

การสังเคราะห์โครงสร้างการควบคุมแบบแผนทัวด์



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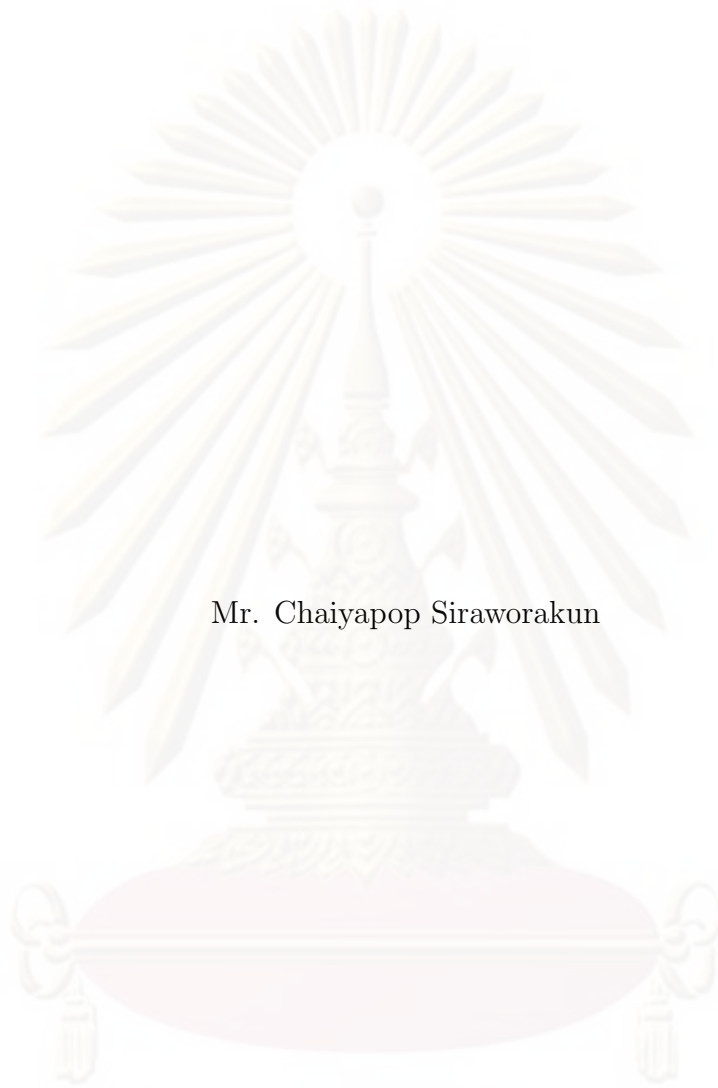
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SYNTHESIS OF THE PLANTWIDE CONTROL STRUCTURE



Mr. Chaiyapop Siraworakun

A Dissertation Submitted in Partial Fulfillment of the Requirements  
for the Degree of Doctor of Engineering Program in Chemical Engineering

Department of Chemical Engineering

Faculty of Engineering

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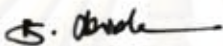
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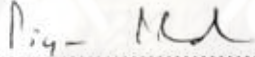
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Field of study        Chemical Engineering  
Advisor                Assistant Professor Montree Wongsri, D.Sc.

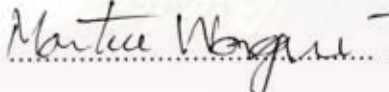
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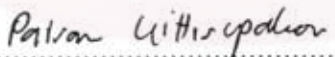
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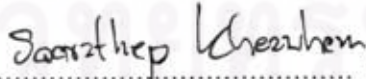
  
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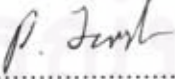
#### THESIS COMMITTEE

  
..... Chairman  
(Professor Piyasan Praserttham, Dr.Ing.)

  
..... Advisor  
(Assistant Professor Montree Wongsri, D.Sc.)

  
..... Examiner  
(Associate Professor Paisan Kittisupakorn, Ph.D.)

  
..... Examiner  
(Soorathep Kheawhom, Ph.D.)

  
..... External Examiner  
(Phisit Jaisathaporn, Ph.D.)

---

ชัยภพ ศิระวรกุล : การสังเคราะห์โครงสร้างการควบคุมแบบแพลนท์ไวด์. (SYNTHESIS OF THE PLANTWIDE CONTROL STRUCTURE) อ.ที่ปรึกษาวิทยานิพนธ์หลัก:  
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วิธีการแบบผสมผสานเชิงคณิตศาสตร์และฮิวริสติกสำหรับการสร้างโครงสร้างการควบคุมแบบแพลนท์ไวด์ถูกนำเสนอในวิทยานิพนธ์ฉบับนี้ วิธีการที่นำเสนอนำข้อดีของทั้งวิธีการเชิงฮิวริสติก และเชิงคณิตศาสตร์เพื่อพัฒนาโครงสร้างการควบคุมแบบแพลนท์ไวด์ที่น่าพึงพอใจ ในส่วนฮิวริสติกชุดของตัวแปรควบคุม และตัวแปรปรับถูกเลือก ตามด้วยการสร้างวงควบคุมที่เป็นได้อย่างชัดเจน ในส่วนคณิตศาสตร์การออปติไมเซชันเชิงสมรรถนะทางพลวัต (dynamic performance-based optimization) ถูกนำเสนอเพื่อสร้างโครงสร้างการควบคุมแบบแพลนท์ไวด์ ปัญหาการออปติไมเซชันถูกกำหนดในรูปแบบของระเบียบวิธีการไม่เป็นเชิงเส้นแบบจำนวนเต็มผสม (mixed integer nonlinear programming) ฟังก์ชันวัตถุประสงค์ถูกนำเสนอด้วยผลรวมของค่าผิดพลาดสัมบูรณ์ถ่วงน้ำหนักโดยเวลา (integral of the time-weighted absolute error) ของตัวแปรวัด และตัวแปรปรับทั้งหมดขณะมีการรบกวนแบบหลากหลาย แบบจำลองปริภูมิสถานะไม่ต่อเนื่อง (discrete state-space model) ถูกใช้เป็นแบบจำลองกระบวนการในปัญหาการออปติไมเซชัน

วิธีการที่นำเสนอถูกทดสอบกับกระบวนการเทเนสซีอีสท์แมน โครงสร้างการควบคุมที่ได้ถูกนำมาเปรียบเทียบกับงานที่ได้นำเสนอก่อนหน้านี้โดย Luyben ในปีค.ศ. 1999 ในการจำลองในสถานะพลวัตสมรรถนะของโครงสร้างการควบคุมแบบแพลนท์ไวด์ถูกประเมินในขณะที่มีการรบกวนแบบหลากหลาย และการเปลี่ยนแปลงค่าเป้าหมาย จากผลการจำลองแสดงให้เห็นว่าโครงสร้างการควบคุมที่ได้ให้การตอบสนองที่น่าพึงพอใจเมื่อเปรียบเทียบกับงานของ Luyben และคณะ ในปีค.ศ. 1999

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The combined mathematic and heuristic based approach is proposed for establishing the plantwide control structure in this dissertation. The proposed approach takes advantages of both heuristic based and mathematic based approaches to develop the appropriate plantwide control structures. In heuristic part, sets of controlled variables and manipulated variables are selected followed by establishing of the obvious control loops. In mathematic part, the dynamic performance-based optimization is proposed for establishing the plantwide control structures. The optimization problem is formulated as a mixed integer nonlinear programming (MINLP). The objective function is presented as an integral of the time-weighted absolute error (ITAE) of all measurements and manipulated variables in the face of disturbances. A discrete state-space model is used as the process model in the optimization problem.

The proposed approach is investigated on the Tennessee Eastman (TE) process. The obtained plantwide control structures are compared with the earlier work given by Luyben et al. (1999). In dynamic simulation, the performance of the plantwide control structures is evaluated in the face of disturbances and set-point changing. The simulation results show that the obtained plantwide control structures give the appropriate responses compares with those of Luyben et al. (1999).

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Field of Study:.....Chemical Engineering....  
Academic Year:.....2008.....

Student's Signature:.....*Chaiyapop*.....  
Advisor's Signature:.....*[Signature]*.....

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## NOMENCLATURES

$K_u$	= Ultimate Gain
$P_u$	= Ultimate Period
$\lambda_{ij}$	= Relative Gain Element
$\Lambda$	= Relative Gain Array
$G$	= Transfer Function
$\sigma_i$	= Singular Value
$\bar{\sigma}$	= Maximum Singular Value
$\underline{\sigma}$	= Minimum Singular Value
$\gamma$	= Condition Number
$A, B, C, D, P, W$	= Constant Matrices in Continuous State Space Model
$\tilde{A}, \tilde{B}, \tilde{C}, \tilde{W}$	= Constant Matrices in Discrete State Space Model
$\tilde{Z}$	= Control Structure Matrix
$\tilde{K}^P, \tilde{K}^I$	= Tuning Parameters Matrices for PI controller
$x$	= State Vector
$u$	= Input (Manipulated Variable) Vector
$d$	= Disturbance Vector
$y$	= Output (Measurement) Vector
$t$	= Time
$T$	= Simulation Time
$w_y$	= Weighting Factor for Measurements
$w_u$	= Weighting Factor for Manipulated Variables
$N_y$	= Number of Measurements
$N_u$	= Number of Manipulated Variables
$N$	= Number of Control loops
$n$	= Number of Disturbances taken to the model

# CHAPTER I

## INTRODUCTION

In a complex chemical process, there are many unit operations which are interconnected together. An important problem is to develop an effective control system for the complex chemical process. In the past, control system design traditionally followed the unit operation approach (Stephanopoulos, 1983). First, all of the controlled loops were established individually for each unit operation. Then the pieces were combined together into an entire plant. This method works well when the processes are in the cascade form (i.e. without material and energy recycles) or large surge tanks are installed for the processes with recycle streams to isolate the individual unit.

Material and energy recycles are used for the reason of process economic and performance improvement. Hence, use of surge tanks should be eliminated from the processes to decrease the capital cost. However, the recycles make a complex behavior within the process. Due to nature of recycle streams, they feature positive feedback to the process. These make the increasing in the overall process gain and time constants. A small change in recycle stream may cause a large change in other stream or we known as snowball effect. Plantwide process control is an appropriate approach to force the complex response corresponding with economic and process limitation. The objective of plantwide process control is to establish the control structure of an entire plant.

### 1.1 Background

Plantwide process control involves the systems and strategies required to control an entire chemical plant consisting of many interconnected unit operations (Luyben, et.al., 1999). The plantwide control problem is quite large and complex.



Generally, there are many measurements and control valves in a chemical plant. Process control engineers have to decide that which measurements should be used as controlled variables and which control valves should be used for manipulating the selected measurements. Due to combinatorial nature, the plantwide control problem is an open-ended problem.

Many researchers proposed a number of methodologies for developing plantwide control structures. These methodologies could be categorized into two main approaches: (1) heuristic approach and (2) mathematical approach. For heuristic approach, chemical engineering knowledge and engineering judgment are used as decision tools for establishing the control structure. For mathematical approach, an optimization problem is formulated and solved for establishing the control structure.

In this work, a new methodology for establishing the plantwide control structure is proposed. The methodology is a combination of heuristic design and mathematical programming. An optimization problem is formulated and solved as the Dynamic Mixed Integer Nonlinear Programming (DMINLP) to establish the control structure. The process disturbances are included in the optimization problem as the treatment of uncertainties. The Tennessee Eastman (TE) process is selected as the test-bed problem, since it consists of . Results are tested by dynamic simulation and compared with the control structures proposed by Luyben.

## 1.2 Objectives of the Research

The objectives of this research are listed below

1. Propose a new methodology based on mathematical approach for plantwide control structure design.
2. Apply the methodology to the Tennessee Eastman (TE) Process.

## 1.3 Scopes of the Research

Scopes of this research are listed below:

1. The proposed methodology is conformed to the class-1 or class-2 which is proposed by Stephanopoulos and Ng (Stephanopoulos and Ng, 2000).
2. The programming languages used in this research is MATLAB.
3. The description of TE process is given by William L. Luyben, Bjorn D. Tyreus, and Micheal L. Luyben (Luyben, et.al., 1998) and original paper by Downs and Vogel (Downa and Vogel, 1993).

#### **1.4 Contributions of the Research**

Contributions of this research are listed below:

1. A new methodology based on mathematical approach for plantwide control structure deisgn is proposed.
2. The plantwide control structures for TE process are developed and evaluated using the proposed methodology.

#### **1.5 Research Procedures**

1. Study of plantwide process control theory, TE process and concerned information.
2. Study of optimization theory and application for plantwide control structure design problem.
3. Simulation of the TE process at steady state and dynamic conditions using MATLAB.
4. Development of control structures for TE process using the proposed methodology.
5. Evaluation of the dynamic control performance of the obtained control structures based on various operating conditions and disturbances.
6. Correction and summarization of simulation results.

## 1.6 Outline of Dissertation

This dissertation has been divided into seven chapters.

In chapter 2, a review of the previous works on plantwide control structure design and on design and control of the Tennessee Eastman (TE) process are given.

In chapter 3, the theories which are related on this dissertation are presented. These include plantwide control fundamental, multivariable control theory, and introduction to optimization.

In chapter 4, the methodology on the synthesis of plantwide control structure is presented. The chapter includes methodology framework, description on the Tennessee Eastman (TE) process, process model development, and optimization problem formulation.

In chapter 5, the the dynamic performance-based optimization for establishing the plantwide control structure of the TE process is proposed. The control structures of the important variables are established by optimization. While the control structures of the remaining variables are established by heuristic. The performances of the obtained control structure are evaluated by the dynamic simulation.

In the chapter 6, the combined mathematic and heuristic approach is proposed for plantwide control structure design. Heuristic rules are used for selecting controlled variables (CVs) and manipulated variables (MVs) sets and for establishing obvious control loops to save computing time. the dynamic performance-based optimization is adopted to establish control structure of the plant. The performances of the obtained control structure are evaluated by the dynamic simulation.

The final summary and overall conclusions of this dissertation are discussed in Chapter 7 followed by suggestions for the future work on this study.

## CHAPTER II

### LITERATURE REVIEW

Plantwide control problem has been increasingly interested for decades. Firstly, Buckley proposed the plantwide control design procedure (Buckley, 1964). The procedure consists of two stages, determining the materials balance control structure for low-frequency disturbances and establishing the product quality control structure for high-frequency disturbances. While Buckley (1964) defined the general problem and provide a practical solution, Foss (1973) brought it to the center of process control research: *"Perhaps the central issue to be resolved by the new theories of chemical process control is the determination of the control system structure"* (Stephanopoulos and Ng, 2000). For many years, a number of methodologies have been proposed in the chemical engineering literatures for the generation of promising plantwide regulatory control structures by several researchers. These methodologies range from pure mathematical programming based methods to heuristic based methods. The purpose of this chapter is to present a review of the previous works of plantwide control design and Tennessee Eastman (TE) process.

#### 2.1 Plantwide Control Structure Design

Price and Georgakis proposed the procedure for developing the coupled system regulatory control system of a CSTR/column example (Price and Georgakis, 1993). The problem was decomposed into two frameworks; (1) modular framework and (2) tiered framework. The procedure is based on a tiered framework for plantwide control system design. The best-performing structures are shown to be self-consistent and designed to minimize the propagation of disturbances through the system.

One of the most significant works in the heuristic based avenue is presented by Luyben et al. (1997). They proposed the nine steps procedure for developing the plantwide control structure. In their textbook (Luyben et al., 1999), they presented the development of plantwide control structure for four chemical processes: (1) Tennessee Eastman (TE), (2) Hydrodealkylation (HDA), (3) Butane Isomerization and (4) Vinyl Acetate.

Wongsri and Hermawan (2005) proposed the plantwide control structure design methodology for controlling a complex energy integration plant. They proposed the heat pathway heuristics (HPH) to use in conjunction with Luyben's nine steps plantwide control procedure to model the heat pathway management and control configuration of hydrodealkylation (HDA) process. An appropriate heat pathway was selected by selective controller with low selector switch (LSS) to direct the disturbance load to the utility units in order to achieve dynamic maximum energy recovery (DMER).

For the past works in the mathematic based approach, Narraway and Perkins proposed a systematic method used to select the economically optimal control structure of a process (Narraway and Perkins, 1993). The problem was limited to selecting optimal control structures for steady-state process model. As the problem is combinatorial in nature, the systematic method uses the integer programming techniques for selecting the optimal control structure.

McAvoy proposed the synthesis of plantwide control structure using the optimization technique (McAvoy, 1999). The objective function is the summation of deviation of all valve positions for their steady-state value. The steady-state gain model was used as process model in optimization. The optimization problem is formulated as mixed integer linear programming (MILP) for establishing the candidate control structures. To establish the candidate control structures, there are three stage of the methodology. For the first and second stage is solved by MILP. The last stage solution is obtained by steps 7-9 of Luyben's nine-step procedure. The candidate control structures are screened by relative gain array.

To extend their previous work, Wang and McAvoy (2001) used the dynamic model in the optimization problem. The plantwide control scheme is synthesized in three stages involving fast and slow safety variables to be controlled, followed by product variables. In each stage, MILP is solved to generate candidate control structures. The objective function involves a tradeoff between manipulated variable moves and transient response area.

Skogestad and Postlethwaite have presented the tasks of control structure design in their textbook (Skogestad and Postlethwaite, 2005). The tasks consist of (1) the selection of controlled outputs, (2) the selection of manipulations and measurements, (3) the selection of control configuration, (4) the selection of controller type. The plantwide control is not only focused on the control structure design but the one of the key challenges is also the selection of controlled variables (CVs). Many researchers have presented variety of approaches to select the proper set of CVs in the chemical processes.

Skogestad (2000) have proposed the idea of self-optimizing control to select the best set of controlled variables. The self-optimizing control is when an acceptable loss can be achieved using constant setpoints for the controlled variables, without the need to reoptimize when disturbances occur.

Although Luyben's nine steps procedure (Luyben et al, 1997) is the guideline for control structure design, it reflects a good guideline for CVs selection, implicitly.

Stephanopoulos and Ng (2000) classified the plantwide control structure problems according to the inclusion of uncertainties in design steps. The uncertainties consist of model uncertainties and process disturbances. They devised three classes based upon the treatment of uncertainties on the selection of controlled variables.

