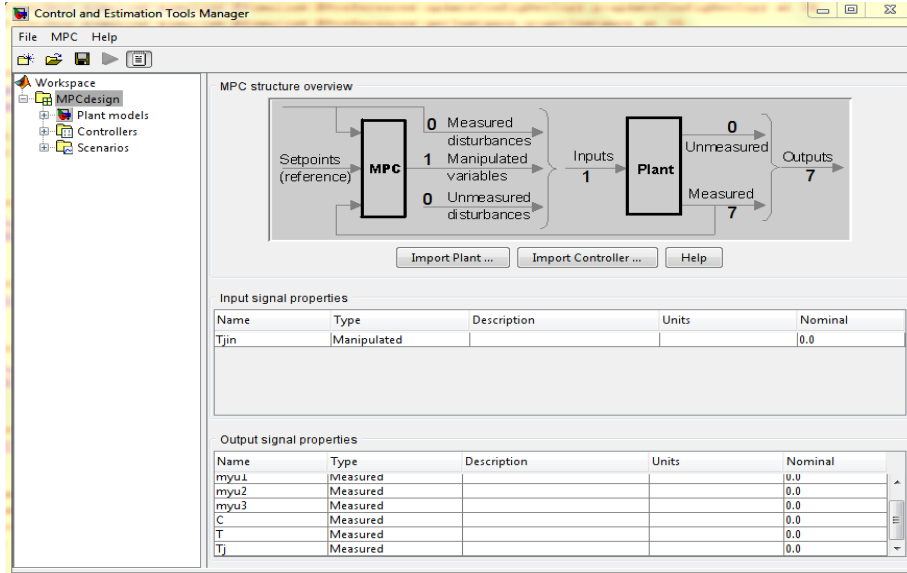

Figure 5.4: Control and Estimation Tools Manager Representing Plant Description

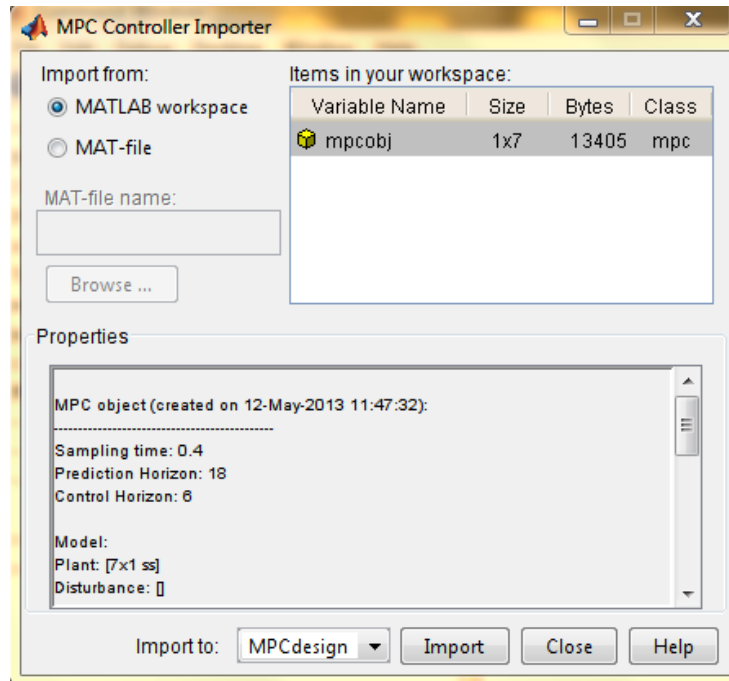Controller is imported in the same manners as a plant shown in figure 5.5.

Figure 5.5: MPC Controller Importer

Control and Estimation Tools Manager after importing controller describes controller with sampling time, number of prediction and control horizon shown in figure 5.6.
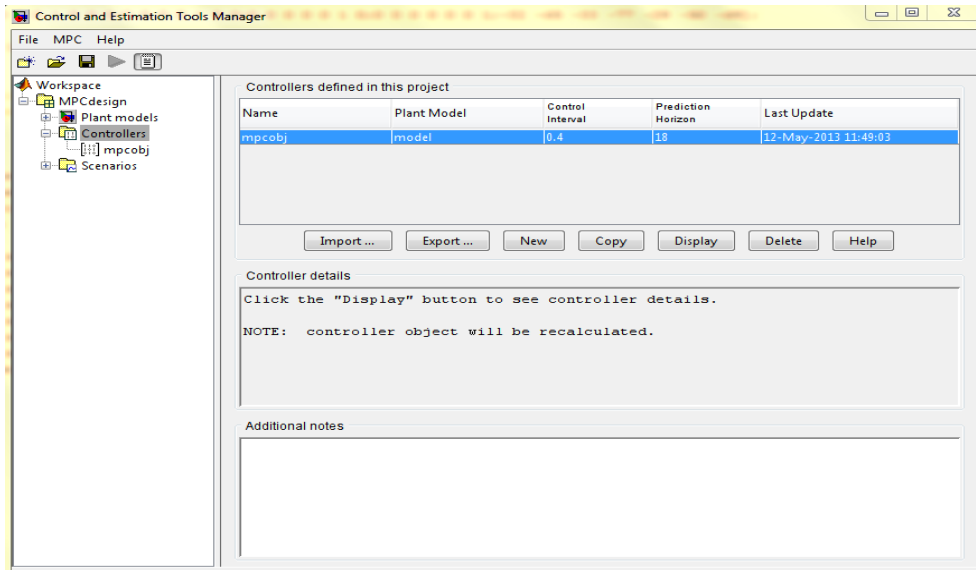

