Modeling & Control of Methoxy-Methyl-Heptane Separation Process

by

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ABSTRACT

A study in Lehigh University Bethlehem, Pennsylvania has proposed the chemical 2-methoxy-2-methylheptane (MMH) as a great alternative gasoline additive to replace methyl *tert*-butyl ether (MTBE) in order to avoid groundwater contamination. In MMH production process, the chemistry involves the liquid phase reversible reaction of methanol with 2-methyl-1-heptene (MH) to form MMH. However, methanol and MH also undergo an undesirable reaction to form dimethyl ether (DME) and 2-methyl-2-heptanol (MHOH). The approach adopted in this paper is to do a modeling and control of the MMH separation process to achieve a specified yield of MMH. The MMH separation process features three distillation columns in series. The first distillation column separate DME from the rest of product, second distillation column separates MH from the rest of product, and the third distillation column separates the final product MMH from MHOH. Process model is obtained through system identification using input-output testing data. A model predictive control strategy would be developed to replace regulatory control in order to sustain production at optimum cost the current regulatory control. This project also explained the function of gasoline additive, why replacement of MTBE with MMH as gasoline additive is needed, and MTBE's effect on environment.

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CHAPTER 1
INTRODUCTION

1.1 Background of Study

Currently, methyl *tert*-butyl ether (MTBE) is used as main gasoline additives. These additives help fuel burns cleaner and more efficient. However, MTBE also caused groundwater contamination, which has become a big environmental crisis that need to be solved immediately. Leakage from gasoline storage tanks has caused MTBE to be found in soil, groundwater and drinking sources. A small of MTBE in water can render the water undrinkable due to its foul smell and taste, besides containing a human and animal carcinogen, a compound that may cause cancer to both human and animal. Latest research has proposed the chemical 2-methoxy-2-methylheptane (MMH) as an alternative gasoline additive to replace MTBE. MMH production process is a really important process in order to solve this groundwater contamination problem. In this process the chemistry involves the liquid phase reversible reaction of methanol with 2-methyl-1-heptene (MH) to form MMH. However, methanol and MH also undergo an undesirable reaction to form dimethyl ether (DME) and 2-methyl-2-heptanol (MHOH). With the introduction of MMH as new gasoline additives, there is potential of MMH to become one of the largest produced and most important chemical in the near future.

1.2 Problem statement

The chemical 2-methoxy-2-methylheptane (MMH) is proposed as an alternative of gasoline additive to replace methy tert-butyl ether (MTBE) in order to avoid groundwater contamination. The chemistry involves the liquid phase reversible reaction of methanol with 2-methyl-1-heptene (MH) to form MMH. However, methanol and MH also undergo an undesirable reaction to form dimethyl ether (DME) and 2-methyl-2-hepthanol (MHOH). We need to construct a modelling of a process that can increase desirable yield MMH and minimize the undesirable reaction. The process itself also needs a base layer control to handle large disturbances in production rate and operating parameters. We then need to construct a model predictive control (MPC) for this process. Model predictive controllers rely on dynamic models of the process, most often linear empirical models obtained by system identification.

1.3 Objectives & Scope of the Study

The objectives of this research are:

1. Construct a steady state and dynamic modeling of Methoxy-Methyl-Heptane Separation Process
2. Construct a model predictive control (MPC) strategy for Methoxy-Methyl-Heptane Separation Process

The whole project would start with the knowledge gathering and theoretical studies. The study on process modeling and model predictive control is to be completed within approximately one year time frame (two semesters).The project can be divided into two phase. The scope of phase 1 is to do steady state modeling and dynamics modeling of the separation process based on MMH production process designed by William L. Luyben. The method is to use HYSYS process simulation software. For phase 2, a model predictive control (MPC) system will be constructed through system identification on the dynamic model using MATLAB and the process will be further analyzed in order to achieve optimized production of MMH. Meanwhile, further research and development would be continuously practiced to ensure satisfactory results are achieved.

CHAPTER 2
LITERATURE REVIEW

2.1 Why MMH is needed to replace MTBE as gasoline additives.

In order to understand the importance of study on MMH process, it is better to understand the reason of MTBE replacement as gasoline additives with MMH. Under this section the author will discuss the origin of gasoline additives, background of MTBE, MTBE in groundwater, and human health effects of MTBE.

2.1.1 The Origin of Gasoline Additives

Ever since the early days of the automobile, petroleum refiners have worked to increase the combustion efficiency of their product, usually by addition of octane-enhancing fuel additives. Based on study by Jacob (2001), one of the earliest fuel additives used is ethanol, which traditionally manufactured by fermentation of plant material. However, ethanol is expensive, due to its popular association with beverage ethanol or whiskey. Industrial ethanol was even taxed for some time in exactly the same manner as beverage alcohol. Tetraethyl lead, another octane-enhancing gasoline additive, eventually became the additive of choice for refiners. Lead was less "bulky" than ethanol, in other words, it took up less space in the gas tank. Tetraethyl lead became the main gasoline additive, until 1970s, when lead's detrimental environmental effects became widely recognized and denounced. The public outcry over these effects, coupled with the discovery of lead's damaging effects on emission control devices, resulted in the phase-out of the use of tetraethyl lead in gasoline. Ethers, such as methyl *tertiary*-butyl ether (MTBE), replaced tetraethyl lead as some of the petroleum industry's additives of choice. The continuing quest for a better gasoline additive, however, still did not end with the introduction of ethers due to some its disadvantages which will be discussed later in this paper.

2.1.2 Background of MTBE

MTBE, or methyl tertiary butyl ether, is an "oxygenate" that makes gasoline burn cleaner and more efficiently. Oxygenates are compounds that contain oxygen. Oxygenates added to gasoline to reduce ozone formation and carbon monoxide emissions and to enhance the octane level in gasoline. Octane enhancement began in the late 1970s with the phase-out of tetraethyl lead from gasoline. According to Green (2000) the use of oxygenates was expanded due to enactment of the Clean Air Act (CAA) Amendments of 1990, which required that oxygen be added to gasoline in areas where concentrations of ozone are most severe or where concentrations of carbon monoxide exceed air-quality standards. The CAA Amendments mandate that gasoline must contain at least 2% oxygen by weight in ozone nonattainment areas and at least 2.7% oxygen by weight in carbon monoxide nonattainment areas.

The CAA Amendments do not specify which oxygenate must be added to gasoline, but the one used most commonly today is MTBE. The second most frequently used oxygenate is ethanol. Under the mandates of the CAA Amendments, two programs of oxygenate use were established:

1. The Oxygenated Fuels Program (OXY) in which 15% MTBE by volume is added for use in carbon monoxide nonattainment areas
2. The Reformulated Gasoline Program (RFG) in which 11% MTBE by volume is added use in severe ozone nonattainment areas.

MTBE is preferred over other oxygenates due to:

1. Low cost
2. Ease of production
3. High octane level
4. Lower evaporative emissions in gasoline
5. Favourable transfer and blending characteristics

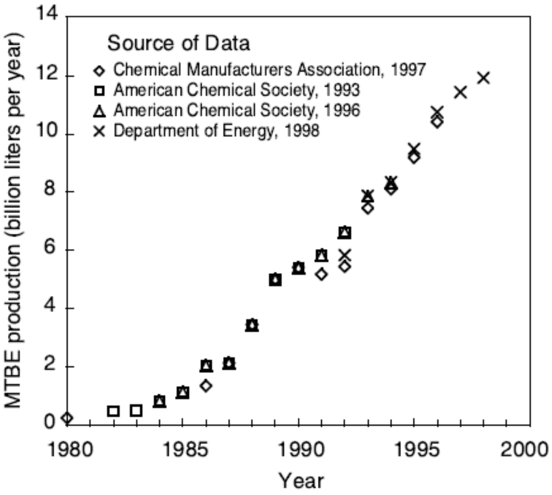


Figure 2.1: Estimated annual production of MTBE in the U.S. from four sources, 1980 to 1998.

Annual production of MTBE has increased from 0.26 billion l/year in 1980 to 11.9 billion l/year in 1998. The production of MTBE was the fourth largest of all chemicals produced in 1996.

2.1.3 Groundwater contamination by MTBE

Usage of MTBE as gasoline additives is originally intended either to boost octane ratings or to reduce the amount of harmful emissions, such as CO and ozone, which are the direct or indirect result of incomplete automobile combustion. However, recent discoveries showed potential of MTBE contribution on water pollution, or more specifically groundwater contamination. MTBE is a foul-tasting, nasty-smelling chemical, probable carcinogen which may cause cancer that spreads rapidly when gasoline escapes from leaky underground storage tanks, contaminating sources of groundwater and drinking water. Under this section the author will summarize current information on the occurrence and distribution of MTBE in groundwater and will be focusing on the MTBE groundwater contamination case in U.S since one of the most popular and severe groundwater contamination case reported is in U.S.

According to studies by Chang (2003), the gasoline containing MTBE has been stored in aboveground and underground storage tanks (ASTs and USTs) at a wide range of facilities, including refineries, terminals, and service stations. As a result of leaks and spills, MTBE, other fuel oxygenates, and other gasoline components have been found in soil and groundwater at these sites. Studies have found that these components, including MTBE, have reached drinking water sources in many locations. Deeb et al (2001) stated that once in soil or water, MTBE breaks down very slowly while it accelerates the spread of other contaminants in gasoline, such as benzene, a known carcinogen. MTBE have powerfully foul taste and smell meant that small concentrations could render water undrinkable, and that once it got into water supplies it was all but impossible to clean up.

Moran et al (2003) stated that the degradation of water supplies by MTBE contamination, specifically with regard to taste and odor considerations, has already seriously affected numerous public well fields across the U.S. Review of some of the reported groundwater contamination cases are as below:

1. In 1997, the City of Santa Monica, California shut down half of its water wells because of MTBE contamination, suffering a 75% loss of the local groundwater supply; the city spent $3 million importing water for its use.

2. In Maine, the presence of MTBE and other gasoline components in groundwater was evaluated in a study issued in 1998 by the State Department of Environmental Protection. Water samples were collected from 951 randomly selected household wells and other household water supplies such as springs and lakes. MTBE was detected in 150, or 15.8%, of the 951 private wells sampled. These numbers suggest that these levels of MTBE were present in 1400 to 5200 private wells in the state.

3. In Denver, Colorado, 79% of groundwater samples had detectable concentrations of MTBE, and in New England, 37% of the samples taken had detectable concentrations. The US Geological Survey (USGS) concluded from the data compiled in this study that MTBE tends to occur most often in shallow groundwater underlying urban areas.

4. In the report, “An Evaluation of MTBE Impacts to California Groundwater Resources,” released in June 1998 by Lawrence Livermore National Laboratory (LLNL), it have presented several conclusions regarding the potential of MTBE to pose a risk to California’s

> groundwater supplies. Among its other conclusions, the report stated that MTBE is a frequent and widespread contaminant in shallow groundwater throughout California, that it moves relatively quickly through groundwater, and that it is difficult to remove from the groundwater. Based on these conclusions, the LLNL report recommended that, while future research on MTBE is needed, groundwater resources should be managed in order to minimize the potential threat of MTBE. As of the date of the LLNL report, there were 32,409 leaking UST cleanup sites in California. Of these sites, 13,278 had groundwater that was impacted by gasoline components. Of the sites undergoing active cleanup studied in the LLNL report, 75% were sites impacted by MTBE, bringing the total of MTBE-impacted sites in the state to 10,000. The report also estimated that there are 6700 MTBE-impacted sites in California within 1/2 mile of a drinking water well.

Based on this study, it is not unreasonable to assume that the groundwater qualities of shallow aquifers in urban areas across the world are threatened with MTBE contamination. Thus, a situation similar to that which shut down half of Santa Monica’s wells may very well arise elsewhere.

2.1.4 Health Effects of MTBE

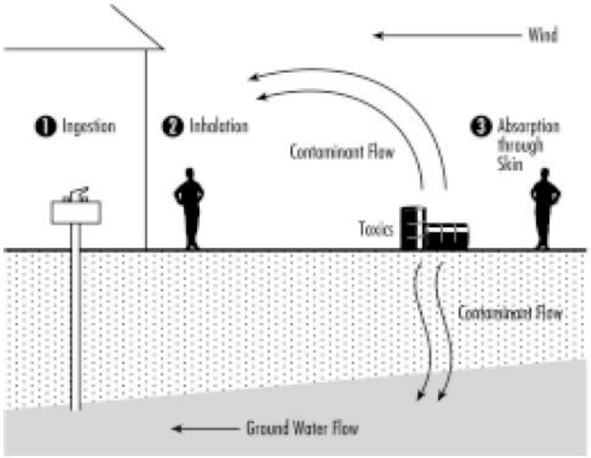


Figure 2.2: Sources and receptors of pollutants.

One of the reason groundwater contamination by MTBE is called this decade environmental crisis is due to its potential to cause cancer in human. This section explores the potential for MTBE to pose a cancer or non cancer human health risk, according to existing but limited data.

This section also compares the level at which MTBE is detected by taste or odor to the level or concentration of MTBE in drinking water that may pose a threat to human health.

James (2003) discussed that MTBE does not stay in the body long; it is released through exhalation and urine excretion. Following an exposure to MTBE, most of the substance will leave the body in about 2 days. The MTBE that is not released from the body is transformed (mostly through hydrolysis) into other compounds such as acetone, *tertiary*-butyl alcohol (TBA), methyl alcohol, formaldehyde, and carbon dioxide. Based on MTBE Risk Assessment Report in 2002, Formaldehyde is classified by the U.S. Environmental Protection Agency, (U.S. EPA) as a probable human carcinogen, and there is some evidence that TBA is an animal carcinogen in male rats and female mice.

2.1.5 Effort to replace MTBE as gasoline additives with alternatives.

a. Ethanol

Shore (2006) has discussed on efforts to replace MTBE as gasoline additives with alternatives such as ethanol. Some of the companies have already moved from MTBE to ethanol. Most companies eliminating MTBE in the short-run will blend ethanol into the gasoline to help replace the octane and clean-burning properties of MTBE. The rapid switch from MTBE to ethanol could have several impacts on the market that serve to increase the potential for supply dislocations and subsequent price volatility on a local basis. These impacts stem mainly from:

- Net loss of gasoline production capacity
- Tight ethanol market, limited in the short-run by ethanol-production capacity and transportation capability to move increased volumes to areas of demand
- Limited resources and permitting issues hampering gasoline supplier’s abilities to quickly get terminal facilities in place to store and blend ethanol
- Loss of import supply sources that cannot deliver MTBE-free product, or that cannot produce the high-quality blend stock needed to combine with ethanol

The different properties between MTBE and ethanol affect not only production, but distribution and storage of gasoline as well. Ethanol-blended gasoline cannot be intermingled with other gasoline during the summer months, and ethanol, unlike MTBE, must be transported and stored separately from the base gasoline mixture to which it is added until the last step in the distribution chain. Many areas of the distribution system cannot handle additional products without further investments. Due to this reasons, ethanol is viewed as not practical to be a replacement of MTBE.

b. Ethyl *Tert*-Butyl Ether (ETBE) and *Tert*-Amyl Ether (TAME).

Gasoline refiners have several others oxygenate options, including ethers such as ethyl *tert*-butyl ether (ETBE), *tert*-amyl methyl ether (TAME). In practice, however, MTBE has emerged as the dominant oxygenate in gasoline due to its lower cost and favorable transfer and blending characteristics. Production volumes of TAME and ETBE are lower than MTBE, however it is steadily increasing. Wezel et al. (2009) stated that in 2006, a third of the European production capacity of MTBE was adapted to produce ETBE.

A study in the Los Angeles area by Shih et al. (2004), concluded that although alternative ether oxygenates (such as TAME and ETBE) are detected in groundwater beneath leaking underground fuel tanks less frequent and at lower concentrations than MTBE, All indications (e.g. physical/chemical characteristics such as high solubility and low biodegradability) suggest that the alternative ethers would pose groundwater contamination threats similar to MTBE if their scales of usage were expanded.

Based on TAME Risk Assessment Report (2006), TAME has a pronounced taste and odour in water at low concentrations. However, there may be significant differences in the odour and taste thresholds depending on individual sensitivity, which can be affected e.g. by smoking. When the odour and taste thresholds in water are exceeded, the contaminated drinking water is normally not used, but another supply of drinking water is then utilized. When large and important reservoir of ground water serving as drinking water supply is contaminated, the consequences can be remarkable in terms of costs and as well as in terms of a need for temporary arrangements for drinking water.

- TAME is not considered to cause adverse health or toxic effects at taste and odour threshold level.

- Even the relatively small amount of TAME may render large reserves of ground water useless.

ETBE also may cause the same problem. Ahmed (2001) stated based on the good solubility of ETBE in water, it can be expected to enter the groundwater when it reaches the soil. Compared with MTBE, ETBE is less economical to produce, and TAME is more toxic. Due to these reasons, ETBE and TAME can be concluded as not the perfect solution to overcome groundwater contamination problem.

2.1.6 MMH as a better replacement to MTBE and other fuel additives.

In order to know why MMH is a better alternatives than MTBE as fuel additives, we would need to take a look at a paper by Gonzalez et al.(2008), which discussed the study on solubility of some fuel oxygenates in aqueous media in function of temperature. Fuel oxygenates studied includes MTBE, ETBE, TAME and diisopropyl ether (DIPE). These fuels oxygenates believed to have similar behaviour into the environment. The solubility of these chemicals is the key thermodynamic information for the assessment of the fate and transport of these pollutants.

According to Gonzalez et al., the ether solubility decreases in the following order: MTBE > ETBE > TAME > DIPE. It was observed that the solubility in water increases, when temperature decrease. The water solubility of ethers is higher for those molecules that show lower occultation of the ether group (higher polar potency) and then are more accessible for water molecules. Due to its molecular configuration, MTBE shows the highest values. MTBE shows a globular structure on the tert-butyl group and then steric hindrance for solvent molecules. Since the other ethers show similar structures, but of higher volume, the hydrogen bond potency into water media decreases towards heavier (as ETBE) and more branched ethers (as TAME and DIPE). Attending to the obtained results it is concluded that the decrease of solubility for rising temperatures is due to two different mechanisms

- Lower temperatures diminish molecular dynamics and then an increase of hydrogen bond potency is produced among polar groups. This fact increases the solubility for the whole ethers into water.
- Higher temperatures produce an increase of internal molecular dynamics. A rising occultation of ether group by steric hindrance was being produced. The probability of build hydrogen bonds is reduced and then lower solubility is observed.