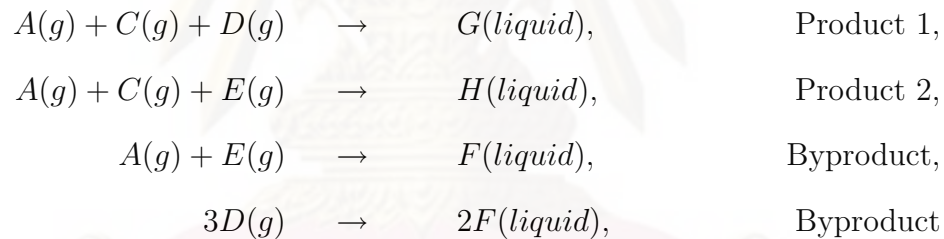
*Class-1:* treatment of uncertainties explicitly. In this approach, model uncertainties are included in the process model. Mathematical techniques are required for the selection of the best structure.

*Class-2:* treatment of uncertainties in the phase of selecting the manipulated variables. Uncertainties are accounted during the actual formation of the control structure, which the set of controlled variables depends on the set of manipulation.

*Class-3:* treatment of uncertainties for the phase of tuning the controller. This approach is the major of the past works. Uncertainties are accounted during the design and tuning of the control laws.

## 2.2 Design and Control of Tennessee Eastman Process

Tennessee Eastman (TE) process was proposed by Downs and Vogel (Downs and Vogel, 1993). The TE Process contains five main unit operations, four feed streams, one product stream and one purge streams. Two products are produced by four reactants as shown below



There are 41 measurements and 12 manipulated variables in the process. The detail of the process is shown in the chapter 4. Several researchers studied the control of the TE process for a decade. There are a number of approaches used for developing the control structure of the TE process such as using optimization technique, heuristic approach, and hierarchical design. The various approaches are discussed below.

McAvoy and Ye proposed the heuristic approach to develop plantwide control structures for the TE process (McAvoy and Ye, 1994). They presented an approach to configure a basic PID control system for the TE process. A multiloop single-input-single-output control structure is used. The control design approach involves using a combination of steady-state screening tools, followed by dynamic simulation of the most promising candidates. The steady-state tools employed are

the relative gain, Niederlinski index and disturbance analysis.

Lyman and Georgakis studied the four plantwide control structures of the TE process (Lyman and Georgakis, 1995). The four control structures were developed in a tiered fashion and without the use of process model. The production rate manipulator is selected first so that it is located on the major process path. Then the inventory controls are arranged in an outward direction from the production rate manipulator (Price and Georgakis, 1993). The four control structures were described and comments were given on their effective handling of the defined disturbances and setpoint changes.

Banerjee and Arkun presented a systematic approach to design the control configuration of the TE process which meets the control objective in the presence of uncertainties (Banerjee and Arkun, 1995). Control configuration design includes the selection and partitioning of measurements and manipulated variables used in the closed loop control. For selection stage, a theorem for establishing a necessary condition for robust stability was used as a selection criterion. For partitioning stage, all sub-systems that pass the selection criterion must be partitioned in the manner of decentralized feedback interaction between the chosen measurements and manipulations.

Ricker determined the optimal steady-state condition for six operating modes of the TE Process (Ricker, 1995). The problem was formulated as nonlinear program and the solutions were obtained using MINOS5.1. The result showed that the base case condition is far from the optimal condition. In the following publication, Ricker and Lee developed and tested the nonlinear model predictive control (NMPC) algorithm for the TE Process (Ricker and Lee, 1995). The model used in NMPC was nonlinear. The unmeasured disturbances and parameters were estimated on-line to eliminate offset of outputs. The results were better than using a typical SISO multiloop strategy. In latter year, Ricker proposed a decentralized control scheme for TE Process (Ricker, 1996). The design procedure begins with the selection of the production rate control method followed by inventory controls and other functions. The performance of the decentralized control scheme was



compared to that of a NMPC developed previously.

Luyben proposed the simple regulatory control for the TE process in heuristic ways (Luyben, 1996). The procedure consists of five parts outlined by Luyben : 1) set production rate, 2) control product quality and constraints, 3) control of inventories, 4) control of overall component balances, and 5) control of the remains. It provided more effective control of the production rate than more complex strategies that were previously proposed in the other literature. Drastic disturbances were easily handled by overrides. An important feature of the structure was the use of proportional-only controllers on all loops in this integrating system.

Model predictive control was used for applying to control TE process (Srinivas and Arkun, 1997). The model used in control algorithm is based on input - output plant data. The model predictive controller acts as a supervisory controller that dictates the setpoints for a lower PID loop structure. Simulations are presented for the case of disturbance rejection and setpoint tracking. The result shown that the MPC with input-output model displays acceptable closed-loop performance and is able to achieve the control objectives.

McAvoy (1998) has developed a steady-state gain matrix that includes the rate of change of integrating variables for TE process. The relative gain and Niederlinski index are used as screening tool for assessing potential level control strategies. McAvoy and Miller (1999) include the integrating variables into steady-state models that use for assessing the operability of the overall plantwide control schemes of TE process. McAvoy (1999) proposed the synthesis of plantwide control structure for the TE process using the optimization technique. The steady-state gain model is used in optimization. Mixed integer linear programming (MILP) was used as optimization technique for establishing the candidate control structures. The candidate control structures are screened by relative gain array. Wang and McAvoy (2001) extended the previous work by using the dynamic model in the optimization problem of the TE process. The objective function involves a tradeoff between manipulated variable moves and transient response area.

Kookos and Perkins (2001) presented an optimization-based method for selecting manipulated variables for regulatory control schemes (Kookos and Perkins, 2001). The proposed methodology is based on the formulation of a MILP for selection the best sets of manipulation variables. The objective of the mathematical programming technique is to minimize the sensitivity of the closed-loop system to disturbances. A general methodology for incorporating heuristics as constraints to the problem is demonstrated. The main advantage of the method is that the plantwide nature of the problem is preserved because decisions related to different levels of the structure of the base control system are obtained.

The concept of self-optimizing control was applied to the TE process (Larsson and et. al. 2001). The paper described the selection of controlled variables. The systematic procedure for reducing the number of candidate control structures was presented. One step is to eliminate variables that, if they had constant setpoints, would result in large losses or infeasibility when there were disturbances (with the remaining degree of freedom reoptimized). The result (controlled variable set and their setpoints) was confirmed by simulations.

## CHAPTER III

### THEORIES

This chapter has collected the basic theories relating to this dissertation. The theories of both in heuristic approach and mathematic approach are described as followed. The chapter consists of three main topics: 1) plantwide control fundamentals, 2) multivariable control and 3) introduction to optimization.

#### 3.1 Plantwide Control Fundamentals

The common topology of the typical chemical plant consists of reaction section and separation section. In the complex plant, additions of recycle streams cause the complex process behaviors both terms of material and energy accumulation. To control the complex plant that consists of many controlled variables and many manipulated variables, appropriate pairing of the controlled variables (CVs) to the manipulated variables (MVs) is needed. The pairing of CVs to MVs is called control structure. The plantwide control problem is to find out control structure for an entire chemical plant.

##### 3.1.1 Incentives for Chemical Process Control

There are three general classes of needs that a control system is called on to satisfy: suppressing the influence of external disturbances, ensuring the stability of a chemical process, and optimizing the performance of a chemical process (Stephanopoulos, 1984).

###### **Suppressing the Influence of External Disturbances**

Suppressing the influence of external disturbances on a process is the most common objective of a controller in a chemical plant. Such disturbances, which denote the effect that the surroundings (external world) have on a reactor, separa-

tor, heat exchanger, compressor and so on, are usually out of the reach of human operator. Consequently, we need to introduce a control mechanism that will make the proper change on the process to cancel the negative impact that such disturbances may have on the desired operation of a chemical plant. In other words, in order to face all disturbances entering the process, the strategies for control are very important.

### **Ensuring the Stability of a Chemical Process**

The process is stable or self-regulating, if the process variable such as temperature, pressure, concentration, or flow rate stay at a certain point or at a desired steady state value as time progresses. Otherwise, the process is unstable and requires external control for the stabilization of their behavior.

### **Optimizing the Performance of a Chemical Process**

Safety and the satisfaction of product specifications are the two principal operational objectives for a chemical plant. Once these are achieved, the next goal is how to make the operation of the plant more profitable. Given the fact that the conditions that affect the operation of the plant do not remain the same. It is clear that we would like to be able to change the operation of the plant (flow rates, pressures, concentrations, temperatures) in such a way that an economic objective (profit) is always maximized.

## **3.1.2 Integrated Processes**

Three basic features of integrated chemical processes lie at the root of the need to consider the entire plant's control system, as follows: the effect of material recycle, the effect of energy integration, and the need to account for chemical component inventories. However, there are fundamental reasons why each of these exists in virtually all real processes.

### **Material Recycle**

Material is recycled for six basic and important reasons

*Increase conversion:* For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints.

Therefore, the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.

*Improve economics:* In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than it is to reach the necessary conversion level in one reactor or several in series.

*Improve yields:* In reaction system such as  $A \rightarrow B \rightarrow C$ , where  $B$  is desired product, the per-pass conversion of  $A$  must be kept low to void producing too much of undesirable product  $C$ . Therefore the concentration of  $B$  is kept fairly low in the reactor and a large recycle of  $A$  is required.

*Provide thermal sink:* In adiabatic reactors and in reactors where cooling is difficult and exothermic heat effects are large, it is often necessary to feed excess material to the reactor so that reactor temperature increase will not be too large. High temperature can potentially create several unpleasant events, such as thermal runaway, deactivation of catalysts, cause undesirable side reaction, etc. So the heat of reaction is absorbed by the sensible heat required to raise the temperature of the excess material in the stream flowing through the reactor.

*Prevent side reactions:* A large excess of one of the reactants is often used that the concentration of the other reactant is kept low. If this limiting reactant is not kept in low concentration, it could react to produce undesirable products. Therefore, the reactant that is in excess must be separated from the products components in the reactor effluent stream and recycled back to the reactor.

*Control properties:* In many polymerization reactors, conversion of monomer is limited to achieve the desired polymer properties. These include average molecular weight distribution, degree of branching, particle size, etc. Another reason for limiting conversion to polymer is to control the increase in viscosity that is typical of polymer solutions. This facilitates reactor agitation and heat removal and allows the material to be further processed.

### **Energy Integration**

The fundamental reason for the use of energy integration is to improve the

thermodynamic efficiency of the process. This translates into a reduction in utility cost. For energy-intensive processes, the savings can be quite significant.

### **Chemical Component Inventories**

A plant's chemical species can be characterized into three types: reactants, products, and inerts. A material balance for each of these components must be satisfied. This is typically not a problem for products and inerts. However, the real problem usually arises when reactants (because of recycle) are considered and accounted for their inventories within the entire process. Because of their value, it is necessary to minimize the loss of reactants exiting the process since this represents a yield penalty. So we prevent reactants from leaving. This means we must ensure that every mole of reactant fed to the process is consumed by reactions.

### **3.1.3 Effects of Recycle**

Most real processes contain recycle streams. The plantwide control problem becomes much more complex and its solution is not intuitively obvious. The presence of recycle streams alters the plant's dynamic and steady-state behavior. Two basic effects of recycle are: 1) Recycle has an impact on the dynamics of the process. The overall time constant can be much different than the sum of the time constants of the individual units. 2) Recycle leads to the "snowball" effect. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates.

### **3.1.4 Snowball Effects:**

Snowball effect is high sensitivity of the recycle flowrates to small disturbances. When feed conditions are not very different, recycle flowrates increase drastically, usually over a considerable period of time. Often the equipment cannot handle such a large load. It is a steady-state phenomenon but it does have dynamic implications for disturbance propagation and for inventory control.

The large swings in recycle flowrates are undesirable in plant because they can

overload the capacity of separation section or move the separation section into a flow region below its minimum turndown. Therefore it is important to select a plantwide control structure that avoids this effect.

### 3.1.5 Basic Concepts of Plantwide Control

#### **Buckley Basics:**

Page Buckley (1964) was the first to suggest the idea of separating the plantwide control problem into two parts: material balance control and product quality control. He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loops is established, using the flowrates of the liquid and gas process streams. Note that most level controllers should be proportional-only (P) to achieve flow smoothing. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of closed-loop product quality loops are estimated. We try to make these as small as possible so that good, tight control is achieved, but stability constraints impose limitations on the achievable performance.

#### **Douglas Doctrines:**

Because the cost of raw materials and the values of products are usually much greater than the costs of capital and energy, Jim Douglas (1988) leads to the two *Douglas doctrines*:

Minimize losses of reactants and products

Maximize flowrates through gas recycle systems

The first idea implies that we need tight control of stream compositions exiting the process to avoid losses of reactants and products. The second rests on the principle that yield is worth more than energy. Recycles are used to improve yields in many processes. The economics of improving yields (obtaining more desired products from the same raw materials) usually outweigh the additional energy cost of driving the recycle gas compressor.

### Down Drill

Chemical component balances around the entire plant are important things, and checking to see that the control structure handles these component balances effectively. The concepts of overall component balances go back to basic principle in chemical engineering, which is how to apply mass and energy balances to any system, microscopic or macroscopic. We check these balances for individual unit operations, for sections of a plant, and for entire processes.

We must ensure that all components (reactants, products, and inert) have a way to leave or be consumed within the process. The consideration of inert is seldom overlooked. Heavy inert can leave the system in bottoms product from distillation column. Light inert can be purged from a gas recycle stream or from a partial condenser on a column. Intermediate inert must also be removed in some way, such as in side stream purges or separate distillation columns.

Most of the problems occur in the consideration of reactants, particularly when several chemical species are involved. All of reactants fed into the system must either be consumed via reaction or leave the plant as impurities in exiting streams. Since we usually want to minimize raw material costs and maintain high-purity products, most of the reactant fed into the process must be chewed up in the reactions.

### Luyben Laws

Three laws have been developed as a result of a number of case studies of many systems:

A stream somewhere in all recycle loops should be flow controlled. This is to prevent the snowball effect.

A fresh reactant feed stream cannot be flow controlled unless there is essentially complete one pass conversion of one of reactants. This law applies to systems with reaction types such as  $A + B \rightarrow \text{product}$  In system with consecutive reactions such as  $A + B \rightarrow M + C$  and  $M + B \rightarrow D + C$ , the fresh feed can be flow controlled into the system, because any imbalance in the ratios of reactants is accommodated by a shift in the amounts of the two products ( $M$  and  $D$ ) that are generated. An



excess of  $A$  will result in the production of more  $M$  and less  $D$ . And vice versa, an excess of  $B$  results in the production of more  $D$  and less  $M$ .

If the final product from process comes out the top distillation column, the column feed should be liquid. If the final product comes out from the bottom of the column, the column feed should be vapor. Changes in feed flowrate or feed composition have less of a dynamic effect on distillate composition than they do on bottoms composition if the feed is saturated liquid. The reverse is true if the feed is saturated vapor: bottom is less affected than distillate.

### **Richardson Rule**

Bob Richardson suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense because it provides more *muscle* to achieve the desired control objective. The largest stream has the biggest effect to volume of vessel. An analogy is that it is much easier to maneuver a large barge with a tugboat than a life raft. The point is that the bigger the handle you have to affect a process, the better you can control it.

### **Tyreus Tuning**

One of the vital steps in developing a plantwide control system is how to determine the algorithm to be used for each controller (P, PI or PID) and to tune each controller. The use of P-only controllers is recommended for liquid levels. Tuning of P controller is usually trivial, that is set the controller gain equal to 1.67. This will have the valve wide open when the level at 80% and the valve shut when the level is at 20%.

For other control loops, the use of PI controllers is suggested. The relay-feedback test is simple and fast way to obtain the ultimate gain ( $K_u$ ) and ultimate period ( $P_u$ ). The Ziegler-Nichols settings or the Tyreus-Luyben settings can be used for tuning the parameters of controller:

$$\begin{aligned} K_{ZN} &= K_u/2.2 & \tau_{ZN} &= P_u/1.2 \\ K_{TL} &= K_u/3.2 & \tau_{TL} &= 2.2P_u \end{aligned}$$

The use of PID controllers should be restricted to those loops were two criteria

are both satisfied: the controlled variable should have a very large signal-to-noise ratio and tight dynamic control is really essential.

### **3.1.6 Luyben's Nine Steps**

The plantwide control procedure has been established based upon heuristics (Luyben et al., 1997). The nine steps of the design procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental, and safety constraints; liquid level and gas pressure inventories; make up of reactants; component balances; and economic or process optimization. This heuristic design procedure is described below.

#### **1. Establish Control Objectives**

Assess steady-state design and dynamic control objectives for the process. This is probably the most important aspect of the problem because different criteria lead to different control structures. These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of operating conditions.

#### **2. Determine Control Degrees of Freedom**

Count the number of control valves available. This is the number of degrees of freedom for control, that is, the number of variables that can be controlled. The valves must be legitimate (flow through a liquid-filled line can be regulated by only one control valve).

#### **3. Establish Energy Management System**

Term energy management is used to describe two functions. First, we must provide a control system that remove exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used elsewhere in the process by other unit operations. This heat, however, must ultimately be dissipated to utilities. If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents propagation of the thermal disturbances and ensures that the exothermic reactor heat is dissipated and not recycled. Process-to-process heat

exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

Heat removal in exothermic reactors is crucial because of the potential for thermal runaways. In endothermic reactions, failure to add enough heat simply results in the reaction slowing up. If the exothermic reactor is running adiabatically, the control system must prevent excessive temperature rise through the reactor (e.g., by setting the ratio of the flow rate of the limiting fresh reactant to the flow rate of a recycle stream acting as a thermal sink).

Increased use of heat integration can lead to complex dynamic behavior and poor performance due to recycling of disturbances. If not already in the design, trim heaters/coolers or heat exchanger bypass lines must be added to prevent this. Energy disturbances should be transferred to the plant utility system whenever possible to remove this source of variability from the process units.

#### **4. Set Production Rate**

Establish the variables that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate. Often design constraints require that production be set at a certain point. An upstream process may establish the feed flow sent to the plant. A downstream process may require on-demand production, which fixes the product flow rate from the plant.