Figure 5.6: Control and Estimation Tools Manager Representing Plant Description

After a succsessful importing of plant and controller, we have to specify the type in which we want output response. In our model, step type is given to state variables in between 0 to1 shown in figure 5.7.
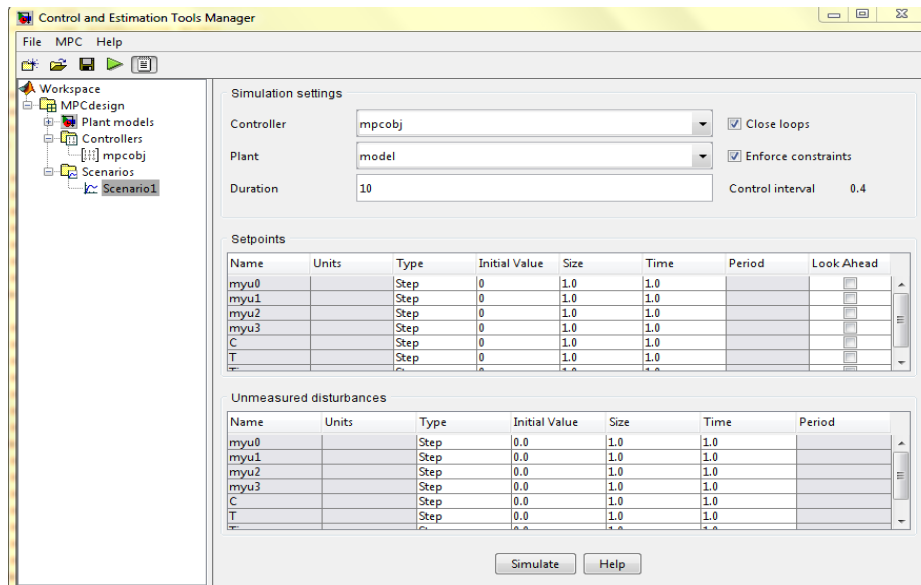

Figure 5.7: Control and Estimation Tools Manager Representing Output Scenario

By designing a MPC controller with prediction horizon as 18 and control horizon as 6 with sampling time of 0.4 second for 10 minutes, controlled state variables of batch crystallization process obtained are given in figure 5.8.
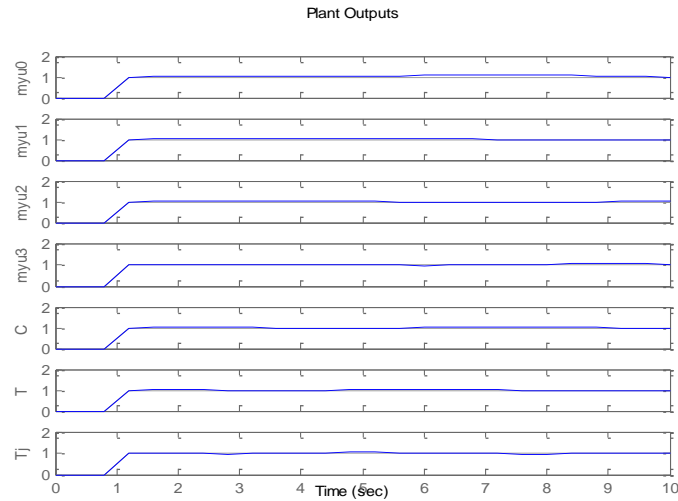

Figure 5.8: Close Loop Response for Batch Crystallizer Using MPC Controller for *P*=18, *M*=6

REFFERENCE

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CHAPTER 6

CONCLUSIONS AND FUTURE RECOMMENDATION

CHAPTER 6
CONCLUSIONS AND FUTURE RECOMMENDATION

Conclusions

The primary research objective of this thesis is to evaluate the opportunities for real-time model-based control to improve product quality and process productivity of industrial batch crystallizers. The model-based control of batch crystallizers is used. The problem of distributed characteristics of PBE is solved by considering moment of crystals. It has been shown that model imperfections and process uncertainties are largely detrimental by the performance of nonlinear model-based controller. But the validation of process models and performance monitoring was cumbersome due to limitations in measurement of process variables. So model predictive controller approach is combined with Kalman filter to measure an unmeasured state variable. Then finally MPC toolbox of MATLAB simulation block is used to obtain desired CSD.

Future Recommendation

Deploying MPC controller for mixed suspension mixed product removal crystallizer (MSMPR) and semi batch crystallization process.