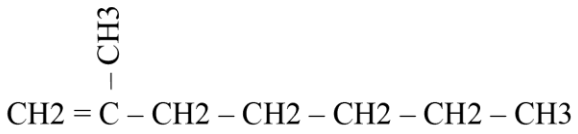
The temperature dependence of the solubility of ethers is a key factor to assess their fate when they are released to surface and groundwater and have to be taken into account in the risk assessments and remediation strategies.

It is concluded that those fuels oxygenates of highest molecular mass and branched structure shows the lowest pollutant character in terms of water solubility. Interestingly, this conclusion is parallel with Griffin et al. (2009) statement that 2-methoxy-2-methylheptane (MMH) which is a higher molecular weight ether will exhibit significantly decreased solubility thus be a good fuel oxygenate alternatives. Based in the results of the work, one can assume that DIPE is the less contaminant ether in terms of potential dispersion into aqueous media. The TBA influence on solubility of MTBE and ETBE is slight. At any case, temperature modifies solubility towards higher values when this magnitude diminishes in the studied temperature range.

2.2 Introduction to Methoxy-Methyl-Heptane

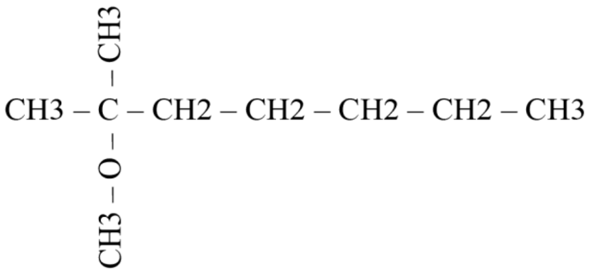
The chemical 2-methoxy-2-methylheptane (MMH) has been proposed as a gasoline additive to replace methyl *tert*-butyl ether (MTBE) in order to avoid groundwater contamination. The chemistry involves the reversible reaction of methanol with the unsaturated compound 2-methoxy-2-methylheptene (MH) to form 2-methoxy-2-methylheptane (MMH). The molecular structures of these components are as below:

MH: 2-methyl-1-heptene (C_8H_{16})



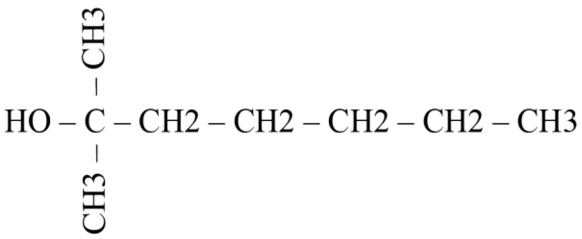
$$\mathrm{CH2} = \overset{\overset{\mathrm{CH3}}{|}}{\mathrm{C}} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH3}$$

MMH: 2-methoxy-2-methylheptane ($C_9H_{20}O$)



$$\mathrm{CH3} - \underset{\underset{\underset{\underset{\mathrm{CH3}}{|}}{\mathrm{O}}}{|}}{\overset{\overset{\mathrm{CH3}}{|}}{\mathrm{C}}} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH3}$$

MHOH: 2-methyl-2-heptanol ($C_8H_{18}O$)



$$\mathrm{HO} - \underset{\underset{\mathrm{CH3}}{|}}{\overset{\overset{\mathrm{CH3}}{|}}{\mathrm{C}}} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH2} - \mathrm{CH3}$$

Figure 2.3: Molecular structures.

2.3.1 Reaction Study

Luyben (2010) (1) stated the chemistry to produce 2-methoxy-2-methylheptane involves the liquid phase reversible reaction of methanol with 2-methyl-1-heptene (MH).

$$CH_3OH + C_8H_{16} \leftrightarrow C_9H_{20}O \qquad (1)$$

There is also undesirable reaction to form dimethyl ether (DME) and 2-methyl-2-heptanol (MHOH).

$$2CH_3OH + C_8H_{16} \rightarrow C_2H_6O + C_8H_{18}O \qquad (2)$$

The overall reaction rates have units of kmol s-1 kg-1. Concentrations are in terms of mole fractions.

$$\mathcal{R}_1 = k_{1F} x_{\mathrm{MeOH}} x_{\mathrm{MH}} - k_{1R} x_{\mathrm{MMH}} \qquad (3)$$

$$\mathcal{R}_2 = k_2 (x_{\mathrm{MeOH}})^2 \qquad (4)$$

Griffin et al. (2009) $^{(2)}$ studied the effect of competing reversible reactions on the optimum operating policies for plants with recycle. Table below gives the kinetic parameters for these reactions on the basis of the information given in Griffin.

		$\mathcal{R}_1$		$\mathcal{R}_2$
		forward	reverse	
k (overall reaction rate)	kmol s^{-1} $kg_{cat.}^{-1}$	6.7×10^{7}	2.1×10^{-6}	1.3×10^{9}
E	kJ/kmol	90000	900	105900
concentrations	mole fraction	$x_{\mathrm{MH}} x_{\mathrm{MeOH}}$	x_{MMH}	$(x_{\mathrm{MEOH}})^2$

Table 2.1: Kinetic Parameters

The activation energy of the forward MMH reaction is larger than that of the reverse reaction, which means that high reactor temperatures should favor conversion. Griffin et al. state that the upper temperature limit of the resin catalyst is about 400 K. To achieve a high yield of MMH, the methanol concentration must be kept low in the reactor, which implies a large recycle of MH from the separation section.

2.3 Methoxy-Methyl-Heptane Process.

2.3.1 Methoxy-Methyl-Heptane Process Background and Optimization

Griffin et al (2009) categorizes Methoxy Methyl Heptane (MMH) production as a case of bounded etherification chemistry with reversible desired reaction. Griffin demonstrates the possible shift in operating policy for a bounded chemistry with a reversible desired reaction having a low equilibrium constant like this reaction.

The chemical 2-methoxy-2-methylheptane (MMH) produced from 2-methyl-1-heptene (MH) and ethanol (MeOH), as shown below. The undesired byproducts are dimethyl ether (DME) and 2-methyl-2-heptanol (MHOH). Water (H_2O) is an intermediate reaction species.

$$\mathrm{MH} + \mathrm{MeOH} \leftrightarrow \mathrm{MMH}$$

$$r_0 = k_0\, x_{\mathrm{MH}} x_{\mathrm{MeOH}} - k_{-0}\, x_{\mathrm{MMH}}$$

$$k_0 = k_{0,0} \mathrm{e}^{-E_{A,0}/RT}$$

$$k_{-0} = k_{-0,0} \mathrm{e}^{-E_{A,-0}/RT}$$

$$2\mathrm{MeOH} \rightarrow \mathrm{DME} + \mathrm{H_2O}$$

$$r_1 = k_1\, x^2_{\mathrm{MeOH}}$$

$$k_1 = k_{1,0} \mathrm{e}^{-E_{A,1}/RT}$$

$$\mathrm{MH} + \mathrm{H_2O} \rightarrow \mathrm{MHOH}$$

$$r_2 = \text{fast}$$

The third reaction is fast compared to the other reactions so the last two reactions can effectively be coupled as a reaction rate law determined by the kinetics of the second reaction. The process chemistry can then be rewritten as

$$\mathrm{MH} + \mathrm{MeOH} \leftrightarrow \mathrm{MMH}$$

$$r_0 = k_0\, x_{\mathrm{MH}} x_{\mathrm{MeOH}} - k_{-0}\, x_{\mathrm{MMH}}$$

$$2\mathrm{MeOH} + \mathrm{MH} \rightarrow \mathrm{DME} + \mathrm{MHOH}$$

$$r_1 = k_1\, x^2_{\mathrm{MeOH}}$$

The process chemistry is now of the form

$$\mathrm{A} + \mathrm{B} \leftrightarrow \mathrm{C}$$

$$2\mathrm{A} + \mathrm{B} \rightarrow \mathrm{D} + \mathrm{E}$$

This is a bounded chemistry because the reactions are in parallel and have the same overall forward reaction order. The kinetic parameters are as given in table below.

Kinetic Parameters for Etherification Chemistry	
$k_{0,0} = 6.7 \text{ x } 10^{10}$ mol/ (kg cat s)	$E_{A,0} = 90$ kJ/mol
$k\text{-}_{0,0} = 2.1 \text{ x } 10^{-3}$ mol/ (kg cat s)	$E_{A,-0} = 0.9$ kJ/mol
$K_{1,0} = 1.3 \text{ x } 10^{12}$ mol/ (kg cat s)	$E_{A,1} = 105.9$ kJ/mol

The equilibrium constant for the desired reaction can be determined by $K = k_0/k_{-0}$. This equilibrium limited chemistry is a possible candidate for a more complicated reactor network or for reactive distillation; but in this case Griffin illustrates the use of a single, isothermal CSTR. The process flow diagram is shown in Figure 4 below and the economic optimization is based on maximizing the economic potential (EP) as described by Douglas.

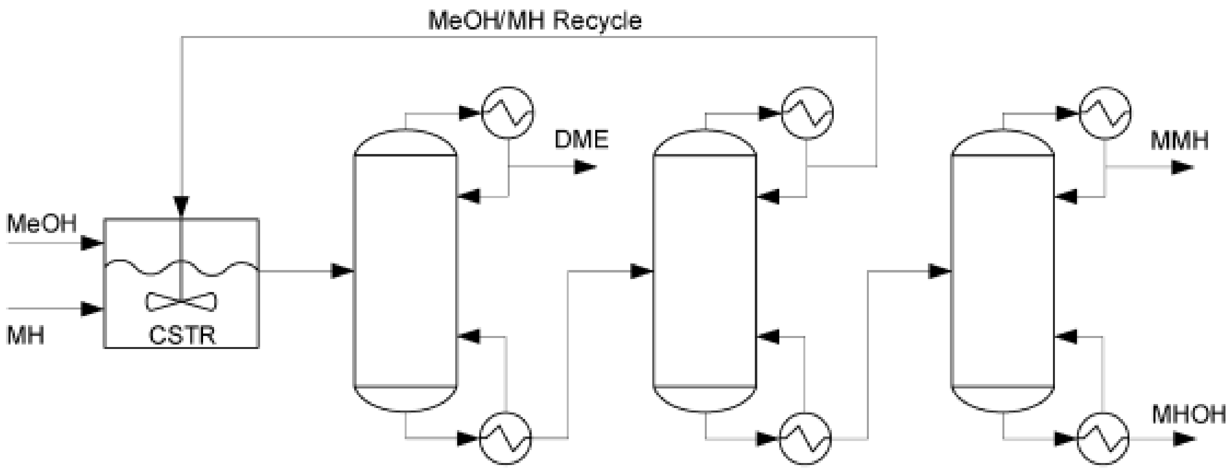


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Figure 2.4: Douglas's Level 4 Process Flow Diagram

2.3.2 Methoxy-Methyl-Heptane Process Design

This is the design of process to produce Methoxy-methyl-heptane studied by William L. Luyben (2010). This paper will use this as basis design. Below is the flowsheet of the design:

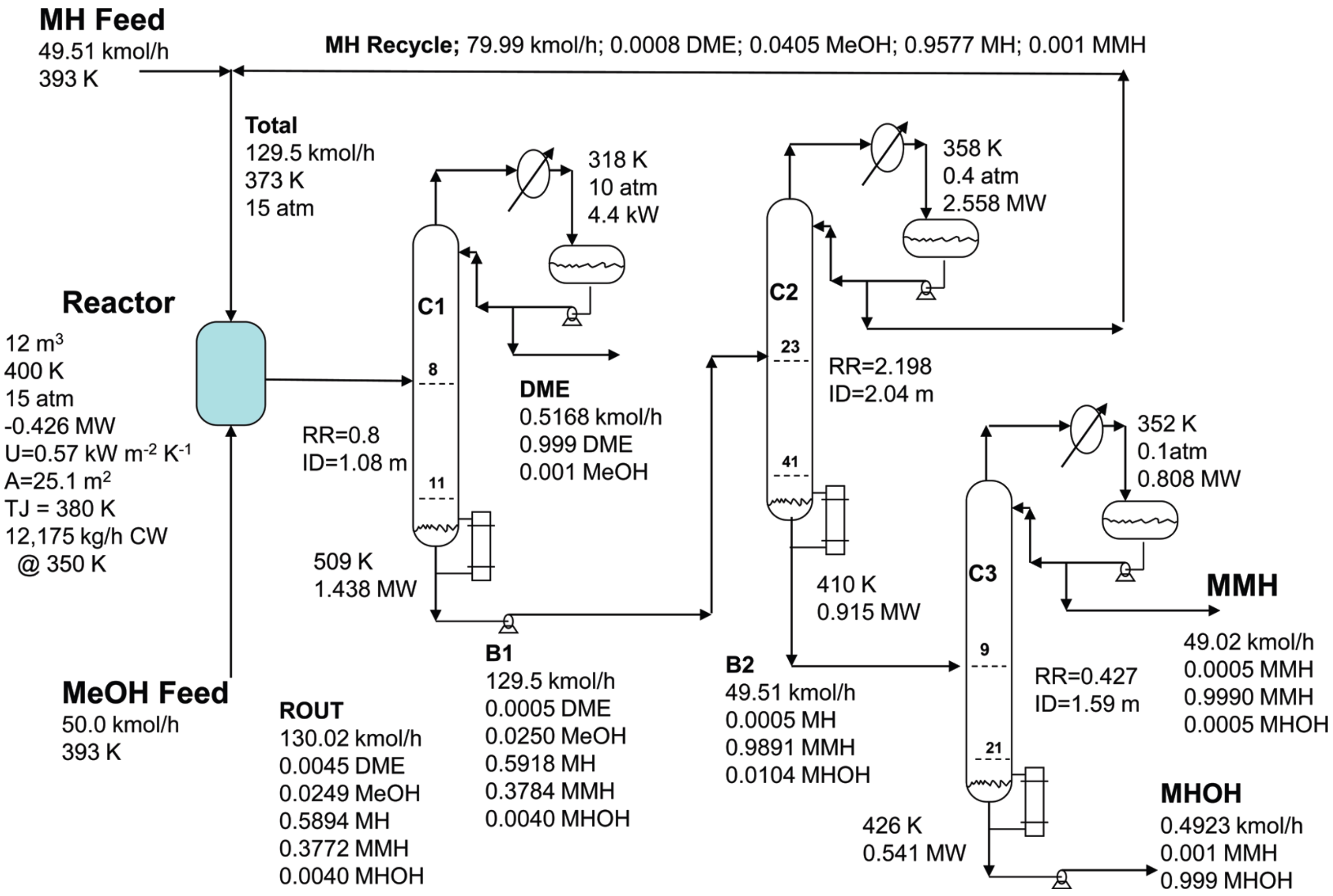


Figure 2.5: Process Flowsheet

2.3.3 Process Control Structure Based on Dynamic Simulations

Alsop et al. (2006) published a paper on what dynamic simulations brings to a process control engineer. The central piece of information required by control engineers for the design and tuning of control strategies is the step response curve(s). This is true for single or multiple input/output processes. Step response curves are used for the design and tuning of dynamic compensators, such as PID regulators and lead/lag blocks within a feedforward or decoupling scheme. In the case of model-based controllers, step response models are embedded within the on line controller algorithm.

In a classical control design procedure, control engineers obtain dynamic response information by a series of plant step tests from which empirical models of the process are identified.

Svrcek et al (2000) state that the quality of the step test data is the most important factor in determining the success of a multivariable control application. Unfortunately, obtaining good quality step test data can be fraught with difficulty for numerous reasons. The main issue is that the process must be excited sufficiently such that the process response signal is seen clearly above the process noise. An acceptable signal to noise ratio may cause unacceptable disturbance to the process and risk off-specification product. In some cases, the time it takes for the process to respond may be so long that the response to the imposed step change becomes drowned by other process disturbances. Another problem with plant tests is that a subset of independent variables, the feedforwards, are not always available for manipulation. This means that a plant test must be of sufficient duration to capture the effect of random movement in feedforward variables in the controlled variables.

Some control practitioners have dared to use dynamic simulation as an alternative to plant testing, as a means of generating the dynamic process response information required for controller design and tuning. On-line model-based controllers have been implemented with minimal or no plant testing. The advantages of conducting step tests on a desktop simulation compared to live plant are obvious. No plant testing is required, the test data is free of noise and valve cycles, all feed forwards can be stepped and engineering time and effort can be minimized especially for processes with many variables and/or long settling times.

Latest process simulation software such as HYSYS has a desktop package for both steady state and dynamic simulation. Within HYSYS, steady state simulations can be cast easily into dynamic simulations by specifying additional engineering details, including pressure/flow relationships and equipment dimensions. Control schemes can also be configured within the HYSYS environment from a pre-built suite of function blocks.

Closed loop simulation can be performed entirely within HYSYS, which provides a far superior test bed for design and tuning than the classical approach of testing a controller against the linear empirical model in a numerical simulation with zero model mismatches. This is because a much richer and realistic picture of the process disturbances can be created by varying the process conditions, such as feed compositions, non-linearities can be observed, and gain conditioning decisions can be validated, even uncertain process parameters like down comer volume and thermal inertia can be varied.