If no constraint applies, then we select the valve that provides smooth and stable production-rate transitions and rejects disturbances. We often want to select the variable that has the least effect on the separation section, but also has a rapid and direct effect on reaction rate in the reactor without heating an operational constraint. This may be the feed flow to the separation section, the flow rate of recycle stream, the flow rate of initiator or catalyst to the reactor, the reactor heat removal rate, the reactor temperature, and so forth.

#### **5. Control Product Quality and Handle Safety, Operational and Environmental Constraints**

Select the best valves to control each of the product-quality, safety, and environmental variables. We want tight control of these quantities for economic

and operational reasons. Hence we should select manipulated variables such that the dynamic relationships between controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants, and the latter prevents problems with the range-ability of the manipulated variable (control-valve saturation).

### **6. Control Inventories (Pressure and Liquid Level) and Fix a Flow in Every Recycle Loop**

Determine the valve to control each inventory variable. These variables include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit.

Proportional-only control should be used in non-reactive control loops for cascade unit in series. Even in reactor-level control, proportional control should be considered to help filter flow-rate disturbances to the down stream separation system. There is nothing necessarily sacred about holding reactor level constant.

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flows in recycle loops are controlled by levels. Two benefits result from this flow-control strategy. First, the plant's separation section is not subjected to large load disturbances. Second, consideration must be given to alternative fresh reactant makeup control strategies rather than flow control. In dynamic sense, level controlling all flows in recycle loop is a case of recycling of disturbances and should be avoided.

### **7. Check Component Balances**

Identify how chemical components enter, leave, and are generated or consumed in the process. Ensure that the overall component balance for each species can be satisfied either through reaction or exit streams by accounting for the component's composition or inventory at some point in the process.

Light, intermediate, and heavy inert components must have an exit path from the system. Reactant must be consumed in the reaction section or leaves as

impurities in the product streams. Fresh reactant makeup feed stream can be manipulated to control reactor feed composition or a recycle stream composition (or to hold pressure or level as noted in previous step). Purge stream can also be used to control the amount of high- or low-boiling impurities in a recycle stream.

## **8. Control Individual Unit Operations**

Establish the control loops necessary to operate each of the individual unit operations. For examples, a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust fuel flow rate to a furnace supplying energy to the reactor. Crystallizers require manipulation of refrigeration load to control temperature. Oxygen concentration in stack gas from a furnace is controlled to prevent excess fuel usage. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

## **9. Optimize Economic and Improve Dynamic Controllability**

Establish the best way to use the remaining control degrees of freedom. After satisfying all of the basic regulatory requirements, we usually have additional degrees of freedom involving control valves that have not been used and setpoints in some controllers that can be adjusted. These can be used either to optimize steady-state economic performance (e.g., minimize energy, maximize selectivity) or to improve dynamic response.

For example, an exothermic chemical reactor can be cooled with both jacket cooling water and brine to a reflux condenser. A valve-position control strategy would allow fast, effective reactor temperature control while minimizing brine use.

## **3.2 Multivariable Control**

### **3.2.1 Design questions for MIMO control systems**

For a general process with several inputs and outputs, several questions must be answered before we attempt to design a control system for such a process.

1. What are the control objectives?
2. What outputs should be measured?

3. What inputs can be measured?
4. What manipulated variables should be used?
5. What is the configuration of the control loops?

For MIMO systems there is a large number of alternative control configurations. The selection of the most appropriate is the central and critical question to be resolved.

### 3.2.2 Degrees of freedom and the number of controlled and manipulated

The degrees of freedom are defined as *the independent variables that must be specified in order to define the process completely*. The number of degrees of freedom is found to be given by the equation

$$f = V - E \quad (3.1)$$

where  $V$  = number of independent variables describing a process

$E$  = number of independent equations physically relating the  $V$  variables

The maximum number of independent controlled variables in a processing system can find from

$$(\text{number of controlled variables}) = f - (\text{number of externally specified inputs}) \quad (3.2)$$

For the design of a control system the number of required independent manipulated variables is equal to the number of independent controlled variables

$$\begin{aligned} (\text{number of independent manipulated variables}) &= (\text{number of controlled variables}) \\ &= f - (\text{number of externally specified inputs}) \end{aligned} \quad (3.3)$$

### 3.2.3 Generation of alternative loop configurations

After the identification of the controlled and manipulated variables we need to determine the control configuration. The selection of the “best” among all possible loop configurations is a difficult problem. Various criteria can be used to select the “best” couplings among the controlled and manipulated variables, such as:

1. Choose the manipulation that has a direct and fast effect on a controlled variable.
2. Choose the couplings so that there is a little dead time between every manipulation and the corresponding controlled variable.
3. Select the couplings so that the interaction of the control loop is minimal.

### 3.2.4 Interaction of Control Loops

The following statement describes the interaction between two control loops:

“The regulatory action of a control loop deregulates the output of another loop (in the same process), which in turn takes control action to compensate for the variations in its controlled output, disturbing at the same time the output of the first loop. ”

### 3.2.5 Relative Gain Array and the selection

The relative-gain array provides exactly such a methodology, whereby we select pairs of input and output variables in order to minimize the amount of interaction among the control loops. Consider a process with two outputs and two inputs. The relative gain,  $\lambda_{11}$ , between output  $y_1$  and input  $m_1$  is defined as

$$\lambda_{11} = \frac{(\Delta y_1 / \Delta m_1)_{m_2}}{(\Delta y_1 / \Delta m_1)_{y_2}} \quad (3.4)$$

Where

$(\Delta y_1 / \Delta m_1)_{m_2}$  = The open-loop static gain between  $y_1$  and  $m_1$  when  $m_2$  is kept constant.

$(\Delta y_1 / \Delta m_1)_{y_2}$  = The open-loop gain between  $y_1$  and  $m_1$  when  $y_2$  is kept constant by the control loop.

The relative gain provides a useful measure of interaction. In particular:

1. If  $\lambda_{11} = 0$ , then  $y_1$  does not respond to  $m_1$  and  $m_1$  should not be used to control  $y_1$ .
2. If  $\lambda_{11} = 1$ , then  $m_2$  does not affect  $y_1$  and the control loop between  $y_1$  and  $m_1$  does not interact with the loop of  $y_2$  and  $m_2$ . In this case we have completely decoupled loops.
3. If  $0 < \lambda_{11} < 1$ , then an interaction exists and as  $m_2$  varies it affects the steady-state value of  $y_1$ . The smaller the value of  $\lambda_{11}$ , the larger the interaction becomes.
4. If  $\lambda_{11} < 0$ , then  $m_2$  causes a strong effect on  $y_1$  and in the opposite direction from that caused by  $m_1$ . In this case, the interaction effect is very dangerous.

### 3.2.6 Selection of loops

For a process with two inputs and two outputs there are two different loop configurations. Let us see how we can use the relative gains to select the configuration with minimum interaction between the loops.

Arrange the four relative gains  $\lambda_{11}$ ,  $\lambda_{12}$ ,  $\lambda_{21}$ , and  $\lambda_{22}$  into a matrix form, which is known as the relative-gain array:

$$\begin{bmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{bmatrix} \quad (3.5)$$

It can be shown that the sum of the relative gains in any row or column of the array is equal to 1. Thus

$$\begin{aligned} \lambda_{11} + \lambda_{12} &= 1 & \text{and} & & \lambda_{11} + \lambda_{21} &= 1 \\ \lambda_{21} + \lambda_{22} &= 1 & & & \lambda_{12} + \lambda_{22} &= 1 \end{aligned} \quad (3.6)$$



We can summarize all the foregoing observations with the following rule for selecting the control loops:

“Select the control loops by pairing the controlled outputs  $y_i$  with the manipulated variables  $m_j$  in such a way that the relative gains  $\lambda_{ij}$  are positive and as close as possible to unity.”

### 3.2.7 Singular value decomposition

Consider a fixed frequency  $\omega$  where  $G(j\omega)$  is a constant complex matrix, and denote  $G(j\omega)$  by  $G$  for simplicity. Any matrix  $G$  may be decomposed into its singular value decomposition (SVD), and we write

$$G = U\Sigma V^H \quad (3.7)$$

$\Sigma$  is the matrix with non-negative singular values,  $\sigma_i$ , arranged in descending order along its main diagonal; the other entries are zero. The singular values are the positive square roots of the eigenvalue of  $G^H G$ , where  $G^H$  is the complex conjugate transpose of  $G$ .

$$\sigma_i = \sqrt{\lambda_i G^H G} \quad (3.8)$$

$U$  is an unitary matrix of output singular vectors,  $u_i$ .

$V$  is an unitary matrix of input singular vectors,  $v_i$ .

Also, the columns of  $U$  and  $V$  are unit eigenvectors of  $AA^H$  and  $A^H A$ , respectively

The singular values are sometimes called the principal values or principal gains, and the associated directions are called principal directions.

Some advantage of the SVD over the eigenvalue decomposition for analyzing gains and directionality of multivariable plants are:

1. The singular values give better information about the gains of the plant.
2. The plant directions obtained from the SVD are orthogonal.

3. The SVD also applies directly to non-square plants.

### 3.2.8 Maximum and minimum singular values

It can be shown that the largest gain for any input direction is equal to the maximum singular value

$$\bar{\sigma}(G) = \sigma_1(G) \quad (3.9)$$

And that the smallest gain for any input direction is equal to the minimum singular value

It can be shown that the largest gain for any input direction is equal to the maximum singular value

$$\sigma(G) \equiv \sigma_k(G) \quad (3.10)$$

Where k denoted the last element of the vector,  $\sigma_i$ .

### 3.2.9 Use of the minimum singular value of the plant

The minimum singular value of the plant,  $\sigma G(j\omega)$ , evaluated as a function of frequency, is a useful measure for evaluating the feasibility of achieving acceptable control. If the inputs and outputs have been scaled, then with a manipulated input of unit magnitude, we can achieve an output magnitude of at least  $\underline{\sigma}(G)$  in any output direction. We generally want  $\underline{\sigma}(G)$  as large as possible.

### 3.2.10 Condition number

Definition of the condition number of a matrix is the ratio between the maximum and minimum singular values,

$$\gamma(G) = \bar{\sigma}(G)/\underline{\sigma}(G) \quad (3.11)$$

A matrix with a large condition number is said to be ill-conditioned. The condition number depends strongly on the scaling of the inputs and outputs. If  $D_1$  and  $D_2$  are diagonal scaling matrices, the minimized or optimal condition number is defined by

$$\gamma^*(G) = \min_{D_1, D_2} \gamma(D_1 G D_2) \quad (3.12)$$

The condition number has been used as an input-output controllability measure, and in particular it has been postulated that a large condition number indicates sensitivity to uncertainty. This is not true in general, but the reverse holds; if the condition number is small, then the multivariable effects of uncertainty are not likely to be serious.

The condition number is large, then this may indicate control problem

1. A large condition number may be caused by a small value of minimum singular value, which is generally undesirable.
2. A large condition number may mean that the plant has a large minimized condition number, or equivalently, it has large RGA-elements which indicate fundamental control problem.
3. A large condition number does imply that the system is sensitive to “unstructured” input uncertainty, but this kind of uncertainty often does not occur in practice. We therefore cannot generally conclude that a plant with a large condition number is sensitive to uncertainty.

### 3.2.11 Self-optimizing Control

Self-optimizing control is when we can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to reoptimize when disturbances occur. (Skogestad and Postlethwaite, 2005)

In the phase of controlled variable selection, two distinct questions arise:

1. What measurements should be selected as the controlled variables?

2. What is the optimal reference value for these variables?

The second problem is one of optimization and is extensively studied. Here we want to gain some insight into the first problem which has been much less studied. It is assumed as following:

1. The overall goal can be quantified in terms of a scalar cost function.
2. For a given disturbance, there exists an optimal value which minimizes the cost function.
3. The reference values for the controlled outputs are kept.

In the following, we assume that the optimally constrained variables are already controlled at their constraints (active constraint control) and consider the remaining unconstrained problem with controlled variables and remaining unconstrained degrees of freedom.

The system behavior is a function of the independent variables  $u$  and  $d$ , so we may formally write  $J = J(u, d)$ . For a given disturbance  $d$  the optimal value of the cost function is

$$J_{opt}(d) = J(u_{opt}(d), d) = \min_u J(u, d) \quad (3.13)$$

Ideally, we want  $u = u_{opt}(d)$ . However, this will not be achieved in practice and we have a loss  $L = J(u, d) - J_{opt}(d) > 0$ .

We consider the simple feedback policy in Figure 3.1, where we attempt to keep  $z$  constant. Note that the open-loop implementation is included as a special case by selecting  $z = u$ . The aim is to adjust  $u$  automatically, if necessary, when there is a disturbance  $d$  such that  $u \approx u_{opt}(d)$ . This effectively turns the complex optimization problem in to a simple feedback problem. This goal is to achieve “self-optimizing control”.

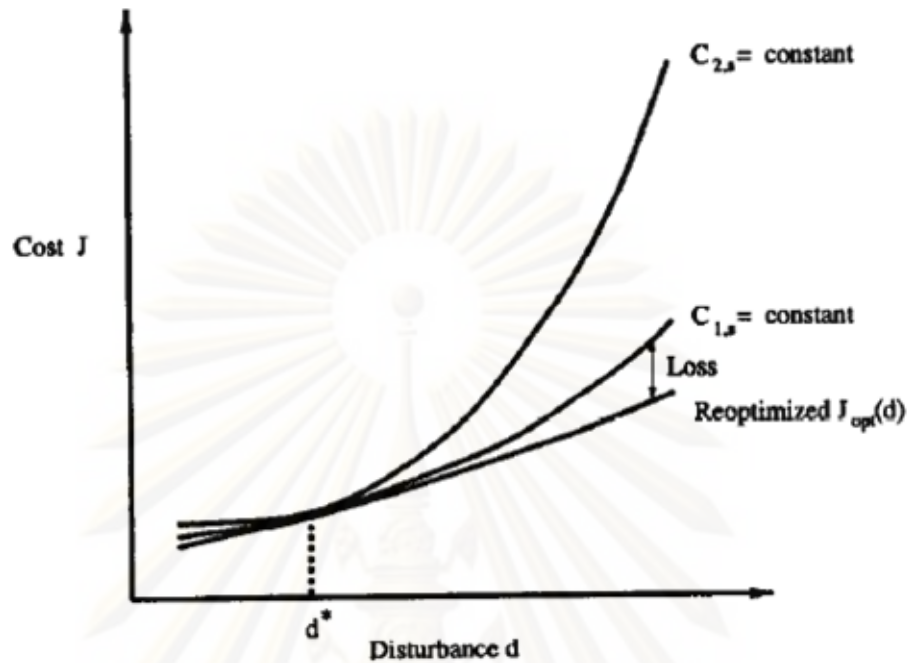


Figure 3.1 Lost imposed by keeping constant setpoint for the controlled variable

### 3.3 Introduction to Optimization

In this section, the concepts of modeling and generic formulations for nonlinear and mixed integer optimization model are described. Section 3.3.1 presents the definition and key elements of mathematical models and discusses the characteristic of optimization models. Section 3.3.2 outlines the mathematical structure of nonlinear and mixed integer optimization problems. Section 3.3.3 describes the mixed integer nonlinear programming (MINLP) overviews.

#### 3.3.1 Mathematical and Optimization Models

Most of applications in areas of science and engineering employ mathematical models. A mathematical model of a system is a set of mathematical relationships which represent an abstraction of the real world system under consideration. A mathematical model of a system consists of four key elements:

1. Variables,
2. Parameters,

3. Constraints, and

4. Mathematical relationships.

The variables can take different values and their specifications define different states of the system. They can be continuous, integer, or a mixed set of continuous and integer. The parameters are fixed to one or multiple specific values, and each fixation defines a different model. The constant are fixed quantities by the model statement.

The mathematical model relations can be classified as equalities, inequalities, and logical conditions. The model equalities are usually composed of mass balances, energy balances, equilibrium relations, physical property calculations, and engineering design relations which describe the physical phenomena of the system. The model inequalities often consist of allowable operating regimes, specification on qualities, feasibility of heat and mass transfer, performance requirements, and bounds on availabilities and demands. The logical conditions provide the connection between the continuous and integer variables.

The mathematical relationships can be algebraic, differential, integrodifferential, or a mixed set of algebraic and differential constraints, and can be linear or nonlinear.

An optimization problem is a mathematic model which in addition to the aforementioned elements contains one or multiple performance criteria. The performance criterion is denoted as objective function, and it can be the minimization of cost, the maximization of profit or yield of a process for instance. If we have multiple performance criteria then the problem is classified as multi-objective optimization problem. A well defined optimization problem features a number of variables greater than the number of equality constraints, which implies that there exist degrees of freedom upon which we optimize. If the number of variables equals the number of equality constraints, then the optimization problem reduces to a solution of nonlinear systems of equations with additional inequality constraints.

### 3.3.2 Structure of Nonlinear and Mixed-Integer Optimization Models

The structure of such nonlinear and mixed integer optimization models takes the following form:

$$\begin{aligned}
 \min_{x,y} \quad & f(x, y) \\
 \text{s.t.} \quad & \\
 & h(x, y) = 0 \\
 & g(x, y) \leq 0 \\
 & x \in X \subseteq \mathcal{R}^* \\
 & y \in Y \quad \text{integer}
 \end{aligned} \tag{3.14}$$

Where  $x$  is a vector of  $n$  continuous variables,  $y$  is a vector of integer variables;  $h(x, y) = 0$  are  $m$  the equality constraints;  $g(x, y) \leq 0$  are  $p$  inequality constraints; and  $f(x, y)$  is the objective function.

The formulation contains a number of optimization problems, by appropriate consideration or elimination of its elements. If the set of integer variables is empty, and the objective function and constraints are linear then the formulation becomes a linear programming LP problem. If the set of integer variable is empty, and there exist nonlinear term in the objective function and/or constraints then the formulation becomes a nonlinear programming NLP problem. If the set of integer variables is nonempty, the integer variables participate linearly and separately from the continuous, and the objective function and constraints are linear, then the formulation becomes a mixed-integer linear programming MILP problem. If the set of integer variables is nonempty, and there exist nonlinear term in the objective function and/or constraints then the formulation becomes a mixed integer nonlinear programming MINLP problem.

### 3.3.3 Mixed Integer Nonlinear Programming Overviews

A wide range of nonlinear optimization problems involve integer and discrete variables in addition to the continuous variables. These classes of optimization problems arise from a variety of application and are denoted as Mixed-Integer Nonlinear Programming (MINLP) problems. (Floudas, 1995).