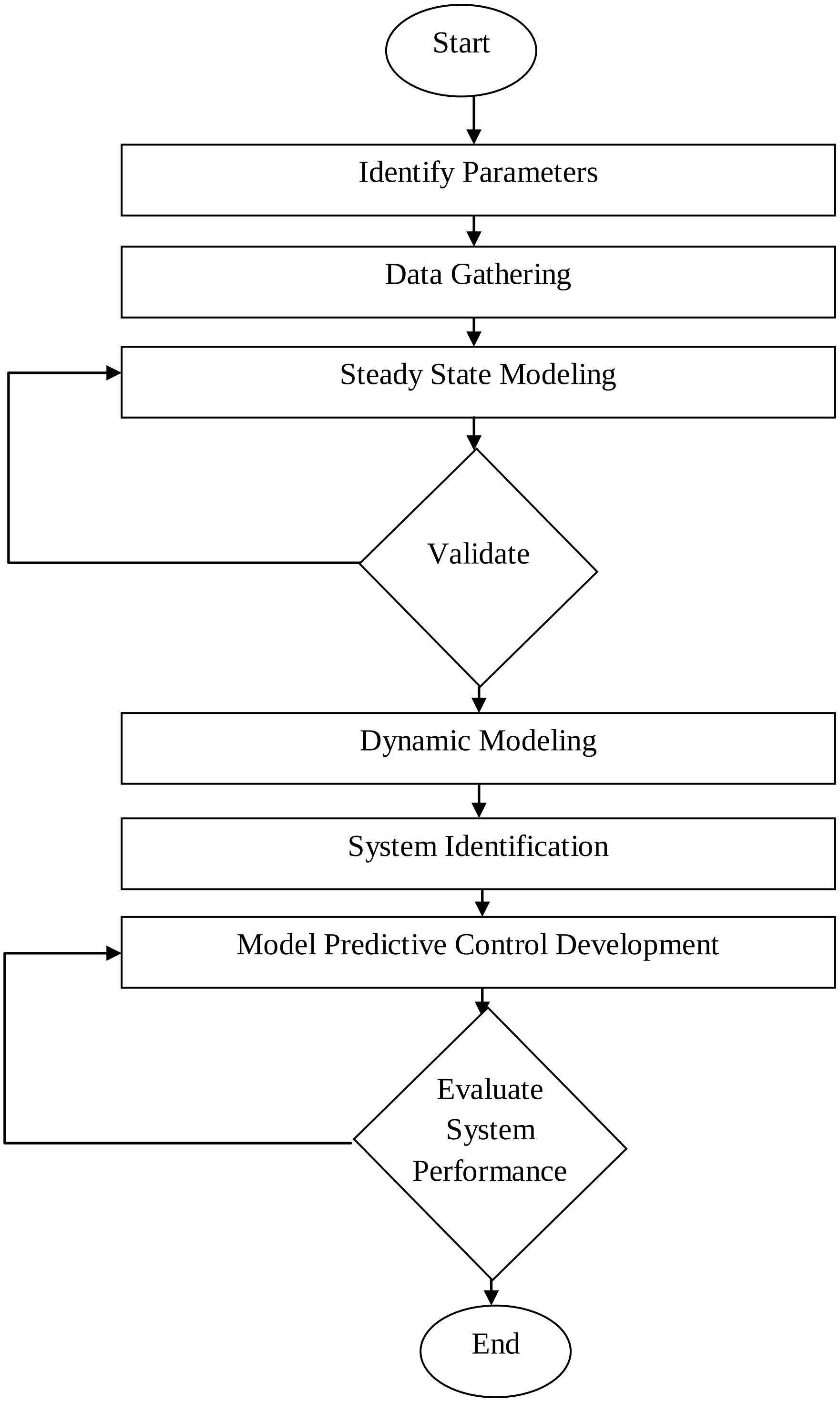
This realistic HYSYS simulation is especially useful to train the operators on the new control scheme and quickly reproduce specific scenarios. Of course, as is the case in all simulation studies, obtaining a high fidelity model that is truly representative of the process is a key issue. Where dynamic models are used, every effort must be made to validate the model against actual process data. It is noted that normal process data from the plant data historian is suitable for this task, and that no special plant tests need be conducted.

2.4 Concluding Remarks

This chapter has presented the origin and function of gasoline additive, why replacement of MTBE with MMH as gasoline additive is needed, and MTBE's effect on environment in form of groundwater contamination. This chapter also covered MMH characteristics and the reaction to produce MMH. Next chapter will present the methodology that is used throughout this project.

CHAPTER 3
METHODOLOGY

Below is the flow chart of methodology adopted for this project. This project is completed within approximately one year time frame (two semesters). This project can be divided into two main phase which are building model for the process and constructing MPC strategy for the process



3.1.1 Identify Parameters

By identifying background and problem statement of the project, conduct a research of the technical and pattern literature for the information on the project such as design of the process, reaction of the process, operating parameters, new technology invention, process modification, process consideration and criteria. The information obtained from the literature is gathered, analyze and applied to achieve the objective of the project.

3.1.2 Data Gathering

The operating parameters for the process can be identified based on the literature. These operating parameters will be used as input for steady state and dynamic modeling in HYSYS. Based on the information obtained from the literature, critical analysis have to be done to analyze the information and relate to this project.

3.1.3 Steady State and Dynamics Modeling

Using all the information on process and operating parameters as an input to steady state modeling and dynamics modeling Methoxy-Methyl-Heptane Process using HYSYS. Steady state modeling by definition is modeling a system in a steady state system which has numerous properties that are unchanging in time. This implies that for any property p of the system, the partial derivative with respect to time is zero:

$$\frac{\partial p}{\partial t} = 0$$

Steady state models can perform steady state energy and material balances and evaluate different plant scenarios. Dynamic modeling differs from steady state in a way where dynamic modeling use properties which evolves over time. Dynamic modeling can be achieved by defining detailed equipment sizing and pressure flow specifications of the process in HYSYS.

3.1.4 System Identification in MATLAB

In control engineering, the field of system identification uses statistical methods to build mathematical models of dynamical systems from measured data. System identification also includes the optimal design of experiments for efficiently generating informative data for fitting such models. MATLAB provides a system identification tools for its users and measured data from HYSYS can be used as input for system identification purposes.

3.1.6 Constructing Model Predictive Control Algorithm for Process

A model predictive control algorithm will be developed that is capable of effectively handling large disturbances in production rate and operating parameters. Model Predictive Control, or MPC, is an advanced method of process control that has been in use in the process industries such as chemical plants and oil refineries since the 1980s. Model predictive controllers rely on dynamic models of the process, most often linear empirical models obtained by system identification. MPC models predict the change in the dependent variables of the modeled system that will be caused by changes in the independent variables. In a chemical process, independent variables that can be adjusted by the controller are often either the setpoints of regulatory PID controllers (pressure, flow, temperature, etc.) or the final control element (valves, dampers, etc.). Independent variables that cannot be adjusted by the controller are used as disturbances. Dependent variables in these processes are other measurements that represent either control objectives or process constraints.

3.1.6 Evaluate System Performance

The system performance can be evaluated based on the working modeling result and the effectiveness of the model predictive control structure to handle disturbance in production rate and operating parameters.

3.1.7 Result Analysis

Analyse the results from modeling and construction of the model predictive control structure. Modeling result is validated against the literature result and MPC result would be analysed on ability to achieve steady output and maintaining set point for the model. Some optimization of the system can be done in order to increase the performance in this section.

3.2 Project Activites

These are some of project activities done throughout this project.

1. Research, information gathering via various resources : online journals, books, etc)
2. Do HYSYS tutorials in order to be familiar using HYSYS.
3. Build steady state and dynamic modeling in HYSYS.
4. Do system identification in MATLAB.
5. Build MPC algorithm in HYSYS
6. Meeting with supervisor regularly for discussions on project.

3.3 Tools

Modeling and MPC algorithm part of this project will be using HYSYS Process Simulation Software. HYSYS is simulation software based on a thermodynamic and physical property calculation mechanism used to predict process behavior for chemical process applications. System identification part of this project will be using system identification tool in MATLAB.

3.4 Concluding Remarks

This chapter explained the methodology, project activities done and tools used throughout this project. A more detail view on modeling construction and result will be explained in the next chapter.

CHAPTER 4

MODELING OF METHOXY METHYL HEPTANE PROCESS

4.1 Introduction

Now a day the process industries are facing an increasingly competitive environment, ever changing market conditions and government regulations. Yet they a still have to increase productivity and profitability. The business objective can be achieved by reducing time required to get new products to market, increasing the quantity and quality of product produced and designing plants for an optimum performance along their life cycle. In industries these complicated problems are often not solved by hand for two reasons which are human errors and time constraints. This is why the usage of steady state and dynamic models based process simulation has been steadily increasing in process engineering. When used to its full capability process simulations can be a very powerful tool for an engineer to achieve major benefits , such as ensuring more efficient and profitability design, improving plant control and operability, eliminating process bottle necks and minimizing process network, and reducing human error and time requirement.

Better technologies available for personal computers ensure the widespread use of process simulation which is beneficial in a lot of fields, especially process engineering and control engineering. Yusoff et al. (2008) stated in general simulation methods are divided into two broad categories which are equation oriented and modular approaches.

Equation oriented simulation requires simultaneous solution of nonlinear equations. In this approach all equations and variables which constitute the model representing the process are generated and gathered together. The equations are solved simultaneously using a suitable mathematical algorithm. These equation oriented simulators contain standard thermodynamic correlations and physical properties that can be employed to develop steady state and dynamic models. Examples of equation oriented simulators are DIVA and DYNSIM.

Yusoff et al. stated that another modeling approach which is close form modular simulation is more attractive for industrial practitioners. Modular approach entails attachment of one solved flowsheet to another. A lot of latest generation simulators using modular approach are commercially available, such as HYSYS, AspenPlus and iCON. Major advantages of using the modular approach are reducing modeling time and efforts and shorter on the job training period.

In subsequent sections, development of steady state and dynamic models of a Methoxy Methyl Heptane process are discussed. The steady state model is used as a basis for developing a dynamic model. Control philosophy is presented according to its purpose.

4.2 Process Description

Below is the design of process to produce Methoxy-methyl-heptane studied by Luyben (2010). This paper will use this as basis design. For this paper the author will not simulate the whole process instead focusing on construction of steady state, dynamics modeling and MPC algorithm only for the area shaded in yellow. The flow sheet of the Methoxy Methyl Heptane process are presented in figure 4.1 and the flow sheet of main process focused in this paper are presented in figure 4.2.

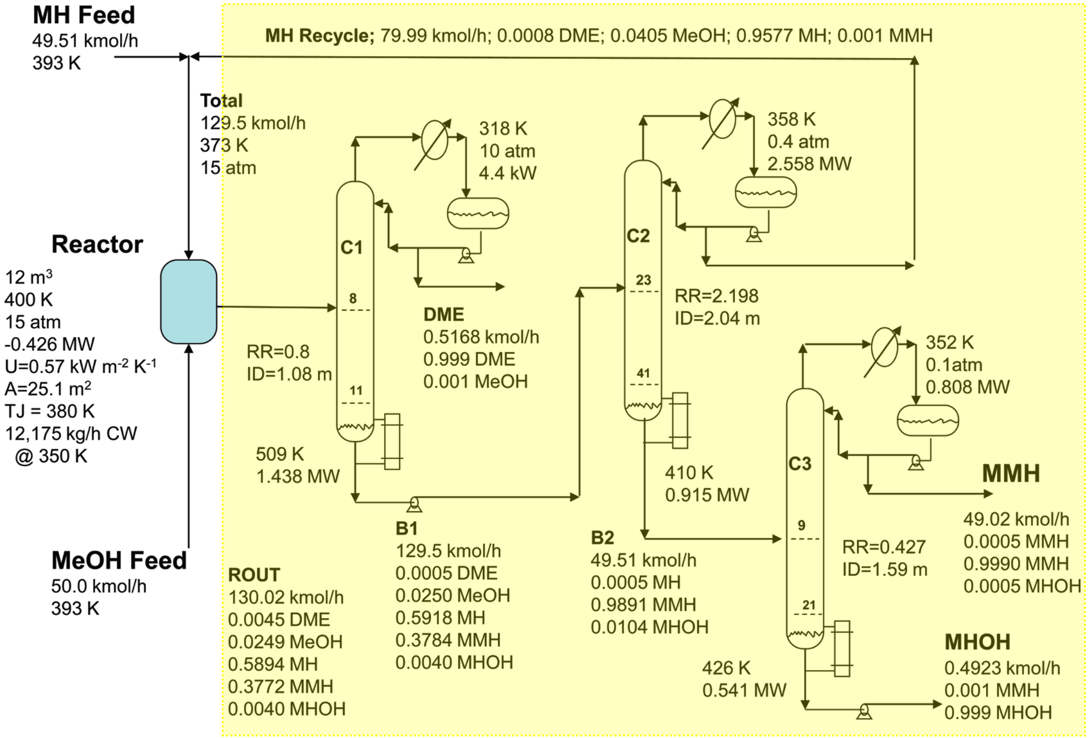


Figure 4.1: Methoxy Methyl Heptane Process Flowsheet

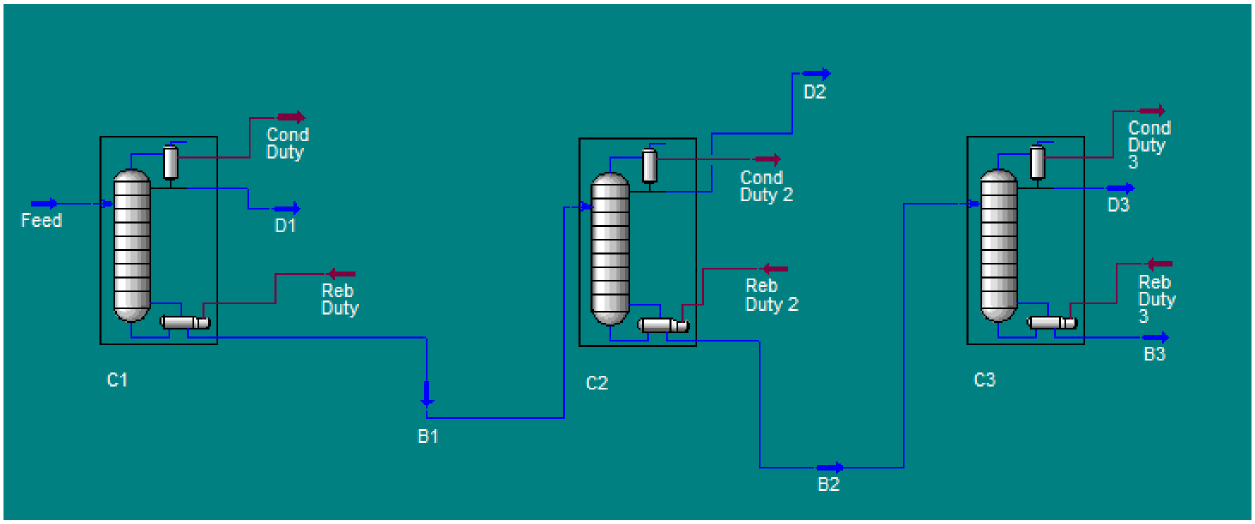


Figure 4.2 : Methoxy Methyl Heptane Process Flowsheet 2

Key operating values are obtained from basis process design from Methoxy-Methyl-Heptane process by Luyben (2010). Feeds to Distillation Column C1 come from CSTR reactor at 350K and 15atm. The feed composition is as listed in Table 4.1.

Table 4.1: Composition of Feed Stream

Component	Compositions
Dimethyl Ether (DME)	0.0045
Methanol (MeOH)	0.0249
2-Methyl-1-Heptene (MH)	0.5894
Methoxy-Methyl-Heptane (MMH)	0.3772
2-Metyl-2-Heptanol (MHOH)	0.0040

Feed composition is fed on distillation column C1 where the separation of most DME from reactor effluents will be done here. Distillate product of C1 is a small stream of 0.5618 kmol/h of 99.9 mol % DME. Since the separation between DME and methanol is easy the reflux ratio is small (RR= 0.8) so only few stages are required. Bottom products of C1 are further processed to separate recycle MH from the product MMH in distillation column C2. The bottom specification is 0.05mol% MH. Reflux ratio of 2.198 is required to achieve the specified separation. Bottom products from C2 will be fed into the third distillation column C3. The distillate is MMH with 99.9 mol% purity and the bottom is byproduct of MHOH with 99.9 mol% purity. The reflux ratio is 1.59. The boiling points of the five components involved in the MMH process are quite different, so the separations are fairly easy. Table 4.2 listed the boiling points of the components involved.

Table 4.2 : Boiling Points of Components Involved.

Component	Boiling Points (K)
Dimethyl Ether (DME)	248.2
Methanol (MeOH)	337.5
2-Methyl-1-Heptene (MH)	392.2
Methoxy-Methyl-Heptane (MMH)	424.4
2-Metyl-2-Heptanol (MHOH)	471.4

4.3 Modeling

Luyben (2010) simulate the process using Aspen but the author will use different test bed which is HYSYS 2006 environment. Thermodynamic properties of the vapors and liquids estimated by UNIQUAC are used in all units of the process. Since MMH and 2-methoxy-2-heptanol (MHOH) are not in the HYSYS databank, hypothetical components were generated by using create a hypo component tool under simulation basis manager in HYSYS. The input submitted for creating hypothetical components are as listed in table 4.3 for MMH and table 4.4 for MHOH. Using these input HYSYS will estimate other unknown properties of the components.

Table 4.3: Input for MMH Hypothetical Component in HYSYS

Component Name	MMH
Chemical Formula	$C_9H_{20}O$
Molecular Weight	144.3
Normal Boiling Point (ºC)	151.2
Ideal Liquid Density (kg/m3)	793

Table 4.4: Input for MHOH Hypothetical Component in HYSYS

Component Name	MHOH
Chemical Formula	C8H18O
Molecular Weight	130.2
Normal Boiling Point (ºC)	198.2
Ideal Liquid Density (kg/m3)	820.0

4.3.1 Steady-state Modeling

Simulation starts with steady state model development. Unit operations and streams are installed in HYSYS process flow diagram from left to right and bottom upwards as shown in figure 4.2.