The integer variables can be used to model, for instance, sequences of events, alternative candidates, existence or nonexistence of units (in their zero-one representation), while discrete variables can model, for instance, different equipment sizes. The continuous variables are used to model the input-output and interaction relationships among individual units/operations and different interconnected systems.

The general MINLP formulation has been shown in equation (3.1)

$$\begin{aligned}
 \min_{x,y} \quad & f(x, y) \\
 \text{s.t.} \quad & \\
 & h(x, y) = 0 \\
 & g(x, y) \leq 0 \\
 & x \in X \subseteq \mathcal{R}^* \\
 & y \in Y \quad \text{integer}
 \end{aligned} \tag{3.14}$$

Where  $x$  represents a vector of  $n$  continuous variables and  $y$  is a vector of integer variables;  $h(x, y)$  denote the equality constraints;  $g(x, y)$  are inequality constraints; and  $f(x, y)$  is the objective function.

The difficulty of MINLP is associated with the nature of the problem, the combinatorial domain (  $y$ -domain) and the continuous domain (  $x$ -domain). As the number of binary variables  $y$  in increase, one faces with a large combinatorial problem, and the complexity analysis results. At the same time, due to the nonlinearities the MINLP problems are in general nonconvex which implies the potential existence of multiple local solutions.

Despite the aforementioned discouraging results from complexity analysis which



are worst-case results, significant progress has been achieved in the MINLP area from the theoretical algorithmic and computational perspective. As a result, several algorithms have been proposed, their convergence properties have been investigated and a large number of applications now exist that cross the boundaries of several disciplines.

The branch and bound algorithm is the one of techniques used for solving the MINLP problem. The branch and bound (BB) starts by solving the continuous relaxation of the MINLP and subsequently perform an implicit enumeration where a subset of the 0-1 variables is fixed at each node. The lower bound corresponds to the Nonlinear Programming (NLP) solution at each node and it is used to expand on the node with the lowest lower bound, or it is used to eliminate nodes if the lower bound exceeds the current upper bound. If the continuous relaxation NLP of the MINLP has 0-1 solution for the  $y$  variables, then the BB algorithm will terminate at that node. With a similar argument, if a tight NLP relaxation results in the first node of the tree, then the number of nodes that would need to be eliminated can be low. However, loose NLP relaxations may result in having a large number of NLP sub-problems to be solved which do not have the attractive update features that LP problems exhibit.

# CHAPTER IV

## SYNTHESIS OF THE PLANTWIDE CONTROL STRUCTURE

The combined mathematic and heuristic based methodology for plantwide control structure design is proposed in this chapter. The methodology can be divided into two parts: 1) heuristic and 2) mathematic. The goal of the methodology is the optimal plantwide control structure of the selected plant. For this dissertation, the Tennessee Eastman (TE) process is selected as the testbed problem. The process description has been given in section 4.2. Moreover, the process model development for using in the optimization and dynamic performance-based optimization problem formulation are described in section 4.3 and 4.4 respectively.

### 4.1 Methodology Framework

Our combined mathematic and heuristic based plantwide control structure design procedure can be divided into two parts, heuristic and mathematic following its namesake. The overall steps are described as follows. Steps 1-3 are included in the heuristic part and steps 4 and 5 are included in the mathematic part. The proposed design procedure is outlined in Table 4.1.

#### **Step 1: Controlled Variable Selection**

Once the control objectives have been identified, we have to select the measurements necessary to monitor the process operation. The control objectives reflect the number of controlled variables that should be controlled at desired values. Generally, the set of CVs consists of process safety, product quality, and plant throughput variables. Several authors have presented guidelines for the selection of controlled variables such as Luyben et al. (1999), Stephanopoulos and Ng (2000), Skogestad and Postlethwaite (2005) and etc.

## **Step 2: Manipulated Variable Selection**

The selection of the appropriate manipulated variables is a very critical problem as some manipulations may have a direct, fast and strong effect on the CVs while others do not. General guidelines for the selection of manipulated variables are given by Stephanopoulos and Ng, (2000). It is assumed that all MVs are measurable and MVs should possess the following properties.

- Ensure controllability of CVs
- Produce input-output relationships with small uncertainties
- Induce small cost on the process operations

## **Step 3: Finding the candidate CV-MV pairings**

All possible CV-MV pairings are determined in this step. However, matching of all candidate CVs to MVs may cause a large number of combinations. To save computing time, first, the obvious control loops such as reactor temperature, product ratio will be determined. Second, unreasonable CV-MV pairings are eliminated from the overall combination. The rest CV-MV pairings are the candidates used in the optimization problem.

## **Step 4: Finding tuning parameters for all candidate pairing**

Once the candidate CV-MV pairings are obtained, tuning parameters of all candidate pairings will be preliminarily determined. PI controllers are used for all control loops. There are many techniques in the literature for determining the tuning parameters. In this paper, the tuning parameters are obtained using the relay feedback testing technique and Tyreus-Luyben tuning method. The obtained tuning parameters are kept constant in the optimization problem.

## **Step 5: Establishing the plantwide control structure via dynamic performance-based optimization**

The plantwide control structure is established using an optimization method. The dynamic performance-based optimization is used as the decision making process for selecting the suitable CV-MV pairings. The number of control loops to be selected is equal to the number of the rest of CVs after selecting the obvious

control loops. The optimization problem formulation has been described in a later section.

Table 4.1: Combined mathematic and heuristic plantwide control structure design procedure

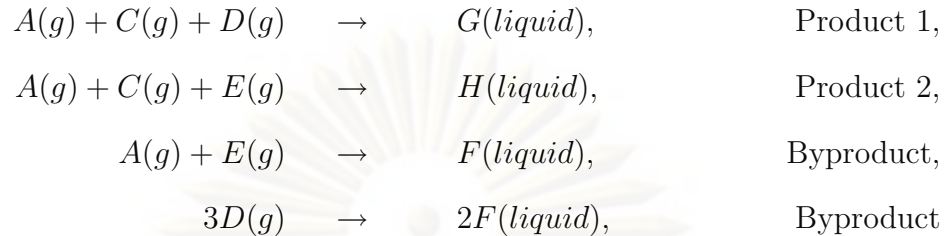
Step	Comments
Heuristic Part	
1. Controlled Variable Selection	<ul style="list-style-type: none"> <li>• Select the CVs set</li> </ul>
2. Manipulated Variable Selection	<ul style="list-style-type: none"> <li>• Select the MVs set</li> </ul>
3. Finding the CV-MV pairings	<ul style="list-style-type: none"> <li>• Determine the possible CV-MV pairings</li> <li>• Close the obvious control loops</li> <li>• Eliminate the unreasonable CV-MV pairings</li> </ul>
Mathematic Part	
4. Finding tuning parameters for all candidate control loops	<ul style="list-style-type: none"> <li>• Determine tuning parameters for candidate CV-MV pairings using relay-feedback testing</li> </ul>
5. Establishing plantwide control structure via dynamic performance-based optimization	<ul style="list-style-type: none"> <li>• Determine control structure corresponding to the rest of CVs using optimization technique</li> <li>• The optimization problem is formulated as the MINLP</li> </ul>

## 4.2 Description of the Tennessee Eastman Process

The Tennessee Eastman Process (TEP) was proposed by Downs and Vogel (1993) as a test of alternative control and optimization strategies for researchers in process control and related fields. The process model has been coded into a set of FORTRAN subroutines which describe the nonlinear relationship in the unit operations and the material and energy balances. The process schematic is shown as Figure 4.1.

The process produces two products from the four reactants. Also present are an inert and a byproduct making a total of eight components:  $A, B, C, D, E, F, G,$

and  $H$ . The reactions are:



All the reactions are irreversible and exothermic. The reaction rates are a function of temperature through an Arrhenius expression. The reaction to produce  $G$  has a higher activation energy resulting in more sensitivity to temperature. Also, the reactions are approximately first-order with respect to the reactant concentrations.

The process has five major unit operations: the reactor, the product condenser, a vapor-liquid separator, a recycle compressor and a product stripper.

The gaseous reactants are fed to the reactor where they react to form liquid products. The gas phase reactions are catalyzed by a nonvolatile catalyst dissolved in the liquid phase. The reactor has an internal cooling bundle for removing the heat of reaction. The products leave the reactor as vapors along with the unreacted feeds. The catalyst remains in the reactor. The reactor product stream passes through a cooler for condensing the products and from there to a vapor-liquid separator. Noncondensed components recycle back through a centrifugal compressor to the reactor feed. Condensed components move to a product stripping column to remove remaining reactants by stripping with  $C$  feed stream. Product  $G$  and  $H$  exit the stripper base and are separated in a downstream refining section which is not included in this problem. The inert and byproduct are primarily purged from the system as a vapor from the vapor-liquid separator.

The reactor product stream passes through a cooler for condensing the products and from there to a vapor-liquid separator. Noncondensed components recycle back through a centrifugal compressor to the reactor feed. Condensed components move to a product stripping column to remove remaining reactants by

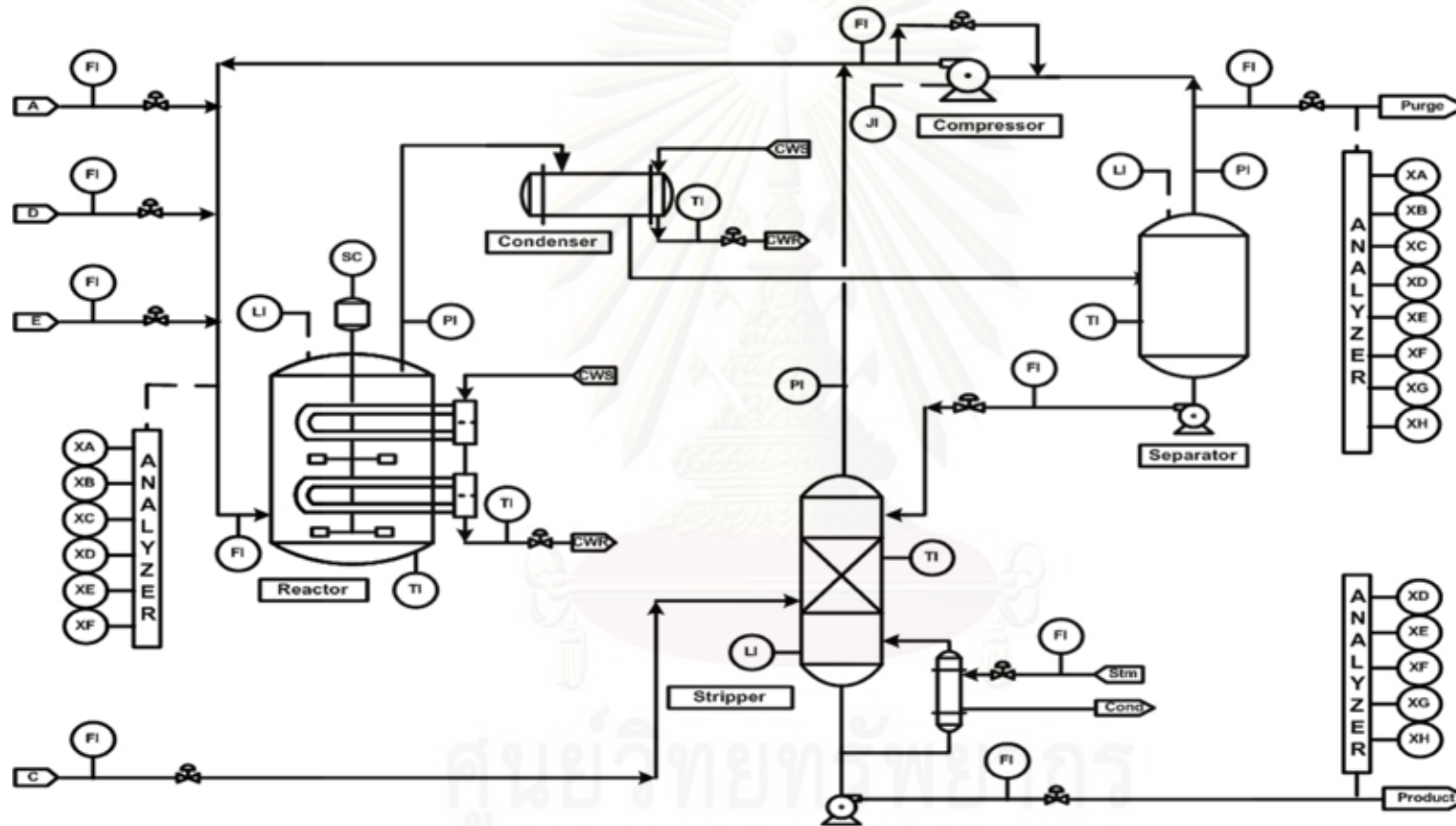


Figure 4.1 Schematic of the Tennessee Eastman Process

stripping with  $C$  feed stream. Product  $G$  and  $H$  exit the stripper base and are separated in a downstream refining section which is not included in this problem. The inert and byproduct are primarily purged from the system as a vapor from the vapor-liquid separator.

There are six modes of process operation at three different  $G/H$  mass ratios (product stream) as shown in table 4.2.

Table 4.2: Six modes of process operation

Mode	G/H mass ratio	Production rate (product stream)
1	50/50	7038 $kg\ h^{-1}G$ and 7038 $kg\ h^{-1}H$ (base case)
2	10/90	1408 $kg\ h^{-1}G$ and 12,669 $kg\ h^{-1}H$
3	90/10	10,000 $kg\ h^{-1}G$ and 1111 $kg\ h^{-1}H$
4	50/50	Maximum production rate
5	10/90	Maximum production rate
6	90/10	Maximum production rate

Mode 1 is the base case. The production mix is normally dictated by product demands. The plant production rate is set by market demand or capacity limitations.

### 4.2.1 Control Objectives

The process has 41 measurements and 12 manipulated variables. The manipulated variables are listed in Table 4.3. A prerequisite for most studies on this problem is a process control strategy for operating the plant. The control objectives for this process are typical for a chemical process:

1. Maintain process variables at desired values.
2. Keep process operating conditions within equipment constraints.
3. Minimize variability of production rate and product quality during disturbances.
4. Minimize movement of valves which affect other processes.

5. Recover quickly and smoothly from disturbances, production rate changes or product mix changes.

### 4.2.2 Process constraints

Table 4.4 lists the specific operational constraints that the control system should respect. These constraints are primarily for equipment protection. The high and low shutdown limits are part of the process interlock strategy and are used to shutdown the process in the event the process conditions get out of hand.

### 4.2.3 Dynamic performance comparisons

The testing and evaluation of various process control technologies can be done with the setpoint changes listed in Table 4.5 or the load changes listed in Table 4.6. These setpoint and load disturbances represent a set of tests that can be used to compare and contrast alternative approaches to operating and automatically controlling this process. Each disturbance illustrates a different aspect of operating the process.

To provide the common basis needed for the purpose of publishing and comparing results, the authors suggest disturbing the process at the base case (Mode 1) with the four setpoint changes listed in Table 4.5 and the following load disturbances from Table 4.6:

IDV(1)	Step change
IDV(4)	Step change
IDV(8)	Random variation
IDV(12),IDV(15)	Simultaneous random variation and sticking valve.

A qualitative comparison of the time responses of at least the following process variables is desired: *A* feed flowrate, *D* feed flowrate, *E* feed flowrate, *C* feed flowrate, product flowrate, product composition and reactor pressure.



Table 4.3: Process manipulated variables

Variable name	Variable number
D feed flow	XMV(1)
E feed flow	XMV(2)
A feed flow	XMV(3)
A and C feed flow	XMV(4)
Compressor recycle valve	XMV(5)
Purge valve	XMV(6)
Separator pot liquid flow	XMV(7)
Stripper liquid product flow	XMV(8)
Stripper steam valve	XMV(9)
Reactor cooling water flow	XMV(10)
Condenser cooling water flow	XMV(11)
Agitator speed	XMV(12)

Table 4.4: Process operating constraints

Process variable	Normal operating limits		Shut down limits	
	Low limit	High limit	Low limit	High limit
Reactor pressure	None	2895 kPa	None	3000 kPa
Reactor level	50% (11.8 $m^3$ )	100% (21.3 $m^3$ )	2.0 $m^3$	24.0 $m^3$
Reactor Temperature	None	150°C	None	175°C
Product separator level	30% (3.3 $m^3$ )	100% (9.0 $m^3$ )	1.0 $m^3$	12.0 $m^3$
Stripper base level	30% (3.5 $m^3$ )	100% (6.6 $m^3$ )	1.0 $m^3$	8.0 $m^3$

#### 4.2.4 Potential Application

This problem can be used for studying a wide variety of topics:

1. **Plant-wide control strategy design** -There are many control strategies that can be used to control this plant. Steady-state analysis tools such as RGA can be used to screen possible schemes. Dynamics simulation can then be used to test the performance of the schemes with the disturbances listed in Tables 4.4 and 4.5. Control strategies can be designed to reject disturbances for all six modes of operation.

Table 4.5: Setpoint changes for the base case

Process variable	Type	Magnitude
Production rate change	Step	-15%
Product mix change	Step	50 G/50 H to 40 G/60 H
Reactor operating pressure change	Step	-60 kPa
Purge gas composition of component B change	Step	+2%

Table 4.6: Process disturbances

Variable number	Process variable	Type
IDV(1)	A/C feed Ratio, B Composition constant	Step
IDV(2)	B Composition, A/C ratio constant	Step
IDV(3)	D feed temperature	Step
IDV(4)	Reactor cooling water inlet temperature	Step
IDV(5)	Condenser cooling water inlet temperature	Step
IDV(6)	A feed loss	Step
IDV(7)	C header pressure loss - reduce availability	Step
IDV(8)	A, B, C feed composition	Random Variation
IDV(9)	D feed temperature	Random Variation
IDV(10)	C feed temperature	Random Variation
IDV(11)	Reactor cooling water inlet temperature	Random Variation
IDV(12)	Condenser cooling water inlet temperature	Random Variation
IDV(13)	Reaction Kinetics	Slow drift
IDV(14)	Reactor cooling water valve	Sticking
IDV(15)	Condenser cooling water valve	Sticking

2. **Multivariable control** - Many of the process measurements respond to many of manipulated variables. Consequently, multivariable control may be benefit for reducing interaction.
3. **Optimization** - Both steady-state and dynamic optimization problem may be studied. Determine the optimum operating conditions for the six modes of operation.
4. **Predictive control** - The application of predictive control techniques containing identification, constraint handling and optimization can be evaluated.