Distillation column C1 is simulated as a 12 tray column with the feed stream fed at tray 8. The condenser pressure is 1013 kPa and reboiler pressure at 1774 kPa. Column C1 use total condenser and active specifications of reflux ratio 0.800 and distillate flow rate 0.5168kmol/hr. Column C1 main aim is to achieve separations between DME and other reactor effluents. The distillate component mole fractions are as listed in table 4.5 and the bottom component mole fractions are as listed in table 4.6. The resulting mole fractions are compared to the component mole fractions in basis design by Luyben (2010). The resulting mole fractions shows low percentage difference, which means it is closely similar to the basis design. The temperature and composition profile of distillation column C1 are presented in figure 4.3 and 4.4. The temperature profile inside column C1 is quite steep ranging from about 45 ºC at the top to 330 ºC at the reboiler. The simulated graph values and pattern closely resemble the values and pattern of the temperature profile of distillation column C1 model designed by Luyben.DME

Table 4.5: Distillate C1 Components Mole Fractions

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
Dimethyl Ether (DME)	0.999	0.999	0

Methanol (MeOH)	0.001	0.001	0

Table 4.6: Bottom C1 Components Mole Fractions

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
Methanol (MeOH)	0.0249	0.0250	0.400
2-Methyl-1-Heptene MH)	0.5917	0.5918	0.016
Dimethyl Ether (DME)	0.000528	0.000500	0.530
Methoxy Methyl Heptane (MMH)	0.378705	0.378400	0.081
2-Metyl-2-Heptanol (MHOH)	0.004016	0.004000	0.398

Figure 4.3: Column 1 Temperature Profile

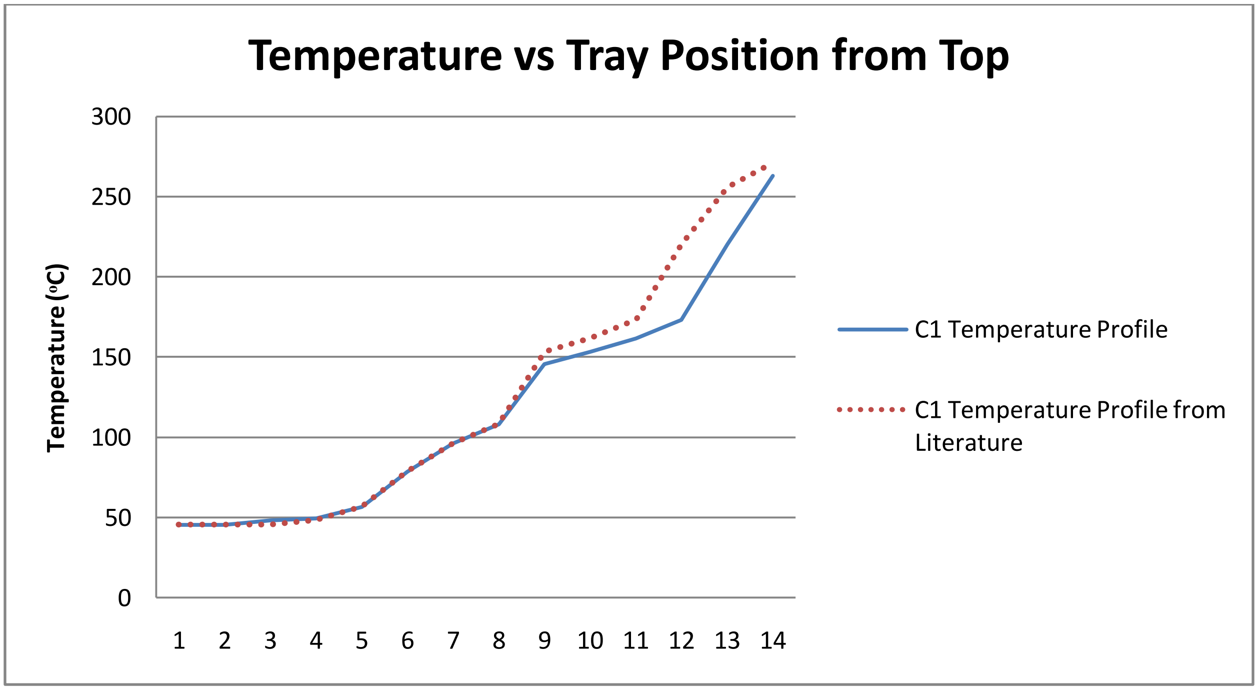
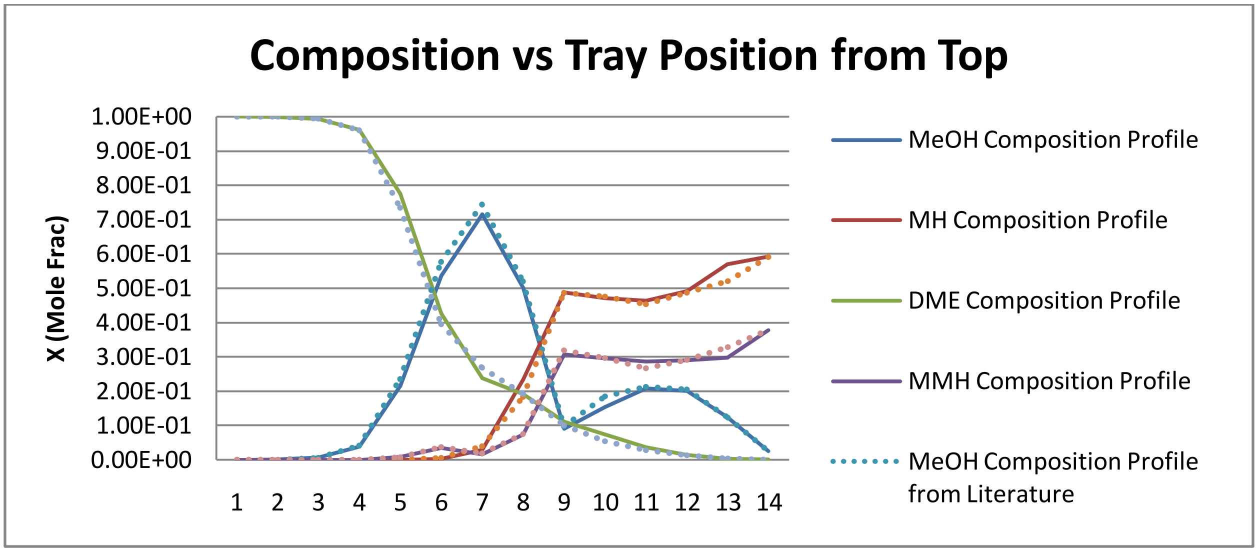


Figure 4.4: Column 1 Composition Profile



Bottom stream of C1 then will be fed to distillation column C2 at stage 23. Distillation column C2 has 42 stages. The pressure assigned for condenser is 1000 kPa and for reboiler is 1013 kPa. Similar to C1, C2 also use total condenser and has active specifications of distillation flowrate 79.99kgmole/hr and distillate component fraction of MH which is 0.9577. Column C2 main focus is to achieve separation of recycle MH from the product MMH. The distillate component mole fractions are as listed in table 4.7 and the bottom component mole fractions are as listed in table 4.8. The resulting mole fractions are compared to the component mole fractions in basis design by Luyben (2010). The resulting mole fractions shows low percentage difference, which means it is closely similar to the basis design. The temperature and composition profile of distillation column C2 are presented in figure 4.5 and 4.6. The temperature profile inside column C2 is quite steep ranging from about 80 °C at the top to 270 °C at the reboiler. The simulated graph values and pattern closely resemble the values and pattern of the temperature and composition profile of distillation column C2 model designed by Luyben.

Table 4.7: Distillate C2 Components Mole Fraction

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
Methanol (MeOH)	0.040473	0.040500	0.0670
2-Methyl-1-Heptene	0.957699	0.957700	0.0012

(MH)			
Dimethyl Ether (DME)	0.000854	0.000800	0.06323
Methoxy Methyl Heptane (MMH)	0.000974	0.001000	2.6694

Table 4.8: Bottom C2 Components Mole Fraction

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
2-Methyl-1-Heptene (MH)	0.000554	0.000500	9.747
Methoxy Methyl Heptane (MMH)	0.988942	0.989100	0.015
2-Metyl-2-Heptanol (MHOH)	0.010504	0.010400	0.99

Figure 4.5: Column 2 Temperature Profile

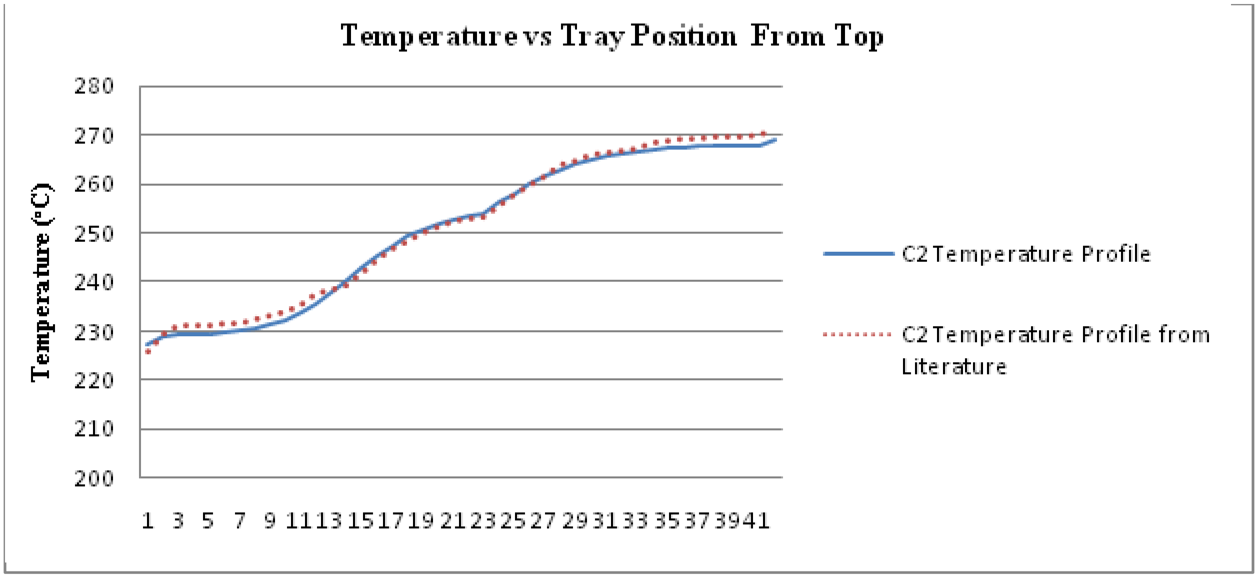
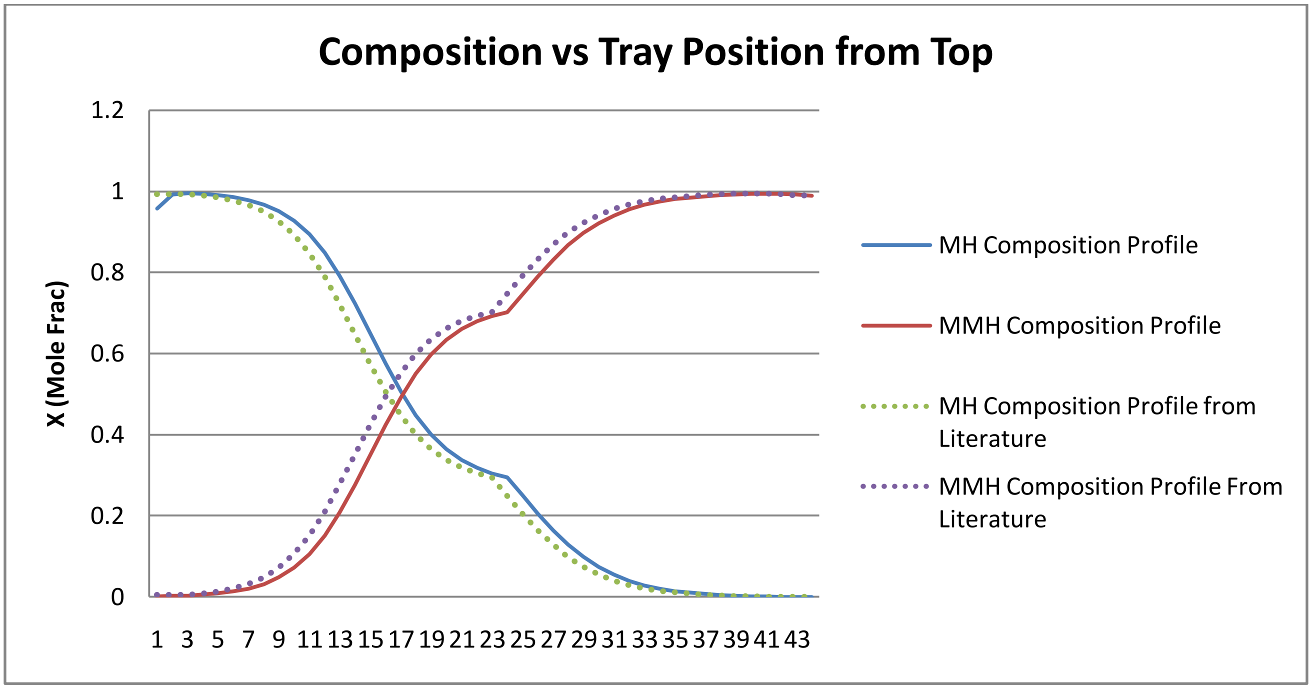


Figure 4.6: Column 2 Composition Profile



Bottom product stream from C2 then will be fed into distillation column C3. The distillation column C3 has 22 stages and inlet stream enters on stage 14. Pressure assigned at condenser is 1000kPa and pressure assigned at reboiler is 1027kPa. Column C3 use total condenser and has active specifications of distillate flow rate 49.02kgmole/hr and bottom component fraction of 0.9990 MHOH. Column C3 main focus is to do a separation that will achieve 99.9% purity of MHOH at bottom and 99.9% purity of MMH at distillate. The distillate component mole fractions are as listed in table 4.9 and the bottom component mole fractions are as listed in table 4.10. The resulting mole fractions are compared to the component mole fractions in basis design by Luyben. The resulting mole fractions shows low percentage difference, which means it is closely similar to the basis design. The temperature and composition profile of distillation column C3 are presented in figure 4.7 and 4.8. The temperature profile inside column C3 is quite steep ranging from about 80 ºC at the top to 330 ºC at the reboiler.

Table 4.9: Distillate C3 Components Mole Fractions

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
2-Methyl-1-Heptene (MH)	0.000559	0.000500	10.0
Methoxy Methyl Heptane (MMH)	0.998881	0.99900	0.01191
2-Metyl-2-Heptanol (MHOH)	0.000559	0.000500	10.0

Table 4.10: Bottom C3 Components Mole Fractions

Component	Mole Fraction	Mole Fraction (Luyben)	Percentage Difference (%)
Methoxy Methyl Heptane (MMH)	0.001	0.001	0
2-Metyl-2-Heptanol (MHOH)	0.999	0.999	0

Figure 4.7: Column 3 Temperature Profile

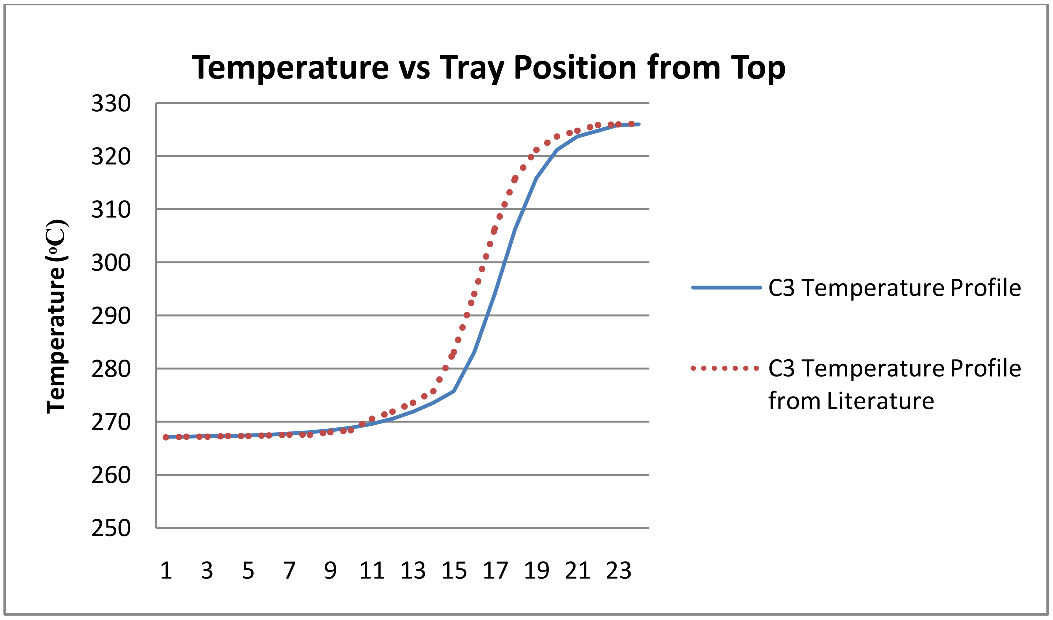
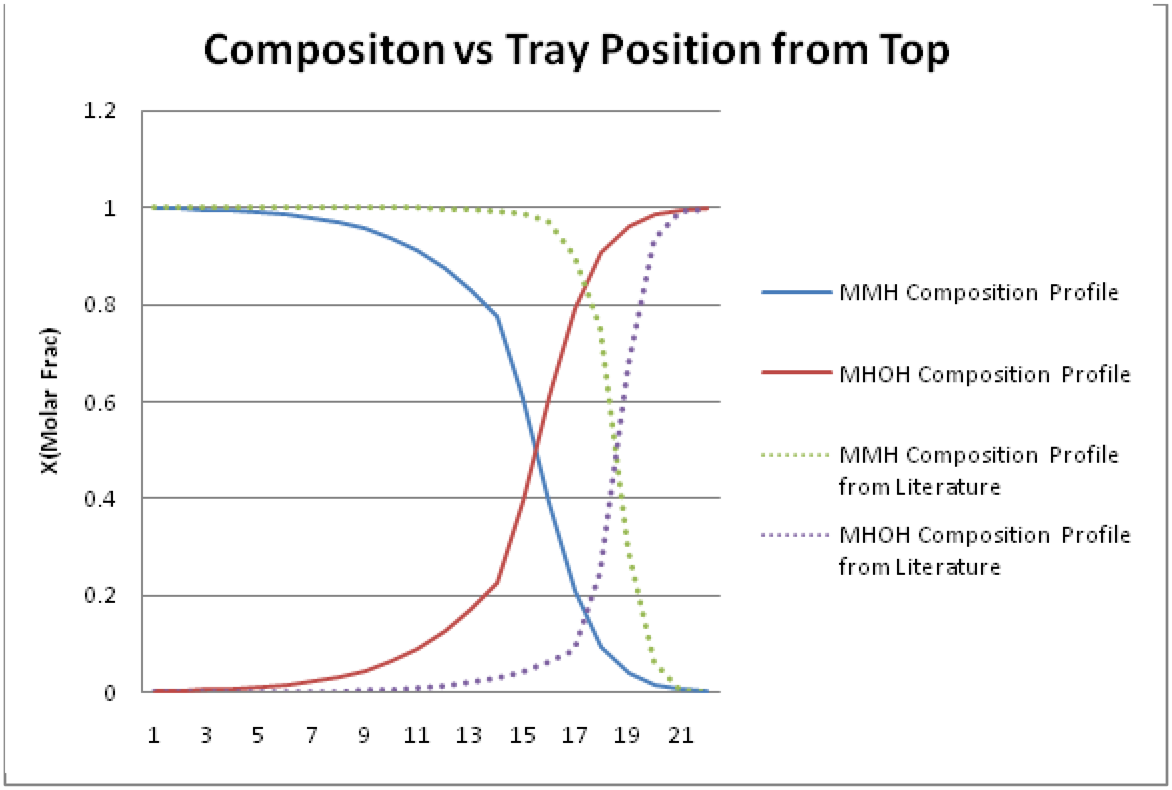


Figure 4.8: Column 3 Composition Profile



4.3.2 Dynamic Modeling

For this paper, author develops dynamic modeling for each main unit operation individually, which is Distillation Column C1, C2, and C3. In order to do a transition between steady state to dynamic model, few steps are needed to be done in HYSYS. These steps are:

a) Sizing of units operations
b) Specification of pressure or flow condition at boundary streams
c) Installation of regulatory control

a) <u>Sizing of units operations</u>

All unit operations need to be sized accordingly. Sizing information for a process can be taken from plant data. Using values from plant data is preferable in order to produce a more realistic dynamic model. In HYSYS an alternative sizing procedure may be used. Yusoff et al. (2008) stated that vessels such as condensers, separators, reboilers should be able to hold 5-15 minutes of liquid accumulation. The vessel volumes can be estimated by dividing the steady state value of the entering liquid flow rates from the holdup time.