5. **Estimation/adaptive control** - Variation in production rate and product mix may cause the process dynamics to change sufficiently to merit on-line controller adaptation.
6. **Nonlinear control** - The reaction and vapor-liquid equilibrium equations are quite nonlinear and control may benefit from a nonlinear approach to the problem.
7. **Process diagnostics** - Expert systems and fault diagnostics can be tested to evaluate their performance and reaction to new or unknown conditions.
8. **Education** - This problem could be used as a study in process control courses to illustrate the concepts of control strategy design, controller tuning, control loop troubleshooting and applications of advanced control.

#### 4.2.5 Model Description

- The vapors all behave as ideal gases.
- The vapor-liquid equilibrium follows Raoult's Law with the vapor pressure calculated using the Antoine equation.
- All the vessels are well mixed and contain no distributed parameters.
- The manipulated variables listed as valve position (%), the flowrate is a function of pressure.
- The reactor is agitated. Agitation speed only affects the heat transfer coefficient.
- The recycle gas compressor is a centrifugal type and has internal surge protection by means of a mechanical bypass arrangement. The relation between flow through the compressor and inlet-outlet pressure difference follows a typical centrifugal compressor curve.
- All process measurements include Gaussian noise with standard deviation typical of the measurement type.

- Table 4.3 lists the process constraints, both normal operating limits and process shutdown limits. The process should be operated within the normal operating limits. If the process exceeds the shutdown limits, it will automatically be shutdown.
- The model is not intended for simulating process start-up and shutdown procedures.

### 4.3 Process Model Development

A process model is a key element that facilitates the design of a plantwide control structure through the use of optimization method. McAvoy (1999) used steady-state model in the optimization. To implement thier previous work, Wang and McAvoy (2001) used the step response coefficient model which is developed from the linear state-space model. To design the plantwide control structure via dynamic performance-based optimization, the dynamic model is required. Originally, the TE nonlinear model is coded as FORTRAN subroutines (Downs and Vogel, 1993). In this work, we use the TE model developed by McAvoy (see, <http://terpconnect.umd.edu/mcavoy>) because this TE model could be used in MATLAB a mathematic modeling and simulation software package. The TE process model has 50 state variables, 22 continuous measurements, 19 sampled measurements and 12 manipulated variables. Process disturbances 1, 2, 4 and 6 are included in the model. Due to the complexity of the problem solving process, a discrete linear state space model is developed and included in the optimization. The discrete linear state space model can be expressed as

$$x_{t+1} = \tilde{A}x_t + \tilde{B}u_t + \tilde{W}d_t \quad (4.1)$$

$$y_t = \tilde{C}x_t \quad (4.2)$$

where  $x$  is the state vector ( $50 \times 1$ ),  $u$  is the vector of manipulated variables ( $12 \times 1$ ),  $d$  is the vector of disturbances ( $4 \times 1$ ),  $y$  is the vector of measurements ( $41 \times 1$ ),  $\tilde{A}$ ,  $\tilde{B}$ ,  $\tilde{C}$ , and  $\tilde{W}$  are the constant matrix and subscripts  $t$  and  $t + 1$

represent current time and future time, respectively. This model can be developed from the following nonlinear dynamic model:

$$\dot{x} = f(x, u, d, t) \quad (4.3)$$

$$y = g(x, u, d, t) \quad (4.4)$$

These functions can be linearized around the nominal condition using two sides perturbation numerical differentiation to obtain a continuous state space model. Then, the obtained continuous model is converted to the discrete model using C2D function in MATLAB. For the selection of the sampling time, the responses of the discrete model with the specific sampling time are compared with the continuous model. To reduce the calculation time, we have to select the maximum sampling time that gives the less deviation response from the continuous model.

In this case, a linear process model is used for establishing the plantwide control structure of the nonlinear process. A chemical process is normally operated around a fix operating condition which does not have variation enough to impact the control structure selection. The nonlinearity of the process can be accommodated by obtaining suitable controller's parameters.

#### 4.4 Dynamic Performance-based Optimization Formulation

The level of uncertainty inclusion of class-2 (Stephanopoulos and Ng, 2000) is selected in this work. The treatment of uncertainties is concerned in the phase of selecting the manipulated variables. In conformance to this work, the process disturbances are included in the optimization problem as the treatment of uncertainties while the model uncertainties are neglected. The dynamic performance-based optimization is formulated to establish the control structure for the selected CVs as follows.

For the objective function, in earlier works, McAvoy (1999) used the summation of deviation of all valve positions from their steady state values. Wang and

McAvoy (2001) used the trade-off between manipulated variable moves and transient response area. These works can be categorized as class-2 of Stephanopoulos and Ng (2000)'s classification. However, the steady-state deviation does not reflect the overall control performance. The objective function proposed by Wang and McAvoy (2001) is adopted from the concept of integral of the absolute value of the error (IAE). In this paper, we present the objective function formulated as an integral of the time-weighted absolute error (ITAE) of all measurements and manipulated variables in the face of disturbances. The ITAE criterion penalizes errors that persist for long periods of time. Weighting factors are multiplied on the ITAE of measurements and MVs separately for giving their importance.

For the optimization constraints, a discrete state space model, which is formulated as discussed above, is used as the process model. In this model, process disturbance matrix is included. A PI controller formulated in velocity form is used in the optimization. The selection matrix  $\tilde{Z}$  is multiplied on the controller model. The  $\tilde{Z}$  matrix consists of  $Z_{j,i}$  which are the binary variables. This matrix represents the pairings of MVs to CVs. The value 1 of  $Z_{j,i}$  means that the  $j^{th}$  MV is paired with the  $i^{th}$  CV, the value 0 means otherwise. The last three constraints allow one MV to be matched with only one CV and limit the number of control loops to be determined to be equal to  $N$ . The formulated optimization problem is shown in Eq. (4.5). The pairing of the selected CVs with the appropriate MVs is represents through the  $\tilde{Z}$  matrix.

$$\begin{aligned}
& \min_{\tilde{Z}} \quad w_y \sum_{d=1}^n \sum_{t=0}^T \sum_{i=1}^{N_y} |y_{i,t}| \cdot t \cdot \Delta t + w_u \sum_{d=1}^n \sum_{t=0}^T \sum_{j=1}^{N_u} |u_{j,t}| \cdot t \cdot \Delta t \\
& \text{s.t.} \\
& \quad x_{t+1} = \tilde{A}x_t + \tilde{B}u_t + \tilde{W}d_t \\
& \quad y_t = \tilde{C}x_t \\
& \quad u_{t+1} = u_t + \tilde{Z} \times \tilde{K}^P(e_t - e_{t-1}) + \tilde{Z} \times \tilde{K}^I(\tau_s \cdot e_t) \\
& \quad Z_{j,i} \in \{0, 1\} \\
& \quad \forall i : \sum_{j=1}^{N_u} Z_{j,i} = 1 \\
& \quad \forall j : \sum_{i=1}^{N_y} Z_{j,i} = 1 \\
& \quad \forall i \forall j : \sum_{i=1}^{N_y} \sum_{j=1}^{N_u} Z_{j,i} = N
\end{aligned} \tag{4.5}$$

The pairing of the selected CVs with the appropriate MVs is represented by the  $\tilde{Z}$  matrix. It is significantly different from that as described in the literature (McAvoy, 1999 and 2001). The results of their previous works report only on the appropriate set of MVs which have to be matched with the CVs in later stage.

ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย

# CHAPTER V

## DYNAMIC PERFORMANCE-BASED DESIGN FOR PLANTWIDE CONTROL STRUCTURE

This chapter illustrates the benefit of dynamic performance-based design for plantwide control structure. The proposed optimization technique is adopted to establish the plantwide control structure of the TE plant. The dynamic performance-based optimization is limited to establish the control structure only for important controlled variables (CVs) of the TE process. The important CVs are defined by those the CVs that relate directly to the process shutdown criteria. While the control structure of the other CVs are established by heuristic.

### 5.1 Introduction

In this chapter, the dynamic performance-based optimization for establishing the plantwide control structure of the TE process is proposed. The controlled and manipulated variable sets are obtained from the literature. The control structure is established via dynamic optimization and heuristics. To save computing time, some obvious CV-MV pairings are obtained using heuristics rules. An optimization problem is formulated and solved as the Mixed Integer Nonlinear Programming (MINLP) to establish the pairing of the important controlled variables (CVs) with the appropriated manipulated variables (MVs). An objective function is the measure of the control performance (ITAE of CVs) and the cost of manipulated variables (ITAE of MVs). The control structures design results are illustrated and evaluated by dynamic simulation and compared with the control structure proposed by Luyben (1999) in the face of various disturbances and setpoint changing.

It is worthwhile to point out our main contribution. First, our objective function is accounted on the dynamic performances of the controlled process. Second,



our process model is more rigorous and accurate compared with those of McAvoy (1999 and 2001) and less complexity compared with the model proposed by Naraway and Perkins (1993). The proposed methodology conforms to the Class-2 of Stephanopoulos and Ng (2000). The process disturbances are included in the optimization problem as the treatment of uncertainties while the model uncertainties are not considered in this work.

## 5.2 Plantwide Control Structure Design of the TE Process

Our plantwide control structure design procedures for the TE process are shown in table 5.1 and the descriptions of each step are given as follows.

Table 5.1: Plantwide control structure design procedure

Step	Comments
1. Controlled Variable Selection	<ul style="list-style-type: none"> <li>• CVs are selected using heuristic.</li> </ul>
2. Manipulated Variable Selection	<ul style="list-style-type: none"> <li>• MVs are selected using heuristic.</li> </ul>
3. Finding of the CV-MV pairings	<ul style="list-style-type: none"> <li>• Determine the possible CV-MV pairings.</li> </ul>
4. Finding of tuning parameters for all candidate control loops	<ul style="list-style-type: none"> <li>• Determine tuning parameters for candidate CV-MV pairings using relay-feedback testing.</li> </ul>
5. Establishing of plantwide control structure via dynamic performance-based optimization	<ul style="list-style-type: none"> <li>• Determine control structure corresponding to the important CVs using optimization</li> <li>• The optimization problem is formulated as the MINLP.</li> </ul>
6. Completing of plantwide control structure	<ul style="list-style-type: none"> <li>• Control structures corresponding to the rest of CVs are designed using heuristic</li> </ul>

### Step 1: Controlled Variables selection

In this paper, a set of controlled variables (CVs) is selected heuristically. A CVs set proposed by Luyben et.al. (1999) is adopted in this work because it is a reasonable way to compare our control structure with theirs. The CVs are

reactor temperature, reactor pressure, reactor level, separator level, stripper level, separator temperature, stripper temperature, product  $G/H$  ratio, component  $A$  and component  $B$ . In this set, there are five CVs related directly to process shutdown criteria: reactor temperature, reactor pressure, reactor level, separator level, and stripper level. Process shutdown conditions are given by Down and Vogel (1993). The control structures involving these five CVs are determined via dynamic optimization while the control structures corresponding to other CVs are determined heuristically.

### **Step 2: Manipulated Variables selection**

There are 12 manipulators in the TE process. Agitator speed is fixed at the constant speed then we do not include it in the set of MVs. To maintain the product  $G/H$  ratio we have to use ratio control of  $D/E$  feed flow. We select  $E$  feed which has larger flowrate to be included in MVs set (Richardson Rule, Luyben et. al., 1999).  $D$  feed will be calculated proportional to  $E$  feed. To use the larger stream, it would give the smooth and fast response. Hence, the set of MVs are  $E$  feed,  $C$  feed, recycle, purge, separator liquid, stripper liquid, stripper steam, reactor cooling water, and condenser cooling water.

### **Step 3: Finding of the candidate CV-MV pairings**

The control structures corresponding to important CVs discussed above will be determined by optimization. For the TE process, the instability arises in the reactor, and closing the reactor temperature loops can be handled it. Apparently, the reactor temperature has to be controlled by reactor cooling water, so this pairing of CV-MV has to be established first. However, this control loop is also included in the optimization problem. Therefore, there are four remaining CVs to be optimized.

The set of MVs used in the dynamic optimization are  $E$  feed,  $C$  feed, recycle, purge, separator liquid, stripper liquid, stripper steam, reactor cooling water, and condenser cooling water. To reduce the computation time, unreasonable pairings of CVs-MVs are eliminated. The possible candidate pairings are shown in the Table 5.2

Table 5.2: Candidate pairing of CVs to MVs

CVs	Candidate MVs			
Reactor Pressure	<i>E</i> Feed	<i>C</i> Feed	Recy. V.	CCW. V.
Reactor Level	<i>E</i> Feed	Recy. V.	Sep. Liq. V.	CCW. V.
Separator Level	<i>C</i> Feed	Recy. V.	Sep. Liq. V.	CCW. V.
Stripper Level	<i>C</i> Feed	Sep. Liq. V.	Str. Liq. V.	Str. Stm. V.

#### Step 4: Finding of tuning parameter for all candidate control loops

Relay feedback technique is used for tuning parameters searching for all candidate control loops shown in the table 5.2. The discrete velocity proportional - integral (PI) control is used for each control loops.

Thus, we have to determine the controller gain ( $K_C$ ) and integral time ( $\tau_I$ ) for all candidate control loops.  $K_C$  and  $\tau_I$  values obtained from relay feedback testing for all candidate control loops are shown in the Table 5.3.

Table 5.3: Tuning Parameter obtained from relay feedback for all candidate control loops

CVs	MVs	$K_C$	$\tau_I$
Reactor Temperature	Reactor Cooling Water Flow	4.14	0.23
Reactor Pressure	<i>E</i> Feed	50.34	0.14
Reactor Pressure	<i>C</i> Feed	11.05	0.12
Reactor Pressure	Recycle Valve	9.96	0.09
Reactor Pressure	Condenser Cooling Valve	58.75	0.33
Reactor Level	<i>E</i> Feed	31.61	0.29
Reactor Level	Recycle Valve	15.08	0.19
Reactor Level	Separator Bottom Valve	55.32	0.31
Reactor Level	Condenser Cooling Valve	28.88	0.86
Separator Level	<i>C</i> Feed	46.38	0.15
Separator Level	Recycle Valve	27.31	0.23
Separator Level	Separator Bottom Valve	5.05	0.15
Separator Level	Condenser Cooling Valve	1.43	1.07
Stripper Level	<i>C</i> Feed	41.49	0.13
Stripper Level	Separator Bottom Valve	2.01	0.15
Stripper Level	Stripper Bottom Valve	2.69	0.13
Stripper Level	Stripper Steam Valve	13.05	2.51

### Step 5: Establishing of plantwide control structure via dynamic performance-based optimization

In this stage, control structures of the important CVs are established by optimization. Parameters of the optimization problem (Eq. 4.5) are specified as followed. The important of CVs and MVs is weighted equally. The number of disturbance  $n$  is 4 (IDV-1, 2, 4 and 6). The details for disturbances are presented in the paper (Downs and Vogel, 1993). There are 4 CVs to be optimized (reactor pressure, reactor level, separator level and stripper level) so the number of control loop  $N$  is 4. The number of measurements  $N_y$  and manipulated variables  $N_u$  are 22 and 12, respectively. The time period  $T$  for the dynamic model is 20 hours with sampling time ( $\Delta T$ ) 1/100 hours.

The Tomlab-MINLP commercial optimization package is used to carry out an optimization result. Each optimization batch takes about 30-45 minutes. Due to the nonlinear problem, a global optimum is not guaranteed. The optimization is solved about 30 times by the result of previous step is set to be the starting point of the next step. All results are ranked to obtain the best control structure corresponding to the important CVs. The three best optimization results are shown in Table 5.4. They represent the CVs-MVs matching established by optimization. In this work, the best and second best control structures will be implemented and evaluated via dynamic simulation.

Table 5.4: Optimization Results

Rank	Reactor Press	Reactor Level	Separator Level	Stripper Level	Obj. Func.
1	$C$ Feed	$E$ Feed	Sep. Liq. V.	Str. Liq. V.	39801
2	$C$ Feed	$E$ Feed	CCW. V.	Str. Liq. V.	45200
3	$C$ Feed	$E$ Feed	CCW. V.	Sep. Liq. V.	58453

### Step 6: Completing of plantwide control structure

Once, the control structure for important controlled variables is determined, the remaining measurements that have to be controlled are product  $G/H$  ratio, separator temperature, stripper temperature, component  $A$  in feed stream and

component  $B$  in purge stream. The pairings of these CVs are configured heuristically. For all cases,  $D/E$  ratio control is used to maintain the  $G/H$  ratio as discussed by McAvoy and Ye (1994).

For the rank 1 (best result, CS1) in Table 5.4 four MVs have been matched with four important CVs. There are six manipulated variables that are not assigned;  $A$  feed, recycle, purge, stripper steam, condenser cooling water and agitator. To control the separator temperature, two choices could be considered: (1) control of the separator temperature directly or (2) control of the separator pressure which has couple effect with the separator temperature. The manipulated variables that affect these two measurements are recycle, purge and condenser cooling water. The recycle stream has to be fixed as mentioned in Luyben et.al. (1999), while the purge will be used to control component  $B$  in the system. The condenser cooling water affects the temperature of the separator feed so that it can be used to control the separator temperature directly. The stripper steam affects the stripper temperature directly while the other manipulated variables around the stripper are assigned for other control loops. Then, the stripper steam is chosen for controlling the stripper temperature. For component balance, the component  $A$  and  $B$  accounted in the process could be measured either in feed and purge stream while the related manipulated variables are  $A$  feed and purge. As discussed by Luyben et.al. (1999), the component  $A$  accounted in the process is measured at the feed stream and controlled by the  $A$  feed directly. The component  $B$  is measured at the purge stream and controlled by the purge. The best control structure (CS1) is shown in figure 5.1.

For the rank 2 (CS2) in table 4, almost control loops are similar with the CS1 except that the separator level is controlled by the condenser cooling water. The remaining manipulated variables that are not assigned are  $A$  feed, recycle, purge, separator bottom, stripper steam cooling water and agitator. To control the separator temperature, the reactor temperature setpoint was used as the manipulated variable. This loop was proposed by Luyben et.al. (1999). The control configurations for other loops are as same as CS1. The second best control structure (CS2)

is shown in figure 5.2.