For this paper, main unit operations to be sized are the three distillation columns C1, C2, and C3. Only internal section needs to be sized and can be achieved by specifying tray/packing type and dimensions. There are five types of trays available in HYSYS which are sieve, valve, bubble cap, chimney, and sump. Estimation of data such as tray diameter, tray spacing, weir length and weir height can be achieved using tray utilities tools in HYSYS. These data then used as input from unit sizing specifications for the distillation columns. Unit sizing specifications are for column C1, column C2, and column C3 are presented in table 4.11, 4.12, and 4.13, respectively.

Table 4.11: Sizing Specifications for Distillation Column C1

Parameter	Value
Tray Space (m)	0.5500
Tray Diameter (m)	1.500
Tray Type	Sieve
Weir Height (mm)	50
Weir Length (mm)	1215

Table 4.12: Sizing Specifications for Distillation Column C2

Parameter	Value
Tray Space (m)	0.6096
Tray Diameter (m)	2.286
Tray Type	Sieve
Weir Height (mm)	50.80
Weir Length (mm)	1568

Table 4.13: Sizing Specifications for Distillation Column C3

Parameter	Value
Tray Space (m)	0.6906
Tray Diameter (m)	1.372
Tray Type	Seive
Weir Height (mm)	50.80
Weir Length (mm)	999

b) Pressure Flow Specifications

The next step in transitioning steady state model to dynamic model is to enter a pressure or flow condition at all boundary streams. This is important because the pressure and material flow are solved simultaneously in HYSYS. In order to do pressure flow specifications one must understand the pressure flow theory which is used by the pressure flow solver in HYSYS.

The simplest way to view the pressure flow solver in HYSYS is to consider the flow sheet as a boundary value problem. Making pressure or flow specifications on all the boundary streams (feed or product streams in a flow sheet) will ensure all the internal pressures and flows to be solved simultaneously at each integration step by the pressure-flow solver. The internal steam pressures and flowrates are calculated from the pressure gradients in the flow sheet. Flow rates are determined from:

1. Changes in vapour pressure nodes within the flowsheet system
2. Resistances across valves
3. Conductance through equipment (coolers, heaters, heat exchangers).

From the flow sheet the boundary streams are stream Feed, Distillate 1 (D1), Distillate 2 (D2), Distillate 3 (D3) and Bottom 3 (B3). Control valves VLV-100, VLV-101, and VLV-102 are placed on the outlet of stream D1, D2, D3 and B3. These valves are sized under rating tab in the valve properties. New streams are attached to the outlet of the valves which are stream D1 Out, D2 Out, D3 Out and B3 Out. Pressure specifications are ticked active at these new streams. Flow specifications are ticked as active at Feed stream. Flow specifications are also set as active at the reflux streams for each distillation column C1, C2, and C3. Figure 4.5 below shown the new flow sheet after addition of valves VLV-100, VLV-101, VLV-102, VLV-103 and streams D1 Out, D2 Out, D3 Out, B3 Out. The flow sheet in figure 4.5 is presented under Dynamic P/F Specs colour scheme in HYSYS where the yellow colour represents active flow specifications and green colour represents active pressure specifications.

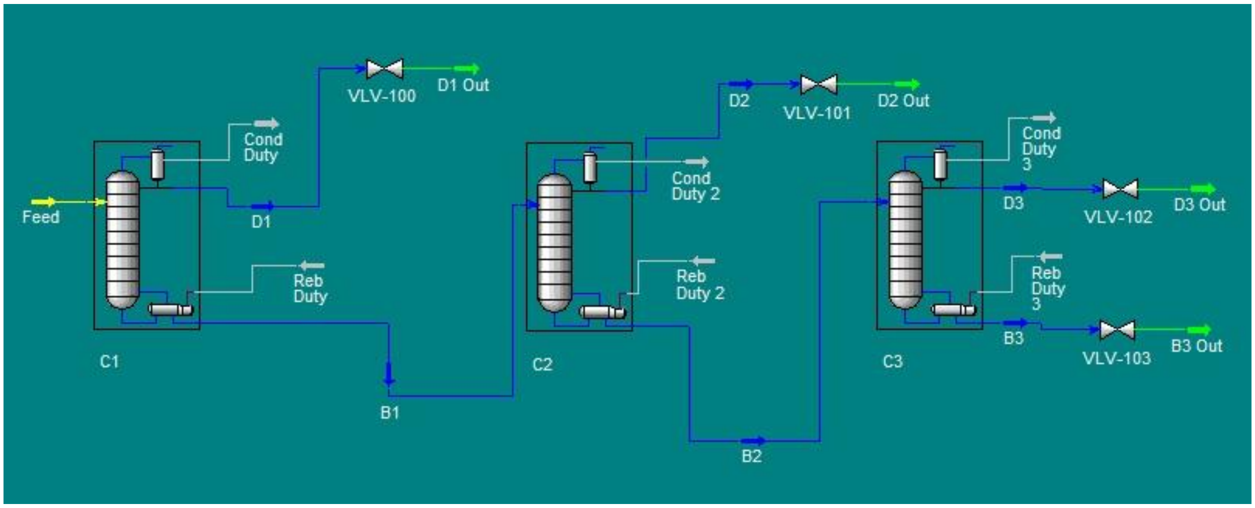


Figure 4.9: Process Flow Sheet for Dynamic Model

c) <u>Installation of Regulatory Controllers</u>

The final step in transitioning steady state model to dynamic model is installation of regulatory controllers. In this case basic regulatory controllers are sufficient for stabilizing a plant model. Composition controllers are not required in columns since temperature controllers provide adequate product quality control. In this work, only the temperature controllers are equipped on the model in order to do step testing for system identification for model predictive control algorithm development. The MMH process plant is equipped with the following controller schemes:

1. Stage 6 temperatures in column C1 is controlled by manipulating the reboiler heat input.
2. Dual temperature control is used in column C2. The stage 8 temperature is controlled by manipulating the reflux flow rate. The stage 28 temperature is controlled by manipulating the reboiler heat input.

3. In column 3 the temperature on stage 19 is controlled by manipulating the reboiler heat input and stage 3 temperatures is controlled by manipulating the condenser heat removal.

Figure 4.10, 4.11, and 4.12 shows temperature control individually for each distillation column.

Figure 4.10: Column 1 Control

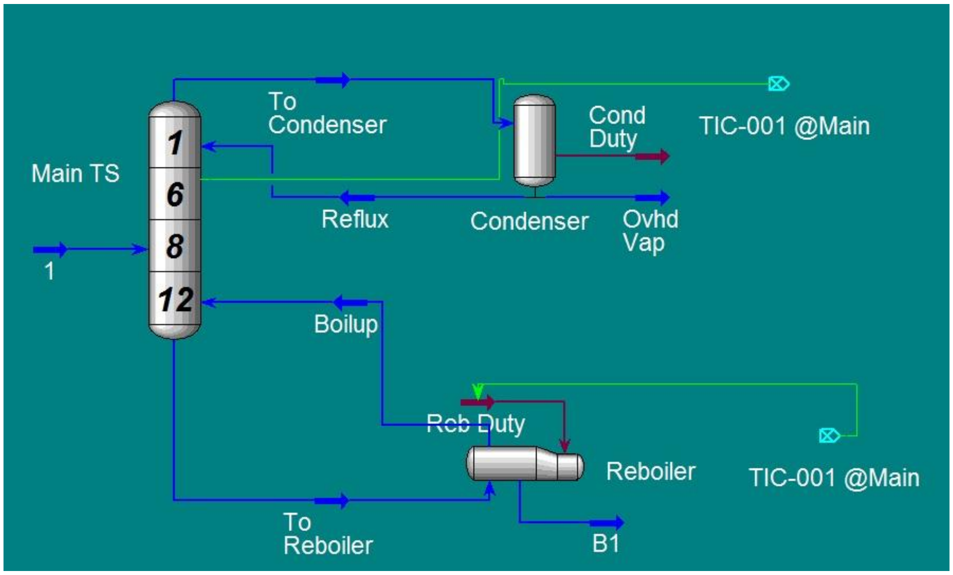


Figure 4.11: Column 2 Control

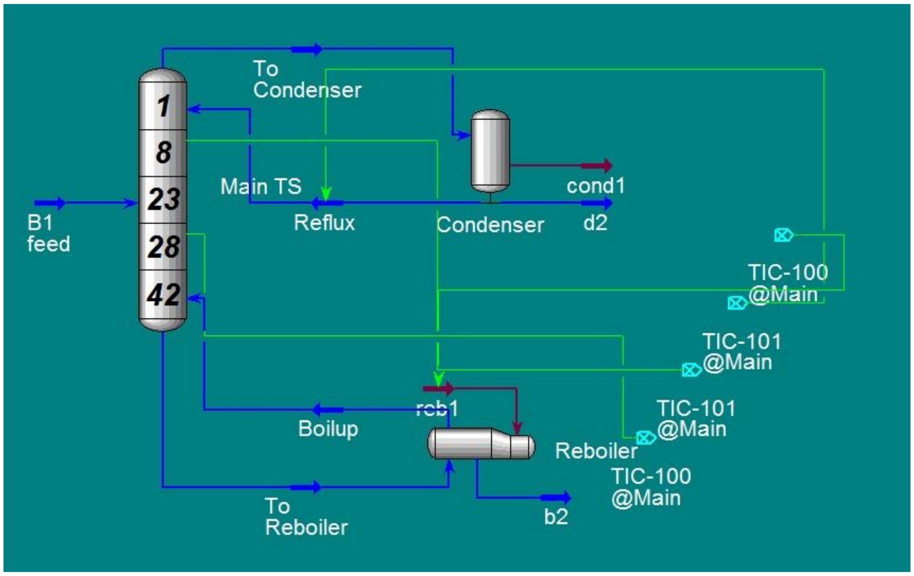
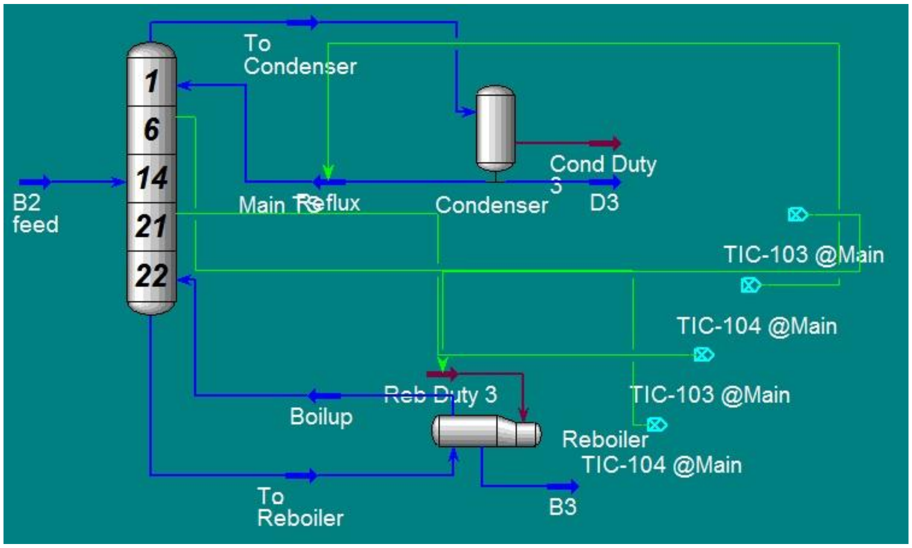


Figure 4.11: Column 3 Control



Below is the table of controller parameters for all the temperature controllers.

Table 4.14: Control & Tuning Parameters

Parameter	TIC-001	TIC-100	TIC-101
Controlled Variable	Stage 6 Temperature in Column C1	Stage 28 Temperature in Column C2	Stage 8 Temperature in Column C2
Manipulated Variable	Reboiler Heat Input	Reboiler Heat Input	Reflux Flow Rate
Action Mode	Reverse	Direct	Reverse
Range	26 to 226ºC	160 to 360ºC	130 to 330ºC
SP	136.7ºC	263ºC	230.5ºC
Kc	0.43	2	2
Ti	30	5	5

Table 4.14: Control & Tuning Parameters (Continued from last page)

Parameter	TIC-103	TIC-104
Controlled Variable	Stage 3 Temperature in Column C3	Stage 19 Temperature in Column C3
Manipulated Variable	Condenser Heat Duty	Reboiler Heat Input
Action Mode	Reverse	Reverse
Range	150 to 350 ºC	200 to 500ºC
SP	266.2ºC	267.5ºC
Kc	2	2
Ti	5	5

4.4 Concluding Remarks

This chapter has presented the developments of steady state and dynamic models of MMH separation process. The model achieved close accuracy when steady state model is validated against result from literature. Dynamic model is initialized and developed based on steady state models. Regulatory controllers are installed to stabilize process and maintain product quality. Next chapter will cover development of MPC strategy based on system identification from step testing data.

CHAPTER 5

MODEL PREDICTIVE CONTROL DEVELOPMENT

5.1 Introduction

Model predictive control (MPC) is a computer control algorithms that utilize a process model to predict future response of a plant. Qin and Badgwell (2003) state that MPC algorithm attempts to optimize future plant behavior at each control interval by computing a sequence of future manipulated variable adjustments. The first input in the optimal sequence is then sent into the plant, and the entire calculation is repeated at subsequent control intervals. The use of MPC technology also has become widespread in various industries such as chemicals, food processing, automotive and aerospace applications. Figure 5.1 shows the basic structure of MPC.

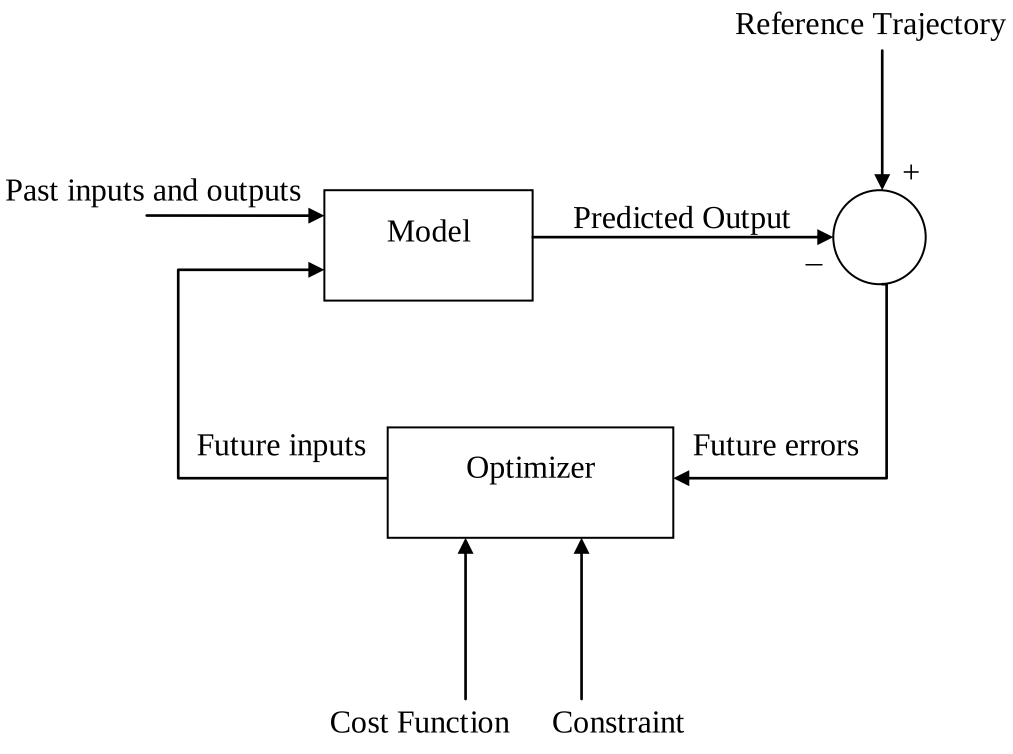


Figure 5.1: Basic Structure of Model Predictive Control

There are 2 types of MPC which are linear MPC and nonlinear MPC. Table 5.1 below highlights the differences between linear MPC and nonlinear MPC.