The control structure of TE process proposed by Luyben et al (1999) was used to compare with our control structures. Luyben et al. (1999) proposed two control structures for TE process: 1) On Supply and 2) On Demand control structure. We select the On Supply control structure as the reference. Figure 5.3 shows the On Supply control structure proposed by Luyben et al.



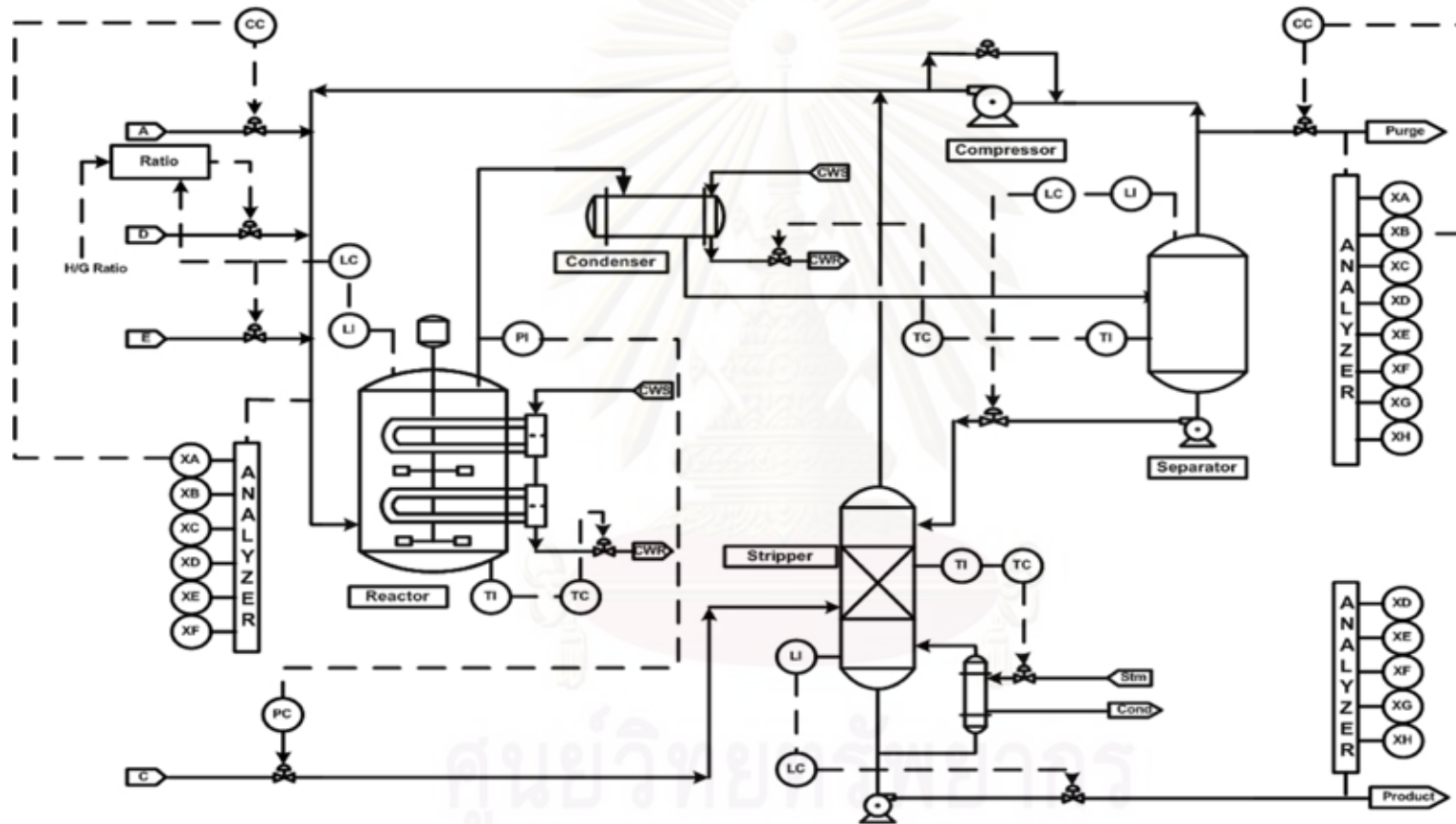


Figure 5.1 Control structure (CS1) for TE process

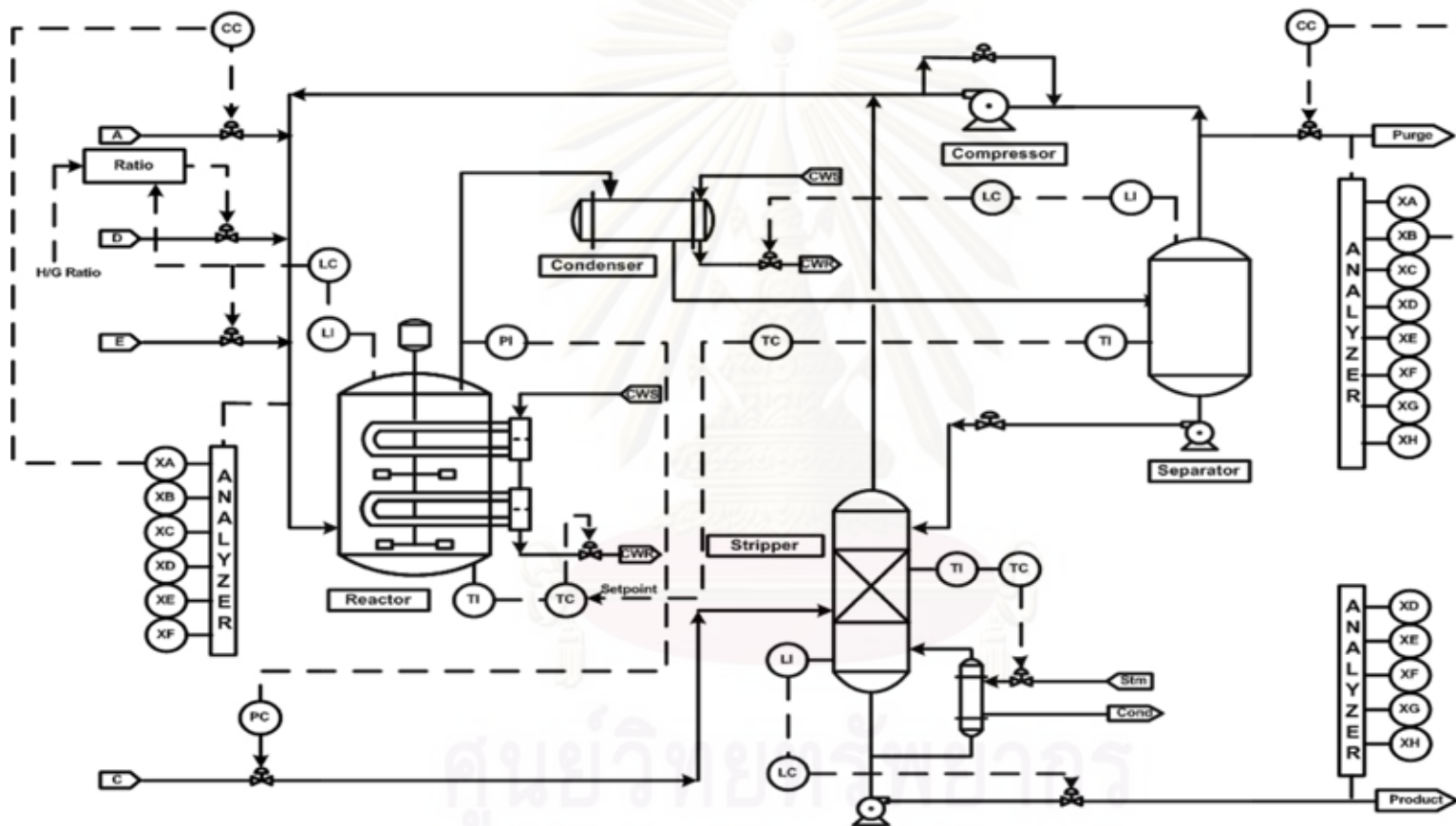


Figure 5.2 Control Structure (CS2) for TE process



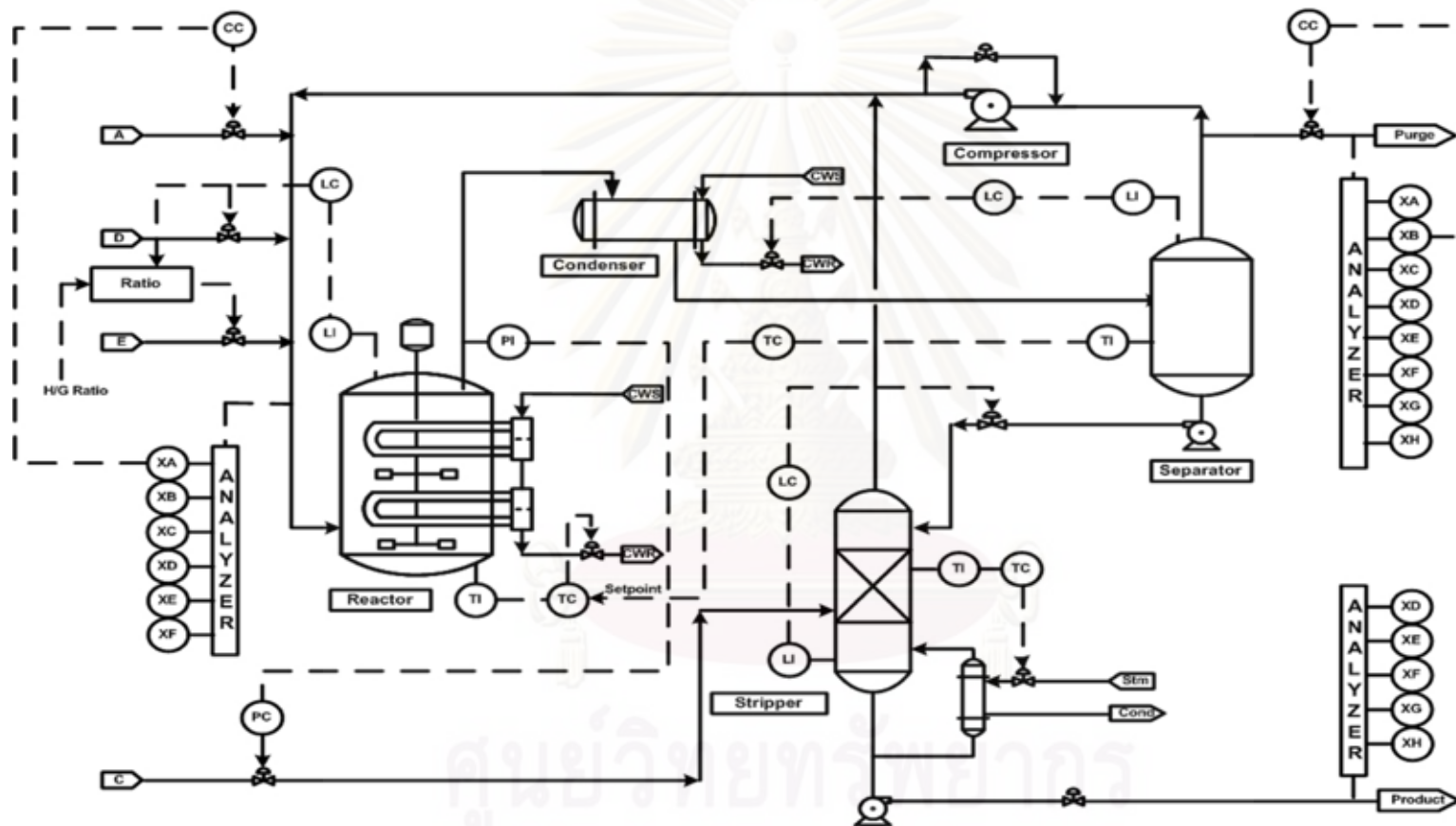


Figure 5.3 Luyben's On Supply control structure for TE process

Table 5.5 compares between Luyben's Control Structure, CS1 and CS2. Most of control loops are familiar. The different control loops are reactor level, separator temperature, separator level and stripper level.

Table 5.5: Comparisons between Luyben's CS, CS1 and CS2

CVs	Luyben's CS	CS1	CS2
	MVs	MVs	MVs
React. Press.	<i>C</i> Feed	<i>C</i> Feed	<i>C</i> Feed
React. Level	<i>D</i> Feed	<i>E</i> Feed	<i>E</i> Feed
React. Temp.	RCWF	RCWF	RCWF
Sep. Temp.	React. Temp. Setp.	CCWF	React. Temp. Setp.
Sep. Level	CCWF	Sep. Liquid Flow	CCWF
Strip. Level	Sep. Liquid Flow	Strip. Liquid Flow	Strip. Liquid Flow
Strip. Temp.	Strip. Steam Flow	Strip. Steam Flow	Strip. Steam Flow
Comp <i>A</i> in Feed	<i>A</i> Feed	<i>A</i> Feed	<i>A</i> Feed
Comp <i>B</i> in Purge	Purge Valve	Purge Valve	Purge Valve

### 5.3 Dynamic Simulation and Discussions

In this section, our control structures and Luyben's control structure are implemented on the nonlinear model of TE process. PI controllers in each loop are re-tuned by relay feedback testing and some trial and error. The tuning parameters for Luyben's CS (CS0), CS1 and CS2 are shown in table 5.6, 5.7 and 5.8, respectively. In dynamic simulation, the performances of three control structures are evaluated for change in operation condition and presence of disturbances. In each case, the performance index (ITAE and IAE) and the dynamic responses of the important CVs with the corresponding MVs are shown and discussed.

Table 5.6: Luyben's CS (CS0) tuning parameters

Controlled Variable	Manipulated Variable	K <sub>c</sub>	$\tau_I$
Reactor Pressure	<i>C</i> Feed	1	0.3
Reactor Level	<i>D</i> Feed	4	0.3
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Reactor Temp Setpoint	0.3	0.2
Separator Level	Condenser Cooling Water Flow	2	1
Stripper Level	Separator Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp <i>A</i> in Feed	<i>A</i> Feed	25	1.5
Comp <i>B</i> in Purge	Purge Valve	100	1.5

Table 5.7: CS1 tuning parameters

Controlled Variable	Manipulated Variable	K <sub>c</sub>	$\tau_I$
Reactor Pressure	<i>C</i> Feed	1	0.3
Reactor Level	<i>E</i> Feed	5	0.1
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Condenser Cooling Water Flow	2	0.1
Separator Level	Separator Liquid Flow	5	0.1
Stripper Level	Stripper Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp <i>A</i> in Feed	<i>A</i> Feed	25	1.5
Comp <i>B</i> in Purge	Purge Valve	100	1.5

Table 5.8: CS2 tuning parameters

Controlled Variable	Manipulated Variable	$K_c$	$\tau_I$
Reactor Pressure	$C$ Feed	1	0.3
Reactor Level	$E$ Feed	5	0.1
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Reactor Temp Setpoint	0.3	0.2
Separator Level	Condenser Cooling Water Flow	2	1
Stripper Level	Stripper Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp $A$ in Feed	$A$ Feed	25	1.5
Comp $B$ in Purge	Purge Valve	100	1.5

### 5.3.1 Change in operation condition

The  $G/H$  ratio setpoint is changed from 50/50  $G/H$  to 1/3  $G/H$ . Table 5.9 and 5.10 show the normalized ITAE and IAE values of CS0, CS1 and CS2. It can be seen that CS1 and CS2 give better ITAE and IAE value than CS0. Figure 5.4-5.6 show the responses for CS0, CS1 and CS2. It can be seen that all control structures achieve appropriate results for most loops. However, CS1 gives better responses for some loops such as product flow, reactor temperature and separator level. As can be seen from figures, CS1 take about 3 hours to reach setpoints while other CSs take much more time.