Table 5.1: Comparison of Linear MPC and Nonlinear MPC

Linear MPC	Nonlinear MPC
1. Uses linear model $\dot{x} = Ax + Bu$	1. Uses nonlinear model $\dot{x} = f(x,u)$
2. Quadratic cost function: $F = x^TQx + u^TRu$	2. Cost Function can be nonquadratic: $F(x,u)$
3. Linear constraints: $Hx + Gy < 0$	3. Nonlinear constraints: $h(x,u) < 0$
4. Quadratic Program	4. Nonlinear Program

Yusoff et al. (2008) discussed there are two ways to obtain a process model in order to use in developing MPC algorithms, which are empirical modeling and first –principle modeling. A first principle model is derived from material and energy balances of an actual plant. The first principle model is generally written in discrete –time implicit form as:

$$\mathbf{x}_{k+1} = \mathbf{f}(\mathbf{x}_k,\mathbf{u}_k,\mathbf{v}_k,\mathbf{w}_k) \tag{5.1a}$$

$$\mathbf{y}_k = \mathbf{g}(\mathbf{x}_k,\mathbf{u}_k) + \xi_k \tag{5.1b}$$

where: $\mathbf{x}\in\Re^{n}$ = vector of state variables
$\mathbf{u}\in\Re^{m_u}$ = vector of manipulated variables or inputs
$\mathbf{y}\in\Re^{m_y}$ = vector of controlled variables or inputs
$\mathbf{w}\in\Re^{m_w}$= vector of unmeasured disturbance variables or process noise
$\xi\in\Re^{m_\xi}$ = vector of measurement noise

An empirical model is developed from input output information that use sequence of systematic testing signals of a plant. One of the common process models used are transfer functions. The simplest form of transfer function is first order model:

$$\frac{y(s)}{u(s)} = \frac{K_p}{\tau_p s+1} \tag{5.2}$$

where: $y(s)$= output K_p= process gain

$u(s)$= input τ_p = time constant

Transfer function models are written in Laplace domain as denoted by transformed variable s. First order and second or second order models with or without time delay are typically used.

5.2 System Identification

Process model can be obtained through system identification using input-output testing data.
For this paper author will do system identification using open loop test which the process inputs stepped independently with various magnitudes.

5.2.1 Step Test

In order to obtain the process model author will use traditional approach of open loop step testing. Qin and Badgwell discussed there are two main requirements during step testing which are tuning of regulatory controllers is prohibited and if operator intervention is required to uphold plant safety or maintaining product quality, synchronizing or correlated input moves are disallowed. The inputs are moved by increasing and decreasing certain percentages of the valves opening. The outputs are measured simultaneously during each input move in order to capture their dynamic responses due to that particular input. In each test the output values would be ensured to reach steady state values before moving on to the next step test. Author would impose a total of 8 step test for column C2 model in this process. Due to the limitation of timeframe of the project, author only implement the MPC strategy on the column C2 model in this process.

a) Column C2 Step Test

The responses of outputs **y**: **y**= [y_1 y_2] are measured where output y1 is the temperature of stage 28 for Column C2 and output y_2 are temperature of stage 8 for Column C2 .The input u_1 is column C2 reboiler duty and input u_2 is Column C2 reflux flow rate. Input u_2 are constant while input u1 moves and the outputs responses are recorded, vice versa. Table 5.2 and 5.3 shows the open loop responses for each u_1 and u_2 move.

Table 5.2: Open Loop Responses with u_1 move (TIC-100)

Input Moves (%)	Output SS Values	
	y_1(°C)	y_2(°C)
53	263.2	230
54.5	264.9	241.7
52.5	247.4	229.4
50	243.4	228.2
535	263.9	229.6
52	246.9	229.1
54	264.4	237.8
55	264.9	242.8
52.8	249.6	229.3

SS= Steady state

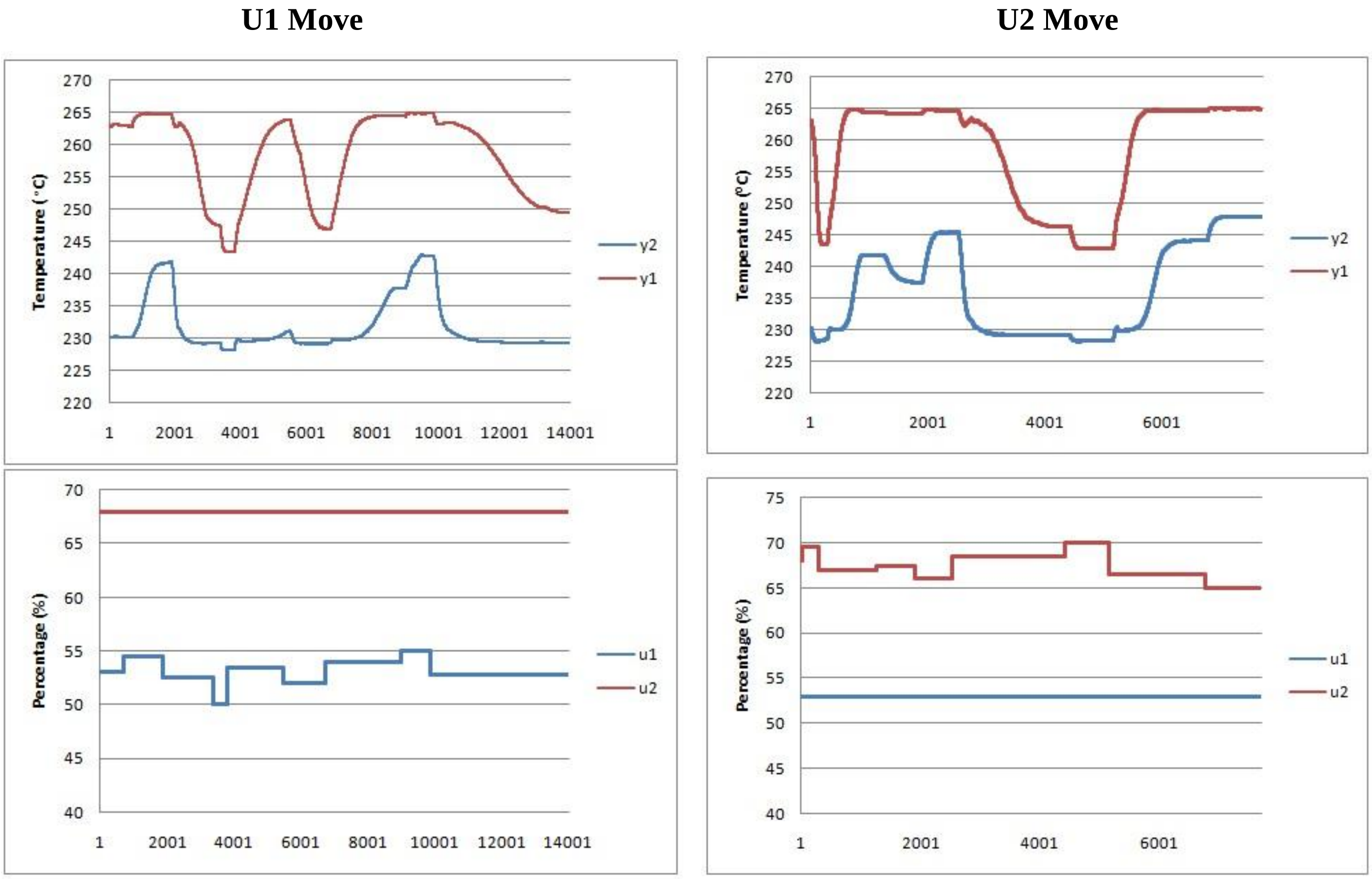
Table 5.3: Open Loop Responses with u_2 move (TIC-101)

Input Moves (%)	Output SS Values	
	y_1(°C)	y_2(°C)
68	263.2	230.4
69.5	243.46	228.4
67	264.5	241.7
67.5	264.2	237.5
66	264.7	245.4
68.5	246.4	229.1
70	242.9	228.2

66.5	264.6	244.1
65	264.9	247.8

SS= Steady state

Below is the open loop response from 8 step test where u1 is moved and u2 is kept constant.

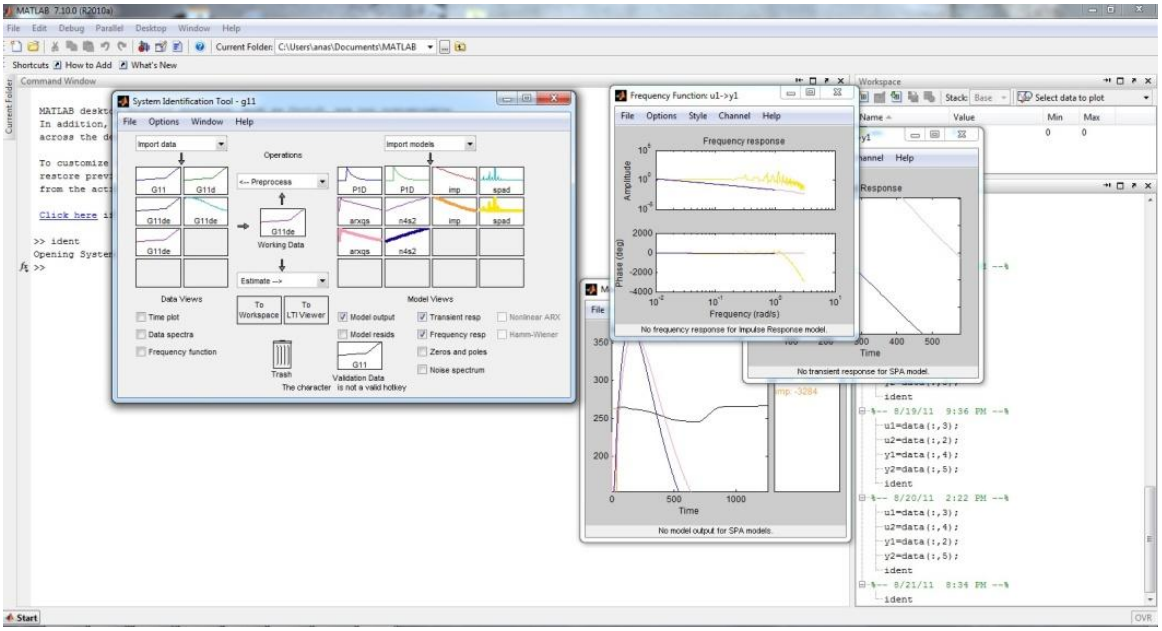

U1 Move

U2 Move

Figure 5.2 : Open Loop Response Graph for 8 Step Tests for u1 move (left) and u2 move (right)

5.2.2 System Identification in MATLAB

This paper use System Identification Toolbox in MATLAB in order to identify the process model. MATLAB provide System Identification Toolbox software which helps construct mathematical models of dynamic systems from measured input-output data. This data-driven approach helps to describe systems that are not easily modeled from first principles or specifications, such as chemical processes and engine dynamics. It also helps to simplify detailed first-principle models, such as finite-element models of structures and flight dynamics models, by fitting simpler models to their simulated responses. Author will use input-output data from step tests done earlier.



```
>> ident
```

```
ident
%-- 8/19/11  9:36 PM --%
u1=data(:,3);
u2=data(:,2);
y1=data(:,4);
y2=data(:,5);
ident
%-- 8/20/11  2:22 PM --%
u1=data(:,3);
u2=data(:,4);
y1=data(:,2);
y2=data(:,5);
ident
%-- 8/21/11  8:34 PM --%
ident
```

Figure 5.3: System Identification Toolbox in MATLAB

Final values of process gains, time constants and time delays obtained from system identification for Column C2 model are presented in Table 5.6.

Table 5.4: Column 2 Model Parameters

Transfer Function	Model Parameters		
	K_p(°C)	τ_p(min)	τ_d (min)
g_{11}	8.3105	552	0
g_{12}	-5.5711	225.787	15
g_{21}	5.065	670.568	0
g_{22}	-5.7155	278.376	0

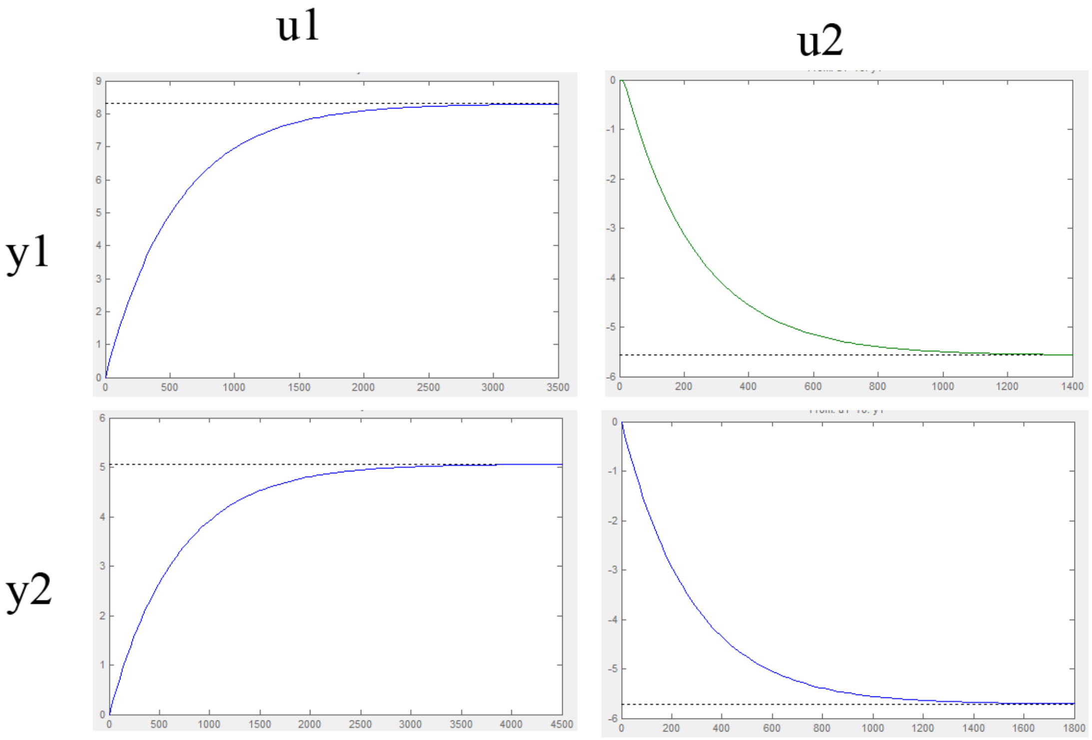


Figure 5.4: Step responses of Column C2 Model.

5.3 MPC Design in HYSYS

Unconstrained MPC controller is designed in HYSYS by specifying: 1. the process model representing plant process, and 2. design and tuning parameters. The previous section has discussed identification of process model. This section will discuss the design and tuning of MPC parameters. A 2x2 MPC controller is built on top of two PI controllers, TC-100, TC-101 for column C2 model and TC-103, TC-104 for Column C3 model. Table 5.8 shows MPC design and tuning parameters. The decision of 1 minute control interval is made so that actual process does not deviate much from model prediction before the next MPC action. Control horizon of length 2 indicates less aggressive MPC actions. Prediction horizon of 25 is sufficient to bring process to a new steady state.

Table 5.5: MPC Design & Tuning Parameters

Parameters	Values
Control interval, t	1 min
Control horizon, M	2
Prediction horizon, P	25

5.3.1 Setpoint Tracking

In order to measure the performance of a control the setpoint tracking method can be used. A good controller should be able to bring an output from its nominal value to another state smoothly. This process is called Setpoint Tracking. Performance of MPC controller than will be measured using integral squared error (ISE) for output changes and total duties for input moves.

Table 5.6: Nominal Input and Output Values.

Index	Input (%)	Output (^{o}C)
1	53	263.2
2	68	230.5

Table 5.7: Range of actual input duty values

Input	Minimum (kW)	Maximum (kW)
1	0	1500
2	0	7800

Eight case studies are carried out in order to determine the performance of MPC controllers which are:

1. y1 + 1^{o}C
2. y1 - 1^{o}C
3. y2 + 1^{o}C
4. y2 - 1^{o}C
5. y1 + 1^{o}C , y2 + 1^{o}C
6. y1 + 1^{o}C , y2 - 1^{o}C
7. y1 - 1^{o}C , y2 + 1^{o}C

8. y1 - 1^{o}C , y2 - 1^{o}C

In all eight cases, outputs are brought to new steady states by coordinated moves of both inputs. The area under the curve for each cases for output are calculated using integral of squared errors (ISE) method. Figure 5.4 shows example of area to be calculated in the response graph. Green shaded area represents the total area under curve need to be calculated. The total area can be calculated through integration of the polynomial trend line estimated from excel or manual calculation of area on the graph.

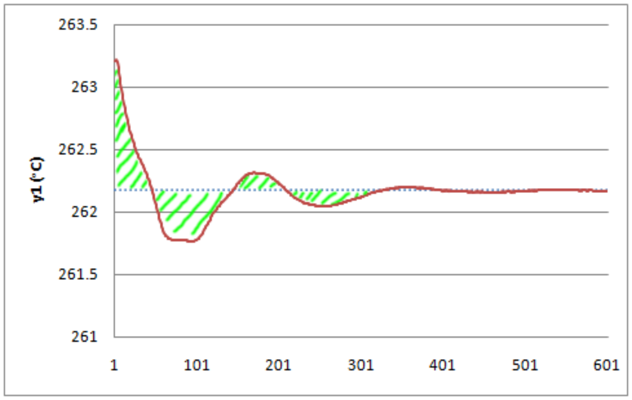


Figure 5.5: Example of the area under closed loop response curve to be calculated (Output)

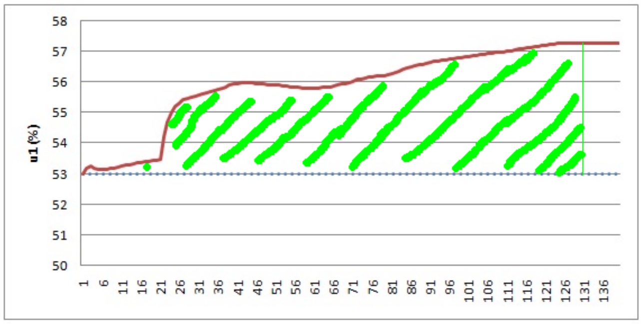


Figure 5.6: Example of the area under closed loop response curve to be calculated (Input)

The area represents the performance of MPC controller, with smaller area means more efficient MPC controller. Area under output curve represents ISE while area under input curve represents total duties needed to change to new set point. Figure 5.7, 5.8, 5.9, 5.10, 5.11, 5.12, 5.13, and 5.14 shows closed loop response for change in all cases.

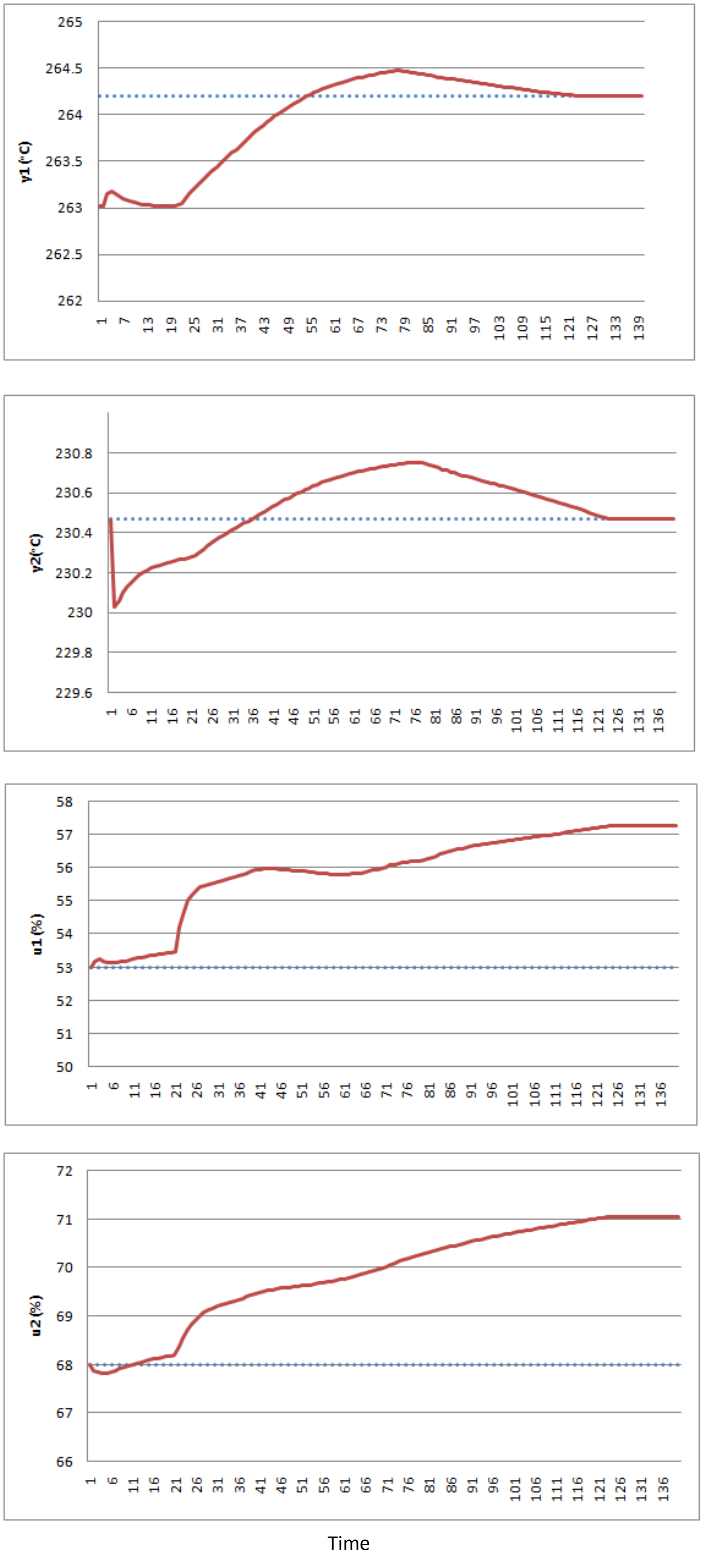


Figure 5.7: Closed Loop responses for y1 + 1°C (Case 1). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

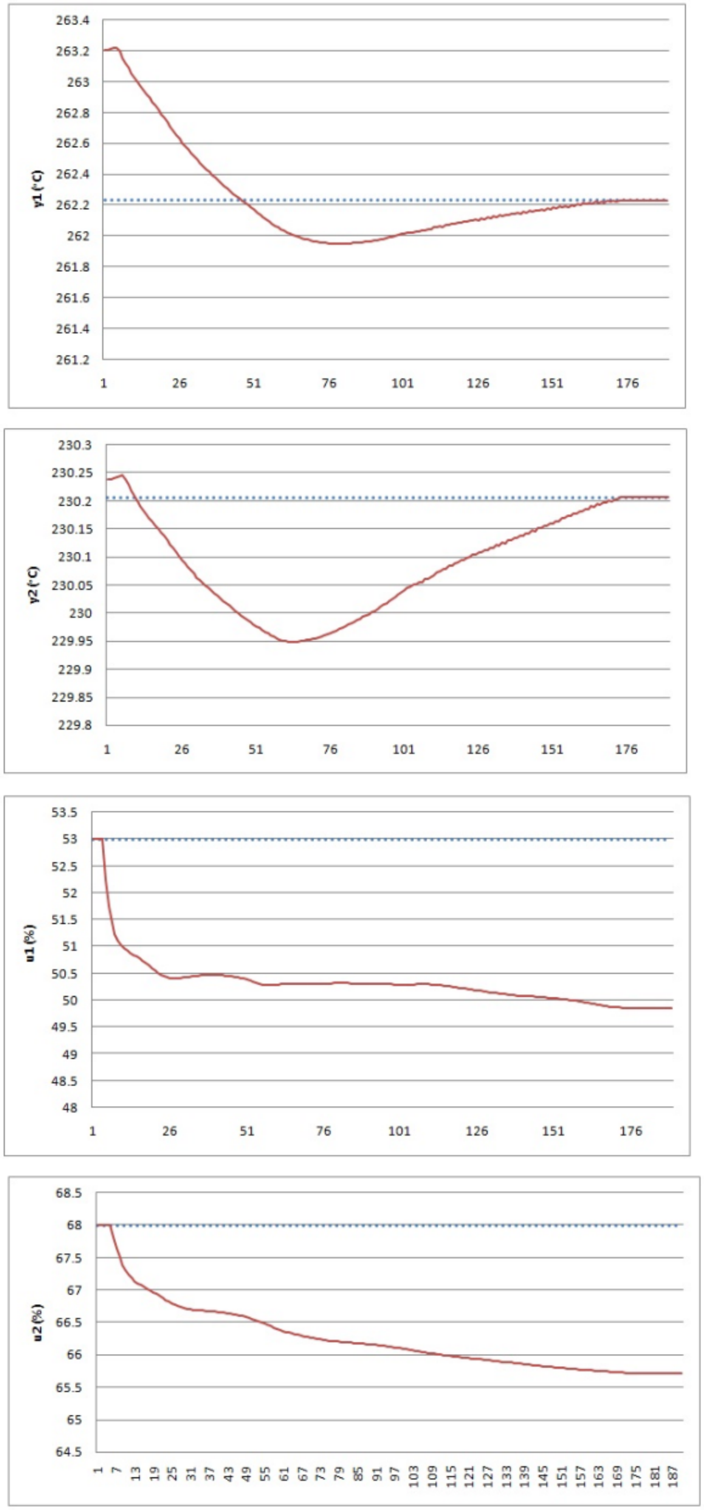


Figure 5.8: Closed Loop responses for y1 - 1°C (Case 2). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

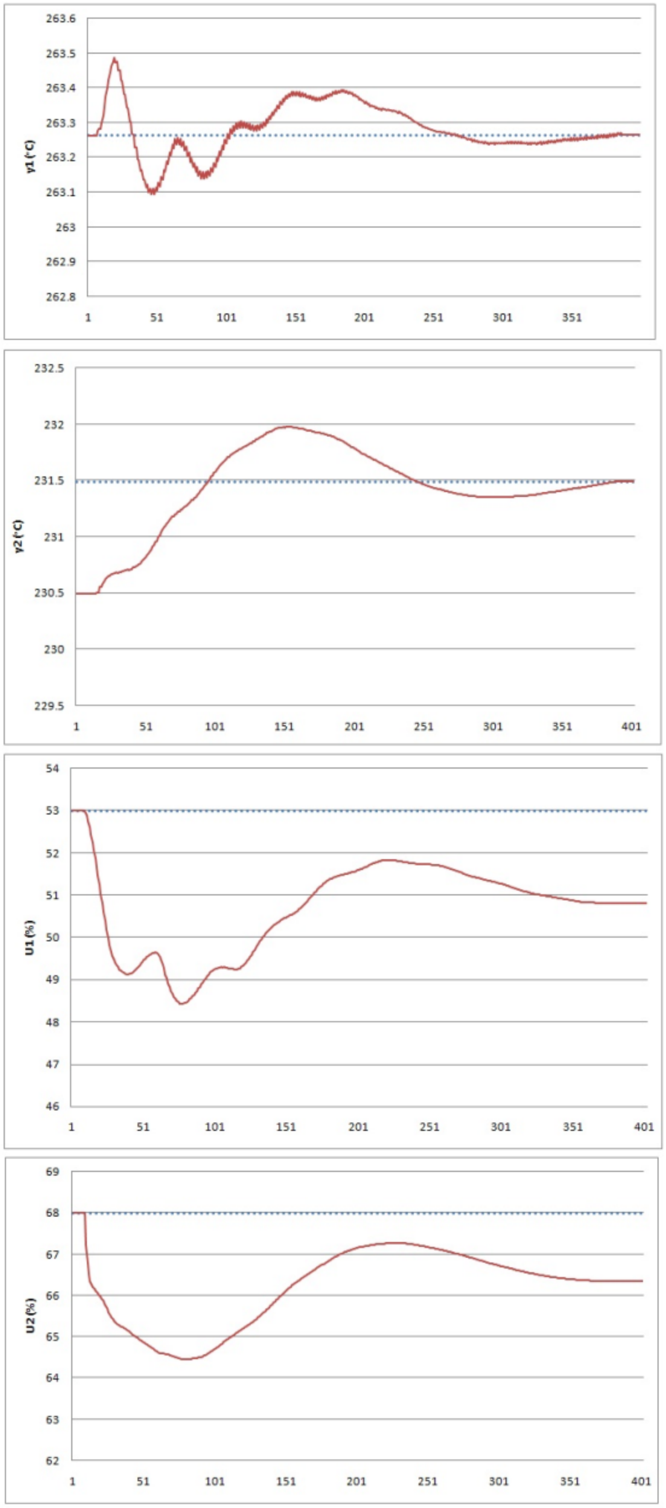


Figure 5.9: Closed Loop responses y2 + 1^{o}C (Case 3). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

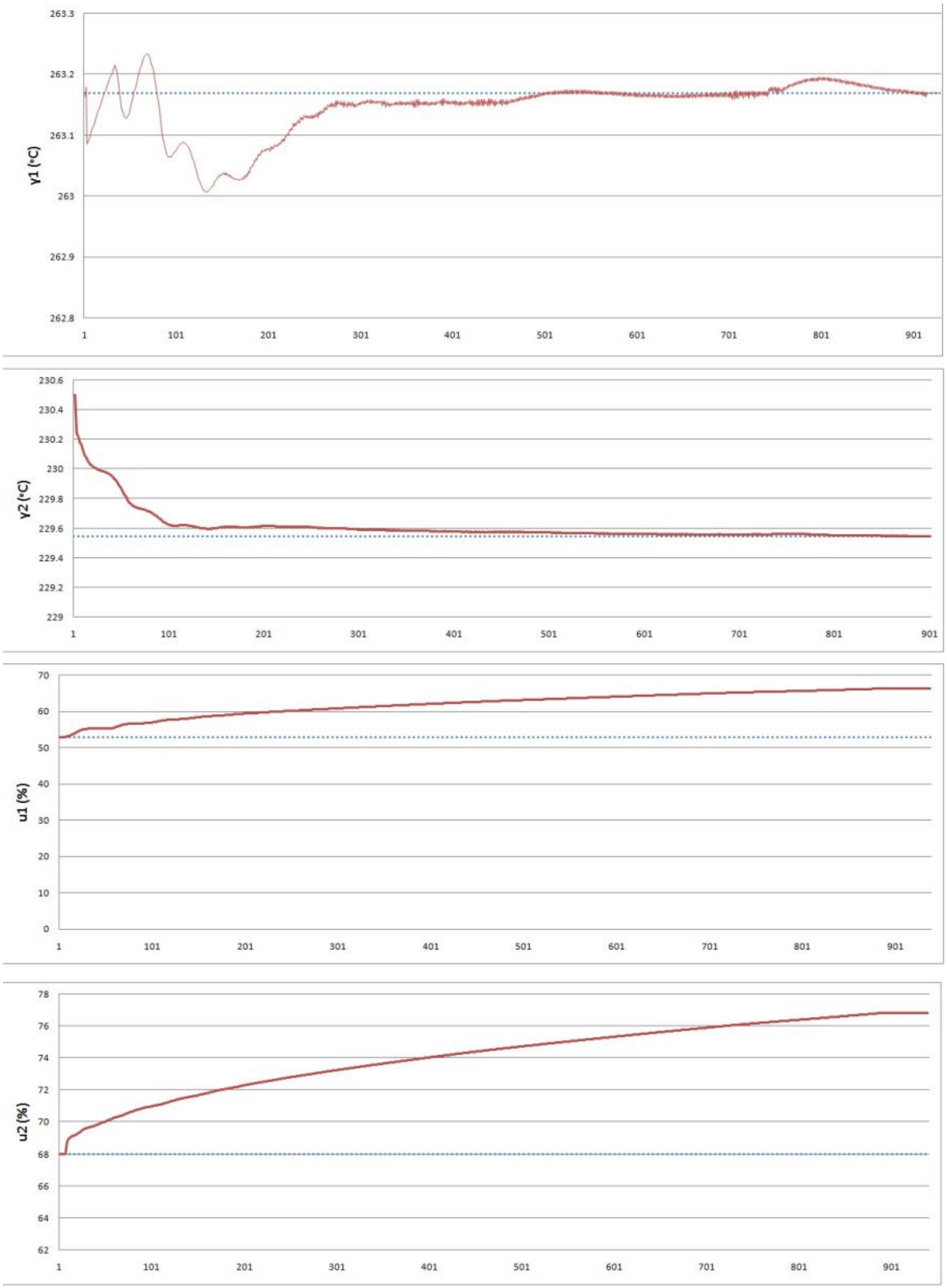


Figure 5.10: Closed Loop responses for y2 -1°C (Case 4). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

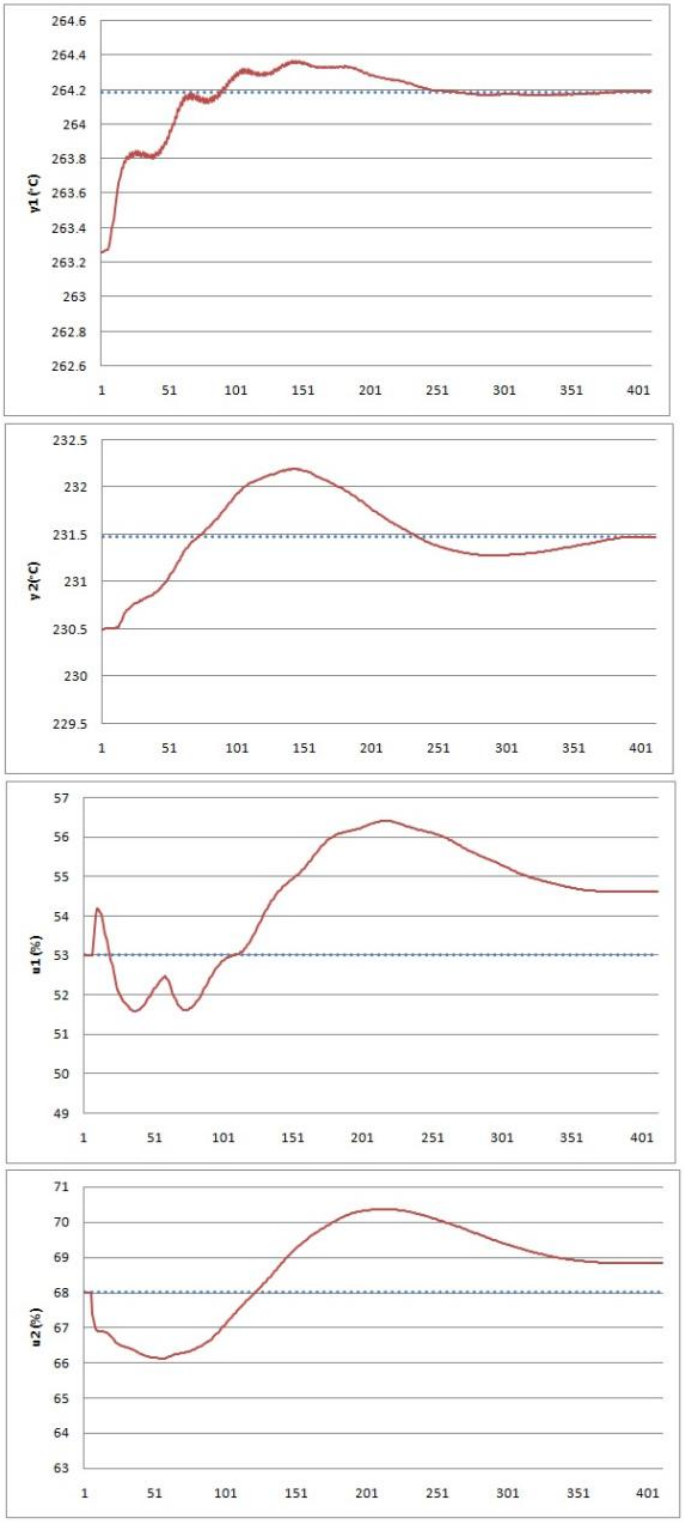


Figure 5.11: Closed Loop responses for y1 + 1°C , y2 + 1°C (Case 5). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