Table 5.9: Normalized ITAE of CS0, CS1 and CS2 for change in  $G/H$  ratio

ITAE	CS0	CS1	CS2
Measurements & MVs	60.61	49.24	46.16
All CVs	12.12	8.03	9.85
Important CVs	5.82	4.04	5.14

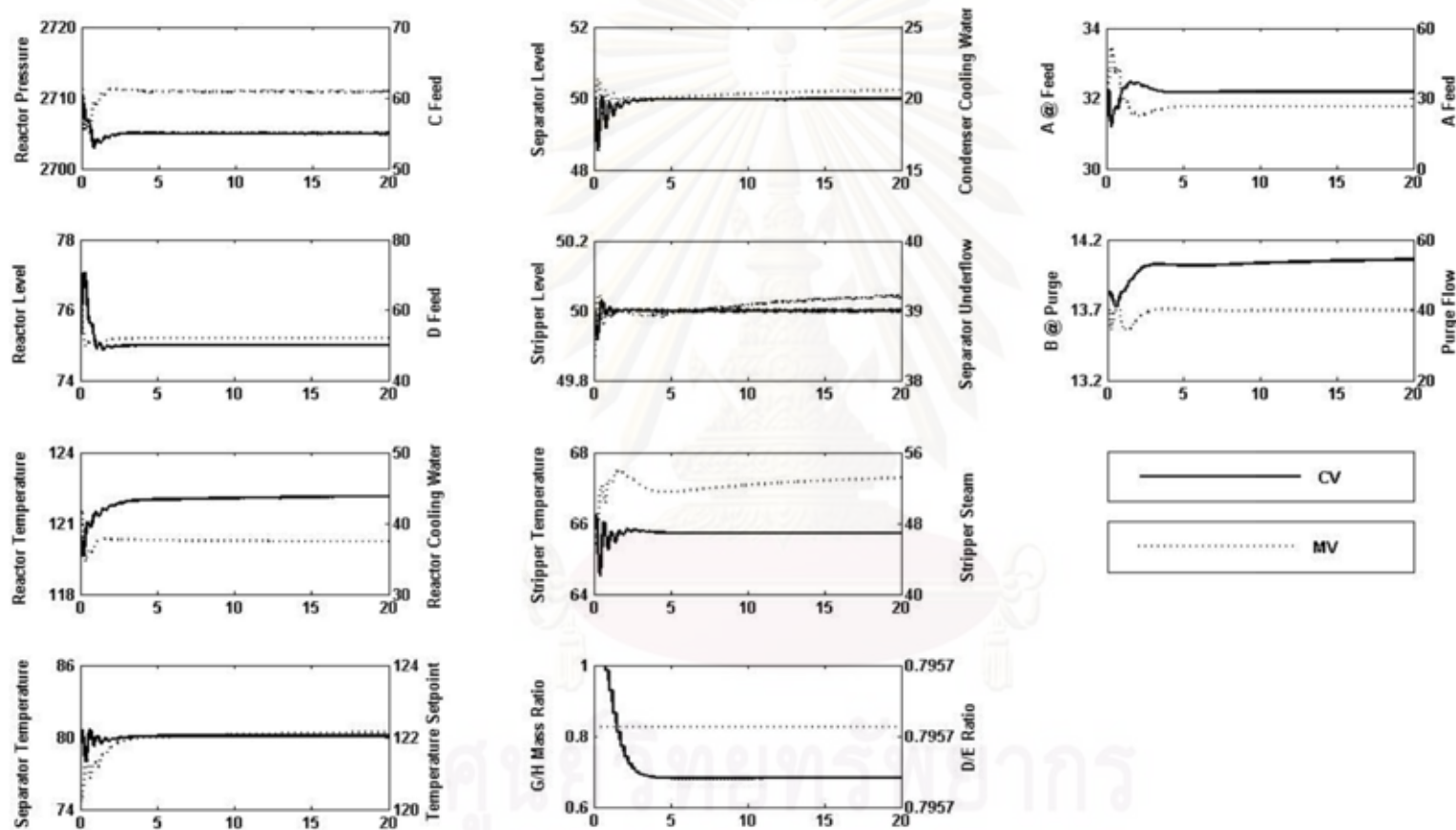


Figure 5.4 Dynamic response of CS0 for change in G/H ratio

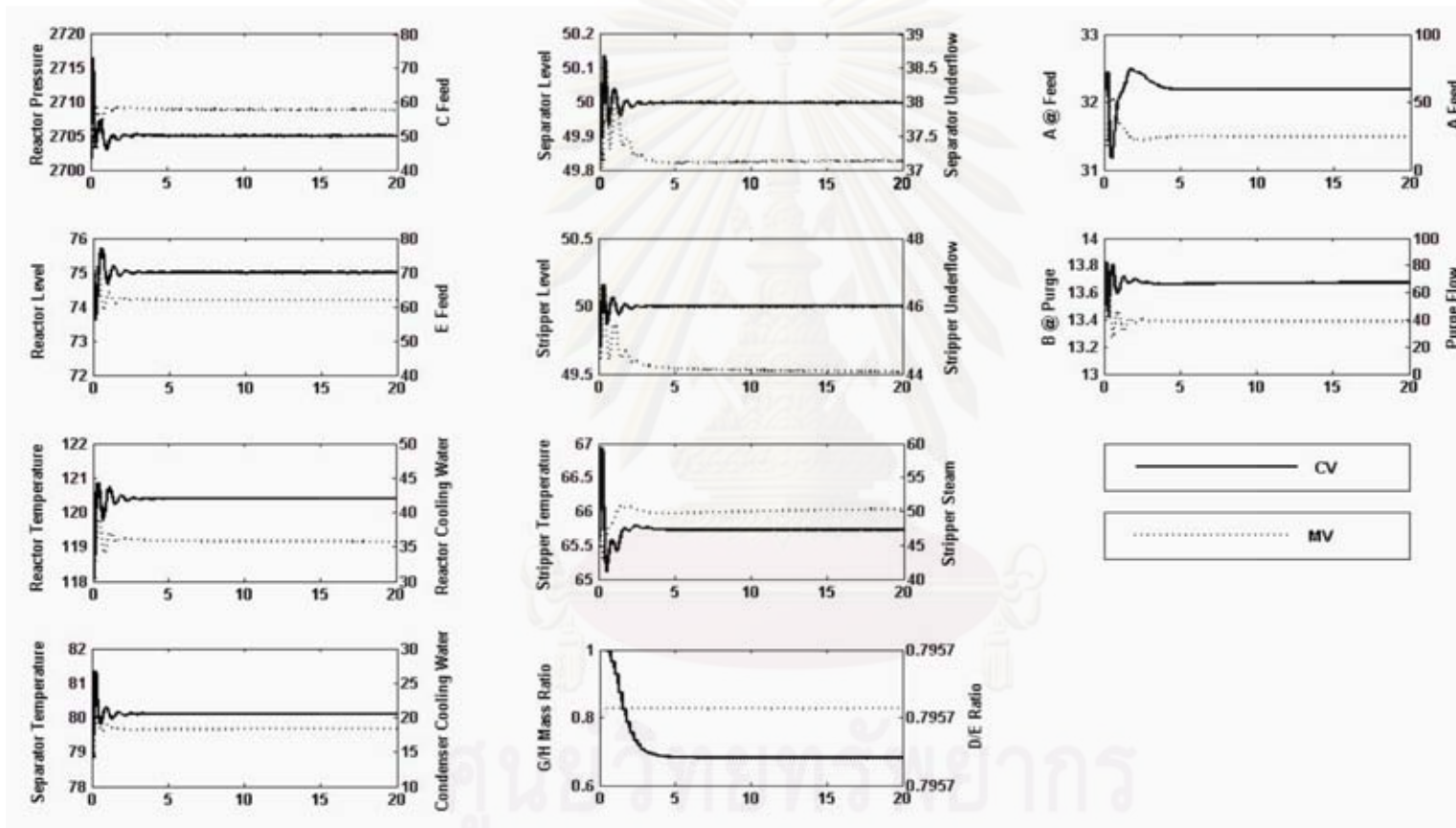


Figure 5.5 Dynamic response of CS1 for change in G/H ratio

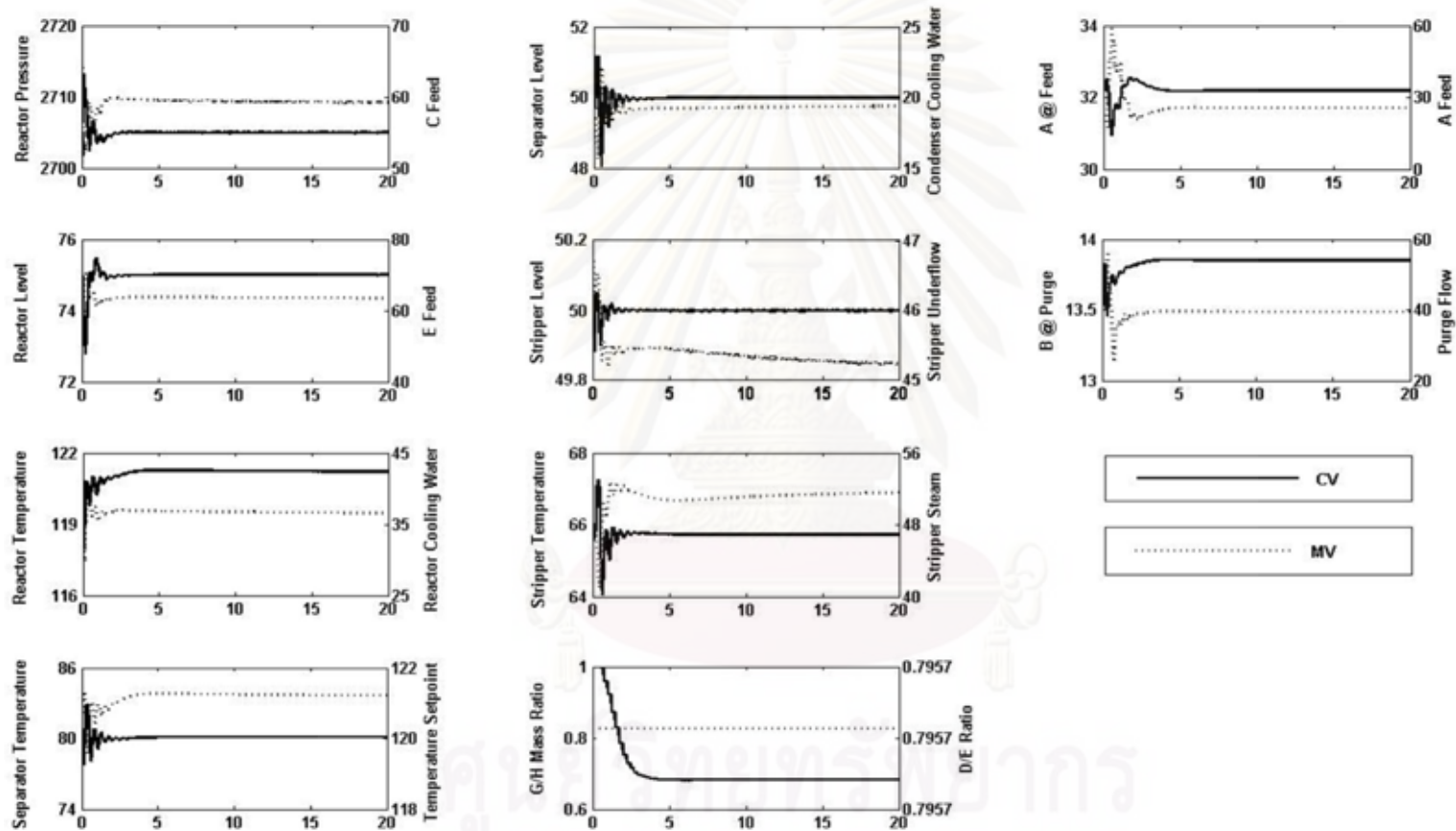


Figure 5.6 Dynamic response of CS2 for change in G/H ratio

Table 5.10: Normalized IAE of CS0, CS1 and CS2 for change in  $G/H$  ratio

IAE	CS0	CS1	CS2
Measurements & MVs	56.94	51.21	47.86
All CVs	10.52	9.11	10.36
Important CVs	4.98	4.74	5.28

### 5.3.2 Presence of disturbances

For presence of disturbances, three kinds of disturbances were studied, 1) change of  $A/C$  ratio in  $C$  feed stream (IDV1) 2) change of  $B$  composition in  $C$  feed stream (IDV2) 3) change of reactor cooling water temperature (IDV4). Responses of these disturbance testing are shown below, separately.

#### - Change of $A/C$ ratio in $C$ feed stream (IDV1)

Table 5.11 and 5.12 show the normalized ITAE and IAE values of CS0, CS1 and CS2. It can be seen that CS1 and CS2 give better ITAE and IAE than CS0. Figure 5.7-5.9 show the response to IDV1, a change of  $A/C$  ratio in  $C$  feed for CS0, CS1 and CS2. CS1 gives smoother responses than CS2 and CS0 except the product flow loop. Especially on reactor temperature, the effects of the IDV1 take about 5 hours to die out while other CSs take more than 5 hours.

Table 5.11: Normalized ITAE of CS0, CS1 and CS2 for IDV1

ITAE	CS0	CS1	CS2
Measurements & MVs	53.18	50.21	52.62
All CVs	11.93	7.88	10.20
Important CVs	6.33	3.83	4.84