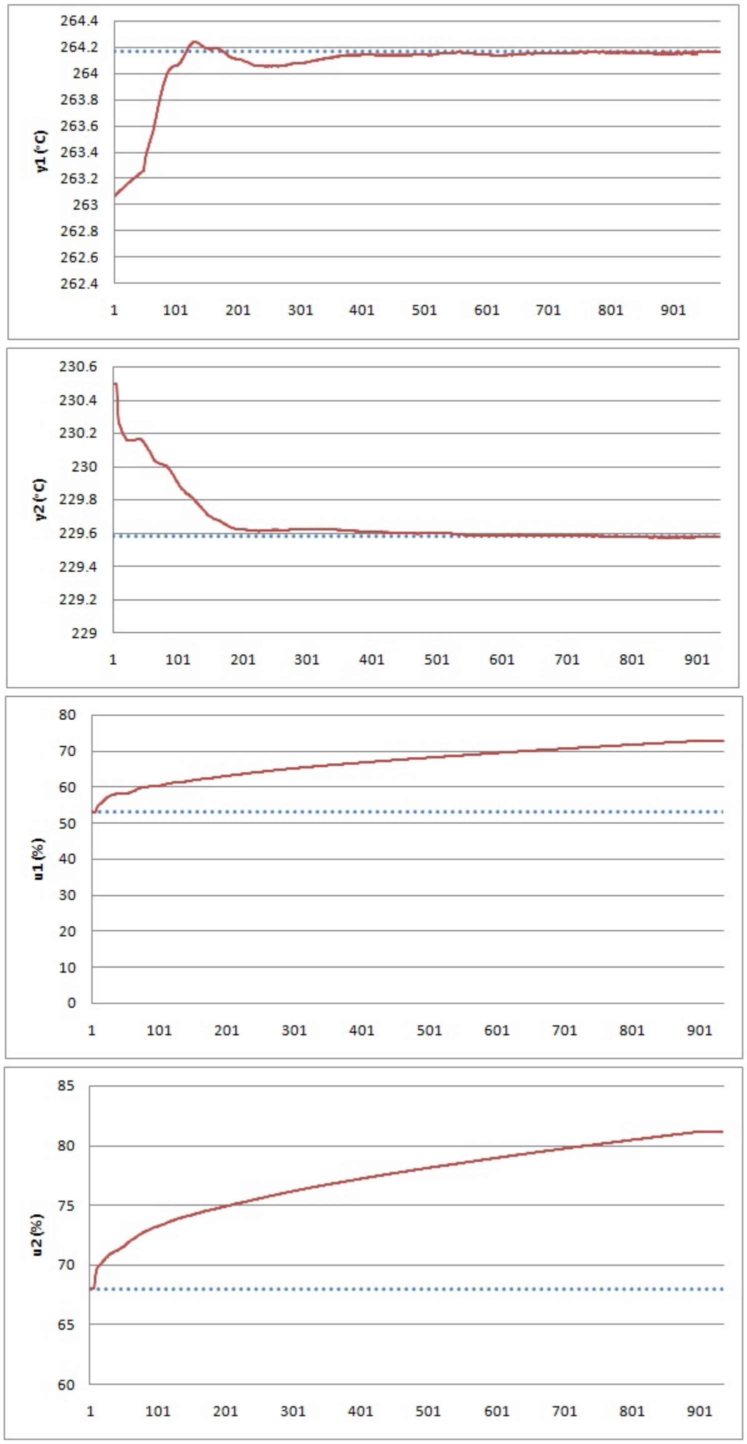


Figure 5.12: Closed Loop responses for y1 + 1°C,y2 - 1°C (Case 6).The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

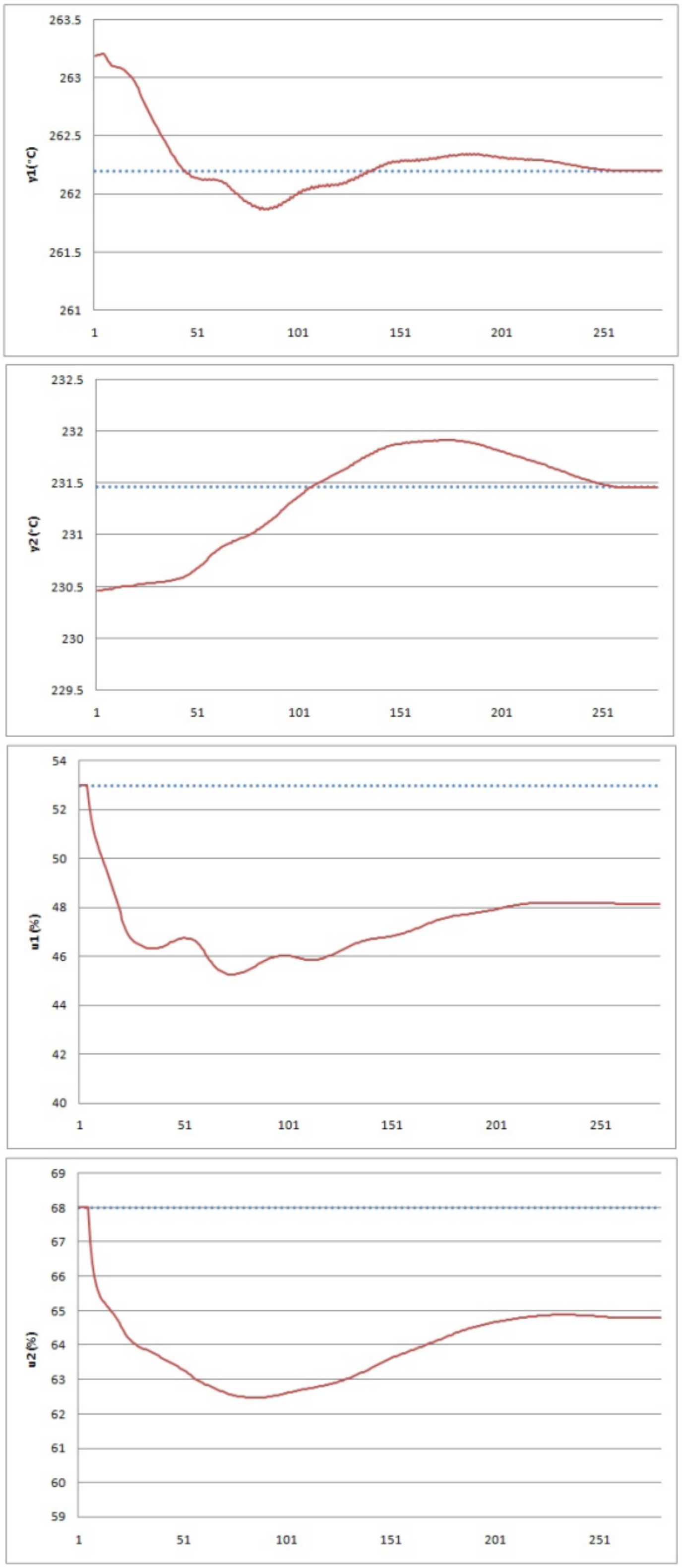


Figure 5.13: Closed Loop responses for y1 - 1°C, y2 + 1°C (Case 7). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

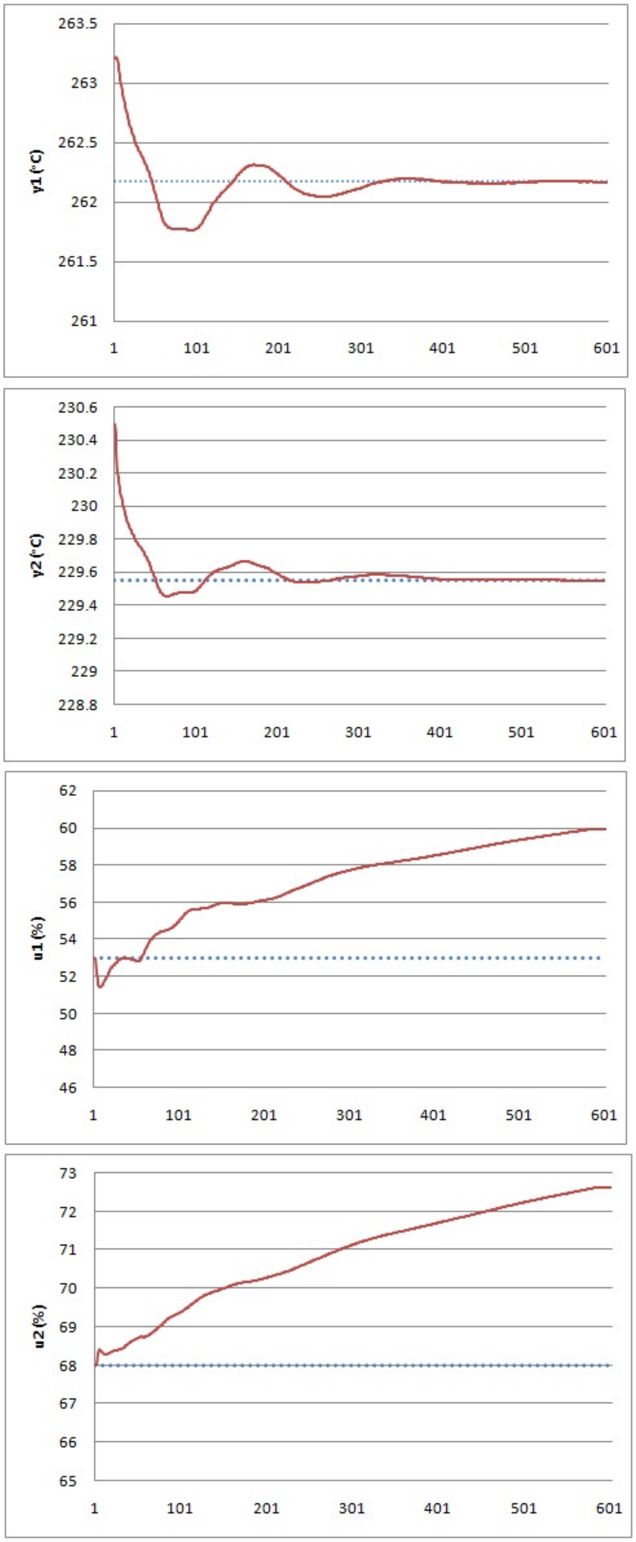


Figure 5.14: Closed Loop responses for y1 - 1^{o}C, y2 - 1^{o}C (Case 8). The response curve (red line) is compared with output set points and input nominal values (dotted blue line)

Integral Square Errors (ISEs) [(°C)^2.min] for different setpoint changes are calculated and the total area or ISEs for each cases are shown in table 5.6 below.

Table 5.6: Integral Squared Errors (ISEs) [(°C)^2.min] values for each cases.

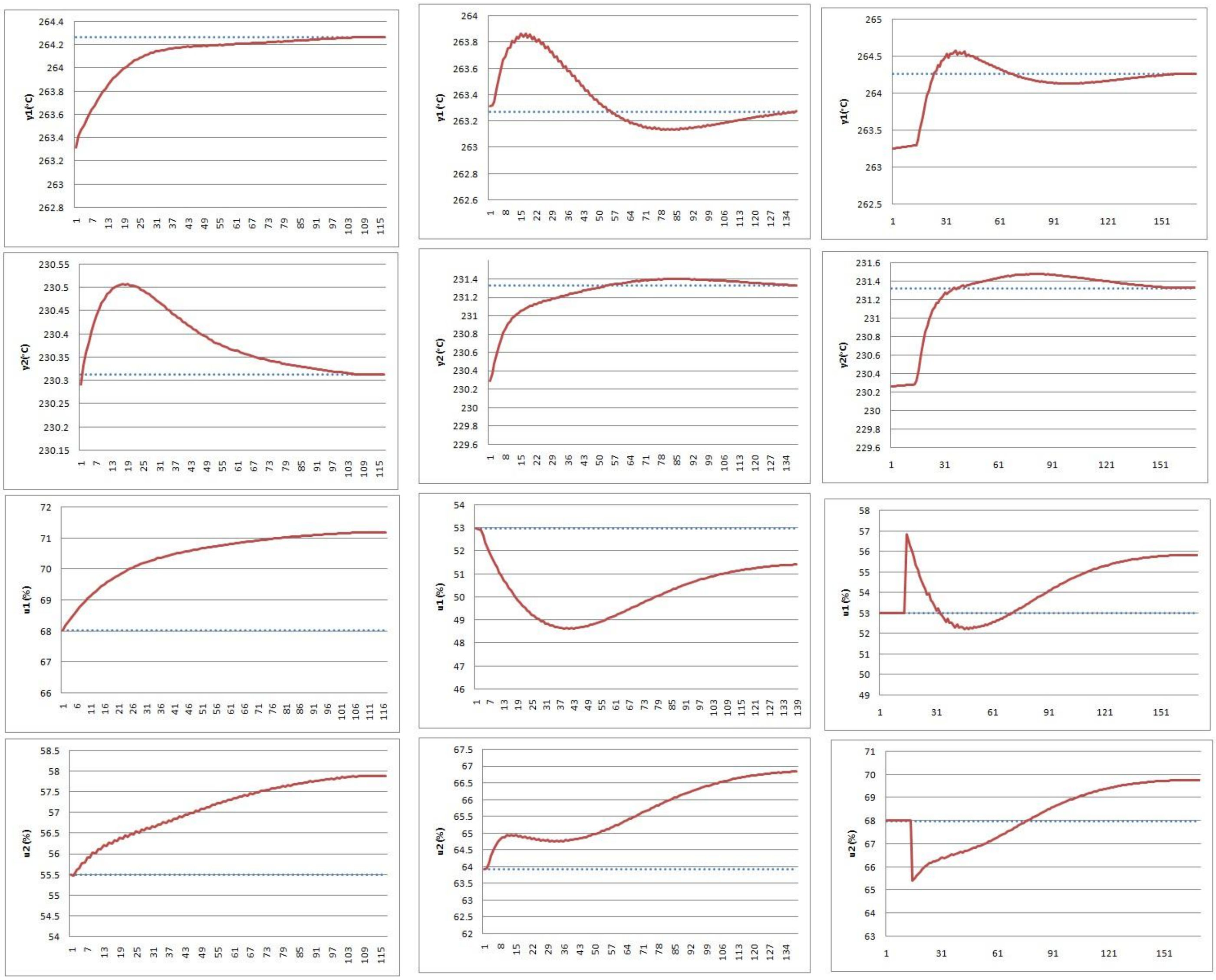
Output	**Case 1**	**Case 2**	**Case 3**	**Case 4**	**Case 5**	**Case 6**	**Case 7**	**Case 8**
y_1	38.015	38.869	18.26	20.937	59.317	77.328	36.0535	57.363
y_2	18.4	20.81	101.424	36.621	110.582	69.387	101.14	31.186

Table 5.7: Total average duties (kW/min) for each cases.

Output	**Case 1**	**Case 2**	**Case 3**	**Case 4**	**Case 5**	**Case 6**	**Case 7**	**Case 8**
u_1	334.8	401.7	451.3	952.5	150.3	1497.7	722.4	517.3
u_2	1187.9	928.2	1284.27	3398	1847.5	5109.3	2925.8	1791.7

The area of ISE represents the performance of MPC controller, with smaller area means more efficient MPC controller. Observing the closed loop response, it can be concluded that the time constants are too high, process took a long time to reach new steady state, and this has caused the ISEs to be high. Large ISE values shows current MPC strategy is not very efficient and some tuning needs to be done on MPC in order to be more efficient.

A comparison between MPC controller and PI controller efficiency also has been done in order to determine better efficiency. Three cases has been compared, which are Case 1 (y1 + 1°C), Case 3 (y2 + 1°C),, and Case 5 (y1 + 1°C, y2 + 1°C),. Figure 5.15 shows the PI closed loop response for set point tracking in each case.



Case 1: y1+1C

Case 3:y2+1C

Case 5: y1+1C y2+1C

Figure 5.15: Setpoint Tracking Responses for PI Controller for Case 1, 3, and 5.

Table 5.8: Comparison of Integral Squared Errors (ISEs) [(^{o}C)^{2}.min] for MPC and PI.

Output	**Case 1**		**Case 3**		**Case 5**	
	MPC	**PI**	**MPC**	**PI**	**MPC**	**PI**
y_1	38.015	21.2	18.26	22.3	59.317	27.28
y_2	18.4	11.5	101.424	18.612	110.582	38.62

Averagely MPC has ISEs that exceeds PI ISEs for each case. Larger ISE means lower efficiency. So currently PI controller is more efficient than MPC controller. MPC controller efficiencies can be increased by a right tuning.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

In conclusion up to this point developments of steady state and dynamic models of MMH process are presented in this chapter. The model achieved close accuracy when steady state model is validated against base reference process from literature. Dynamic model is initialized and developed based on steady state models. For this process the dynamic model is developed individually for each main unit operation. Regulatory controllers are installed to stabilize MMH process and maintain product quality. A system identification has been done on the process model in MATLAB using step testing data on model and the process gains and time constants has been identified. In order to sustain production at optimum cost MPC strategy has been implemented and the performance is measured, however need more tuning to be more efficient. Comparison with PI controller performance shows PI controller is more efficient than MPC controller at the moment.

This study can be further improved by developing the reactor model for MMH process. The current model only focus on separation process of MMH while integrating reactor model into the separation model would result a complete model for MMH process. Integration between MPC tools in HYSYS which construct unconstrained MPC strategy and MPC tools in MATLAB which construct constrained MPC strategy will lead to a better MPC scheme that is closer to real life process plant.

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