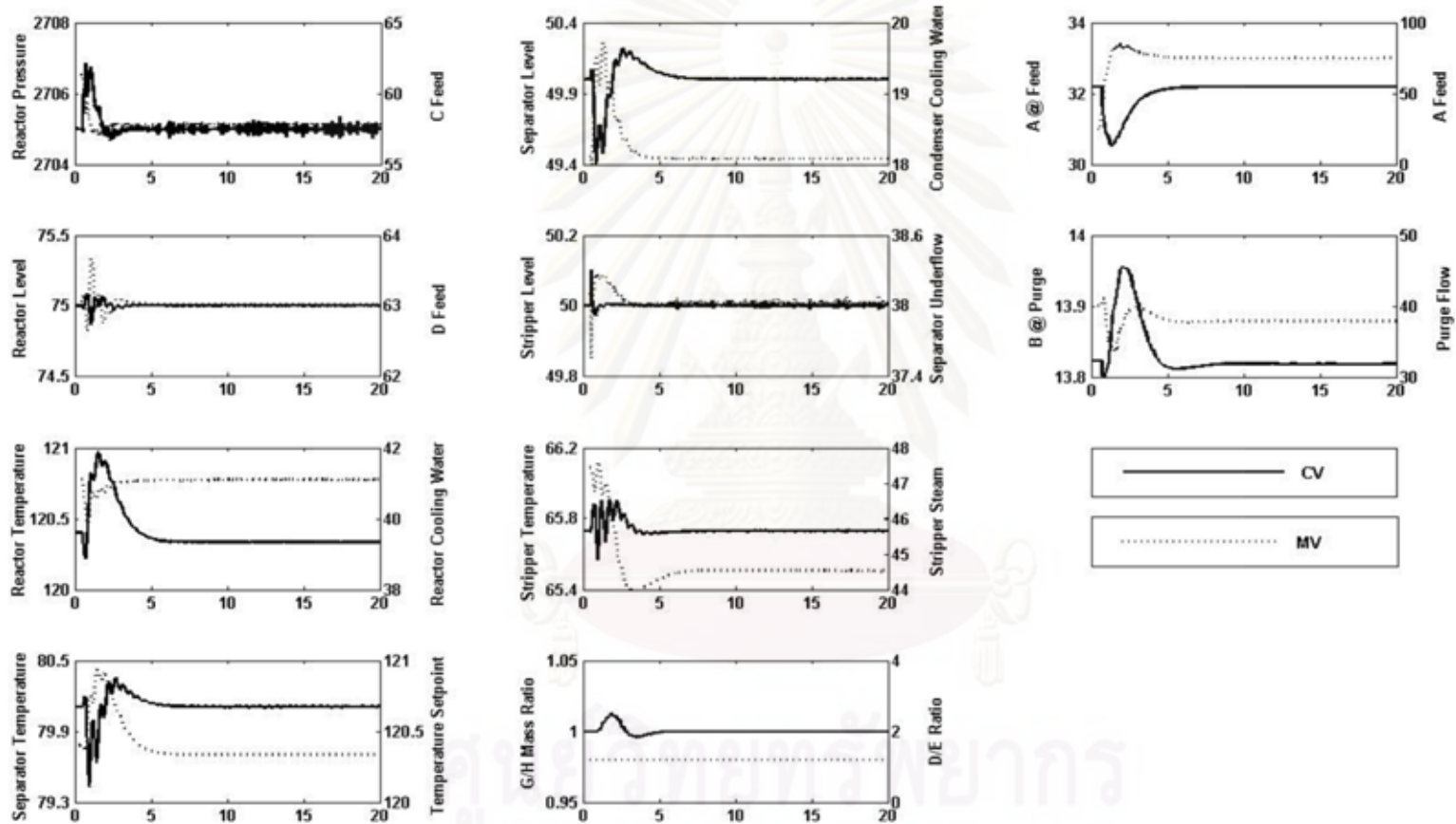


Figure 5.7 Dynamic response of CS0 for IDV1

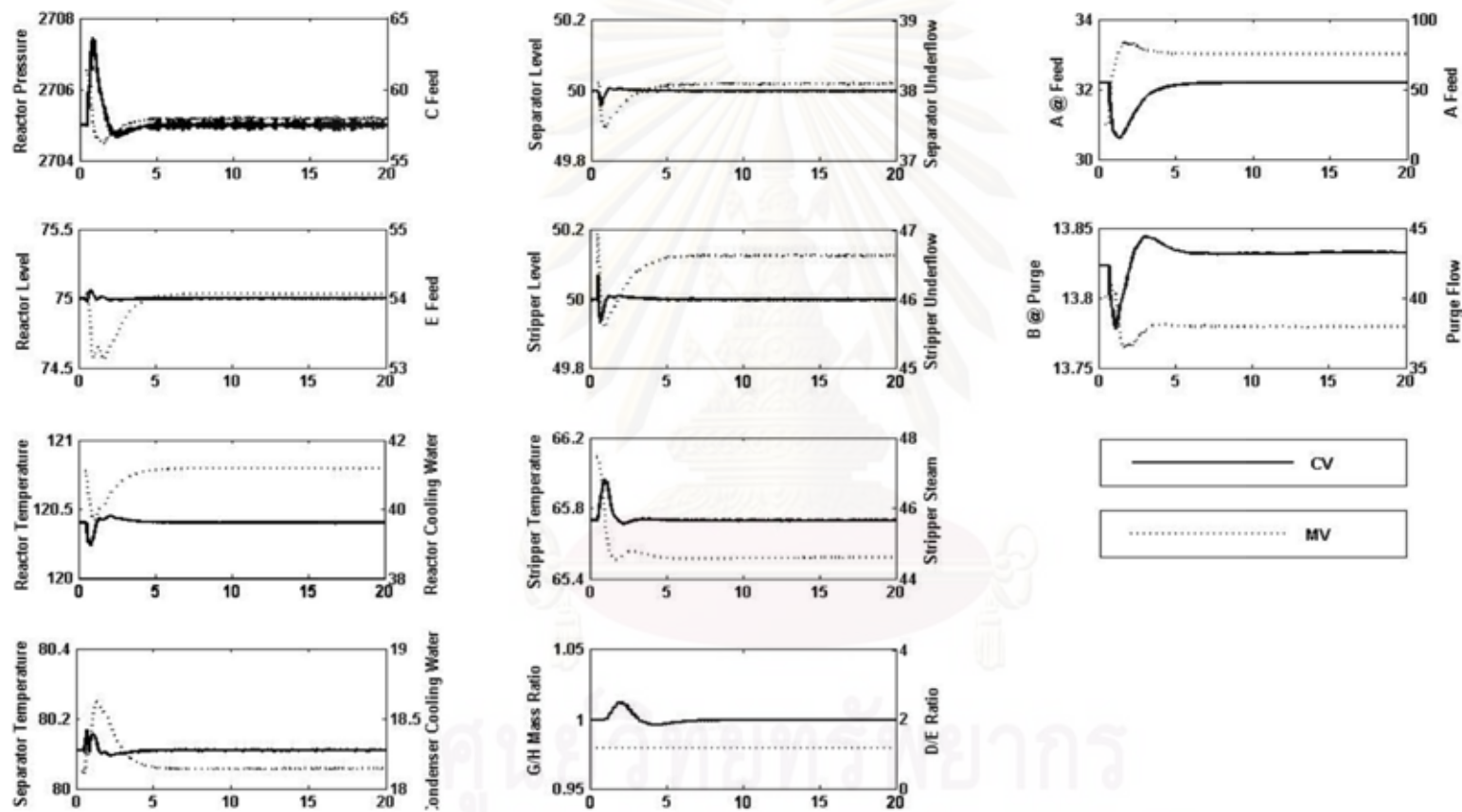


Figure 5.8 Dynamic response of CS1 for IDV1

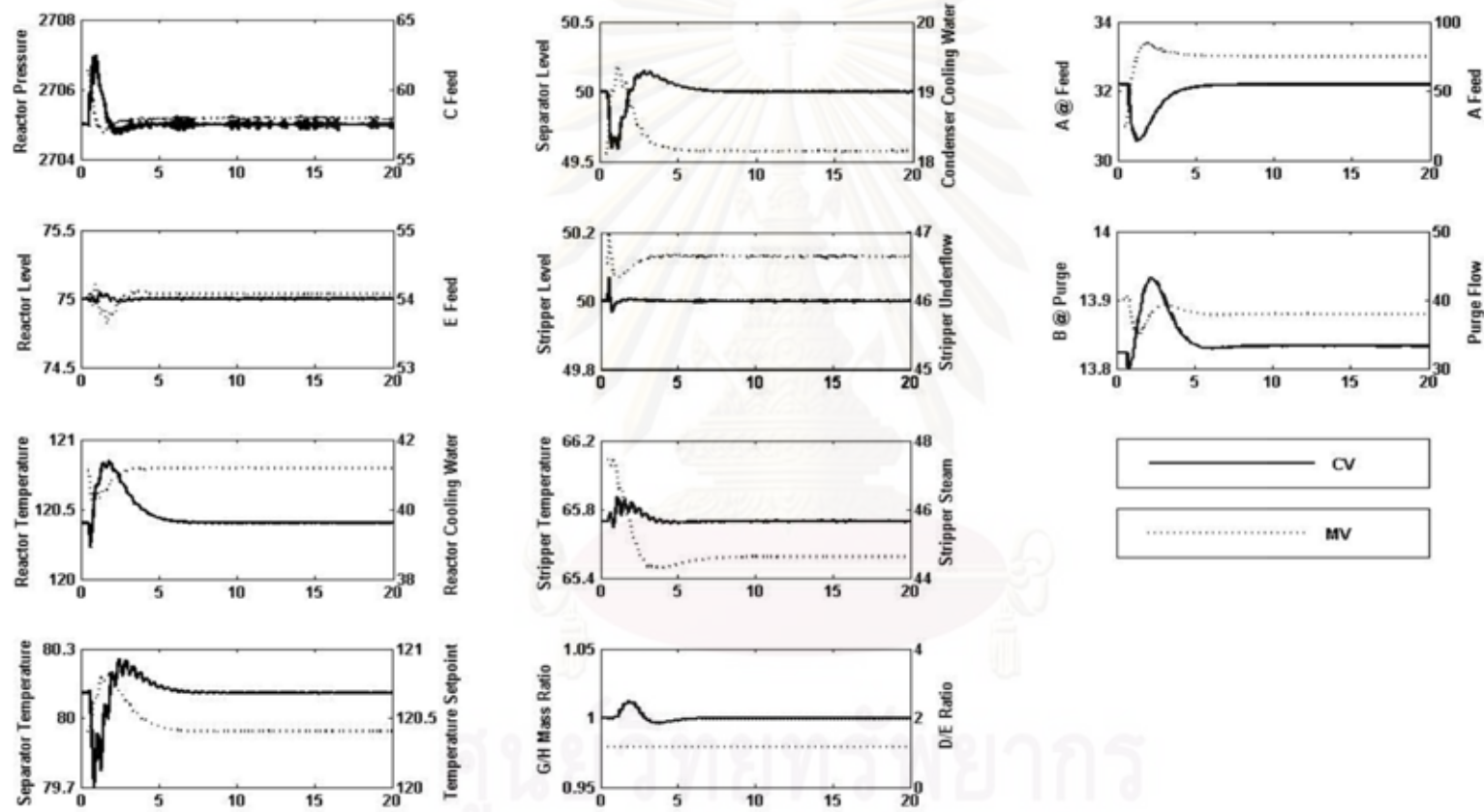


Figure 5.9 Dynamic response of CS2 for IDV1

Table 5.12: Normalized IAE of CS0, CS1 and CS2 for IDV1

IAE	CS0	CS1	CS2
Measurements & MVs	51.71	53.37	50.92
All CVs	11.81	8.10	10.09
Important CVs	5.91	4.30	4.79

### - Change of $B$ composition in $C$ feed stream (IDV2)

Table 5.13 and 5.14 show the normalized ITAE and IAE values of CS0, CS1 and CS2. It can be seen that CS1 and CS2 give better ITAE and IAE than CS0. Figure 5.10-5.12 show the response to IDV2, a change of  $B$  composition in  $C$  feed for CS0, CS1 and CS2. CS1 gives smoother responses than CS2 and CS0. The IDV2 effects reactor temperature and product flow significantly. On reactor temperature of CS1, the effects of disturbance take less than 5 hours to die out while other CSs take much more time. However, all control structures cannot maintain  $G/H$  ratio because of composition changing in feed stream.

Table 5.13: Normalized ITAE of CS0, CS1 and CS2 for IDV2

ITAE	CS0	CS1	CS2
Measurements & MVs	53.50	51.04	51.46
All CVs	13.37	7.10	9.53
Important CVs	6.78	3.03	5.18

Table 5.14: Normalized IAE of CS0, CS1 and CS2 for IDV2

IAE	CS0	CS1	CS2
Measurements & MVs	52.85	51.64	51.51
All CVs	12.45	7.64	9.91
Important CVs	6.56	3.33	5.11

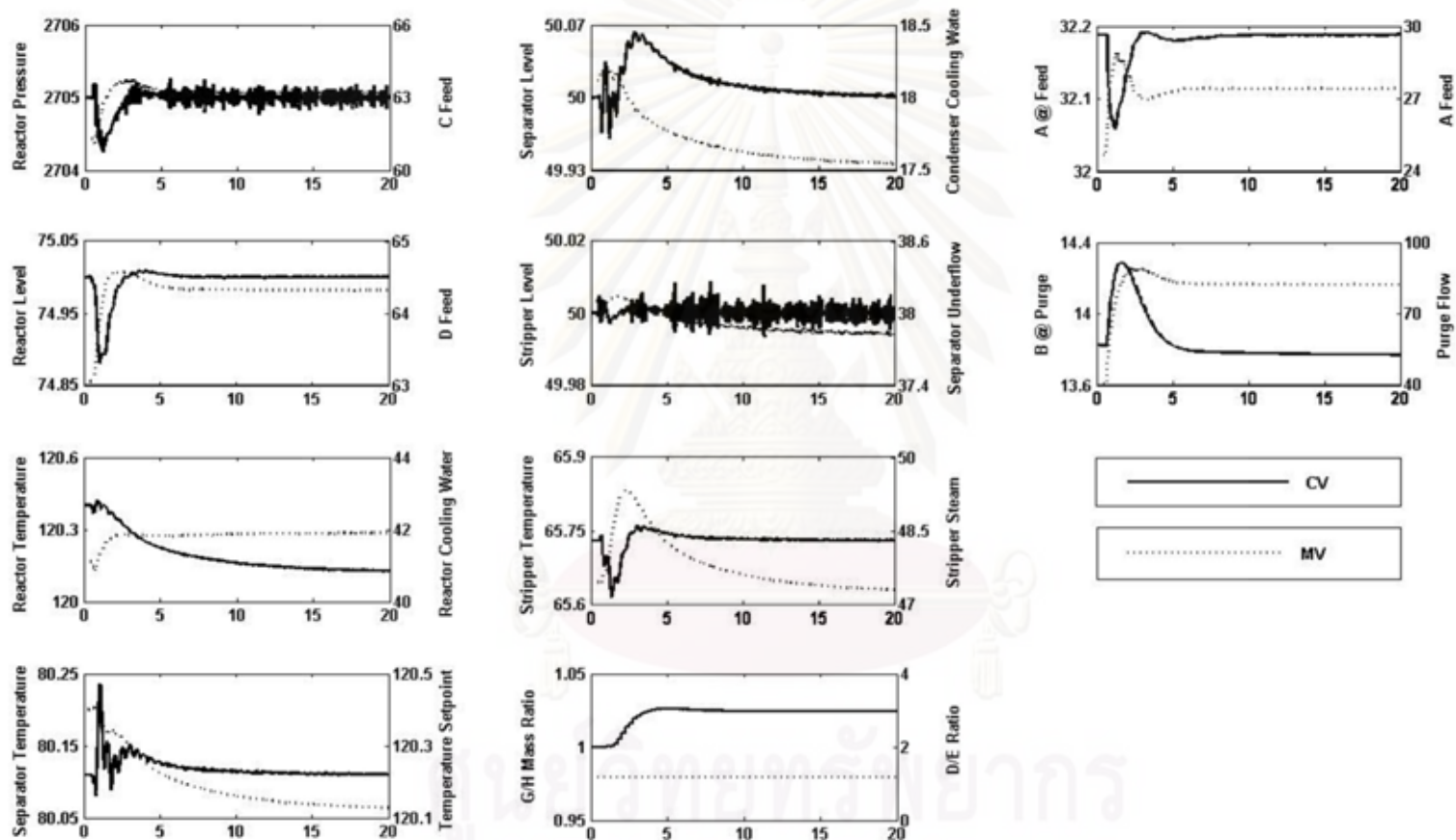


Figure 5.10 Dynamic response of CS0 for IDV2

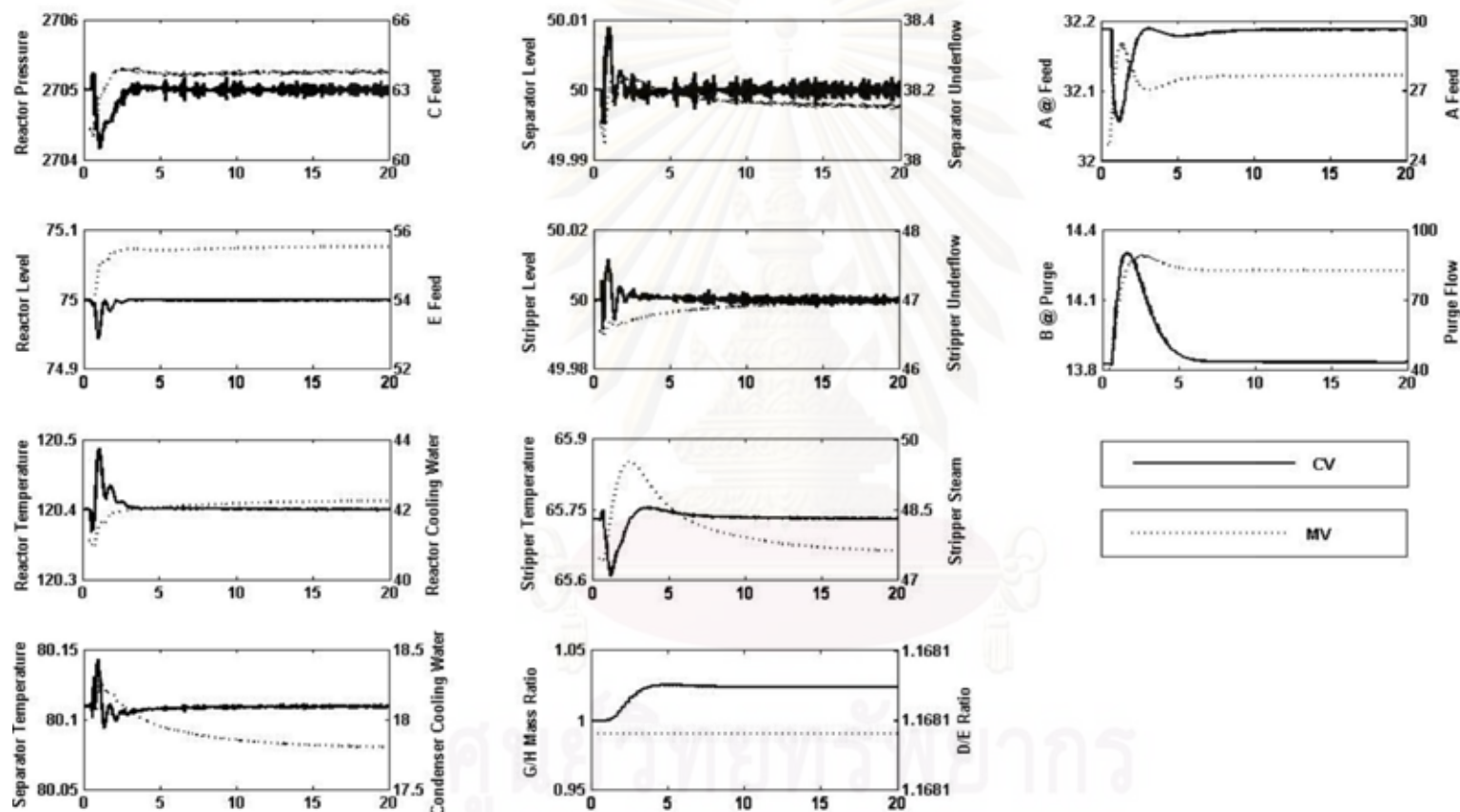


Figure 5.11 Dynamic response of CS1 for IDV2

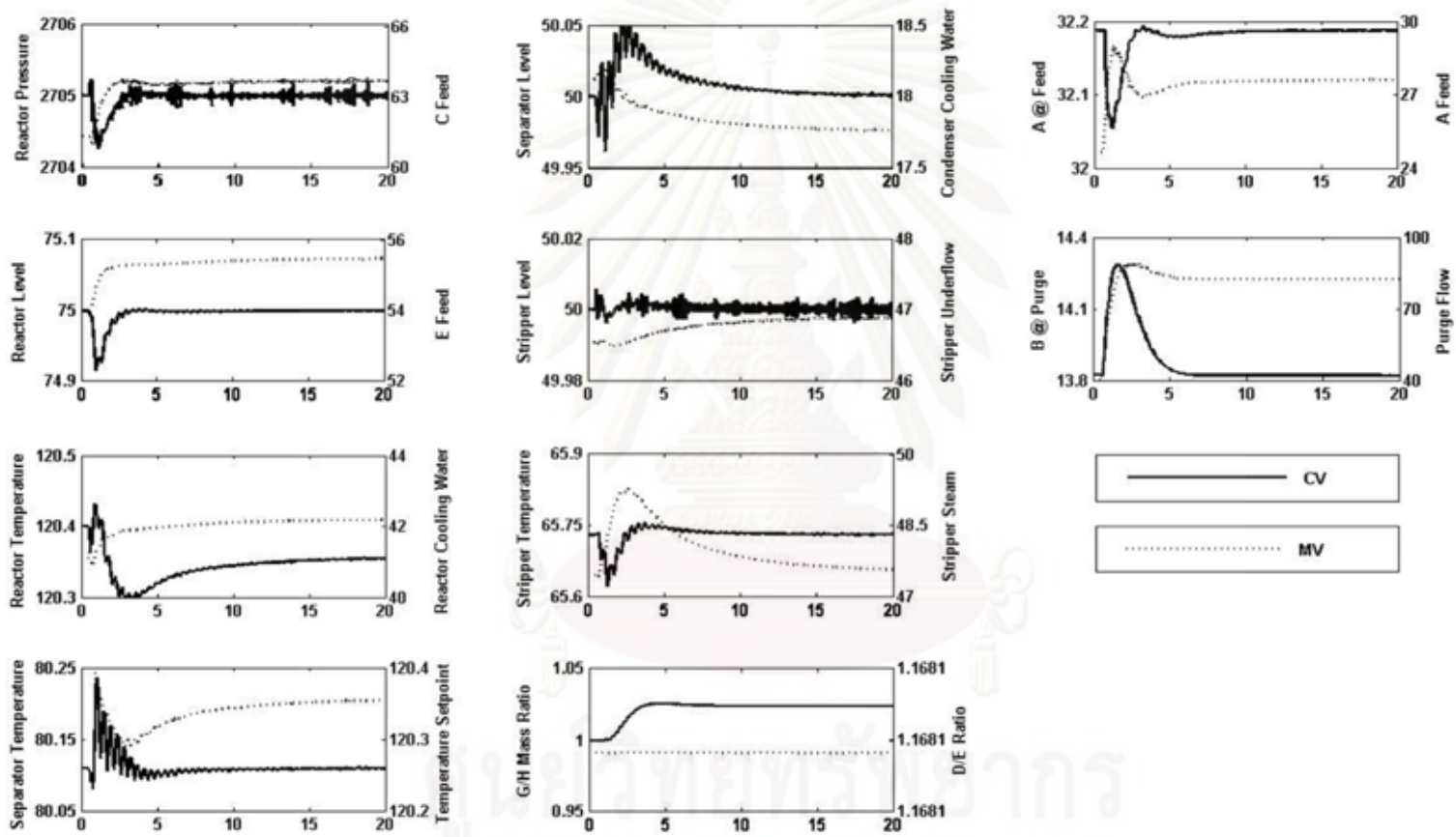


Figure 5.12 Dynamic response of CS2 for IDV2

#### - Change of reactor cooling water temperature (IDV4)

Table 5.15 and 5.16 show the normalized ITAE and IAE values of CS0, CS1 and CS2. It can be seen that CS1 gives smaller ITAE than CS0 otherwise CS0 gives smaller IAE than CS1 while CS2 gives quite large ITAE and IAE. Figure 5.13-5.15 show the response to IDV4, a change of reactor cooling water temperature for CS0, CS1 and CS2. CS1 gives small oscillation compared with CS2 and CS0. The effects of IDV4 on all three CS take about 5 hours to die out. However, it can be noted that CS1 can maintain the setpoint faster than the others.

Table 5.15: Normalized ITAE of CS0, CS1 and CS2 for IDV4

ITAE	CS0	CS1	CS2
Measurements & MVs	40.03	41.21	74.77
All CVs	8.15	5.45	16.40
Important CVs	4.21	2.87	7.92

Table 5.16: Normalized IAE of CS0, CS1 and CS2 for IDV4

IAE	CS0	CS1	CS2
Measurements & MVs	41.48	48.65	65.87
All CVs	8.58	7.20	14.22
Important CVs	4.05	4.15	6.80



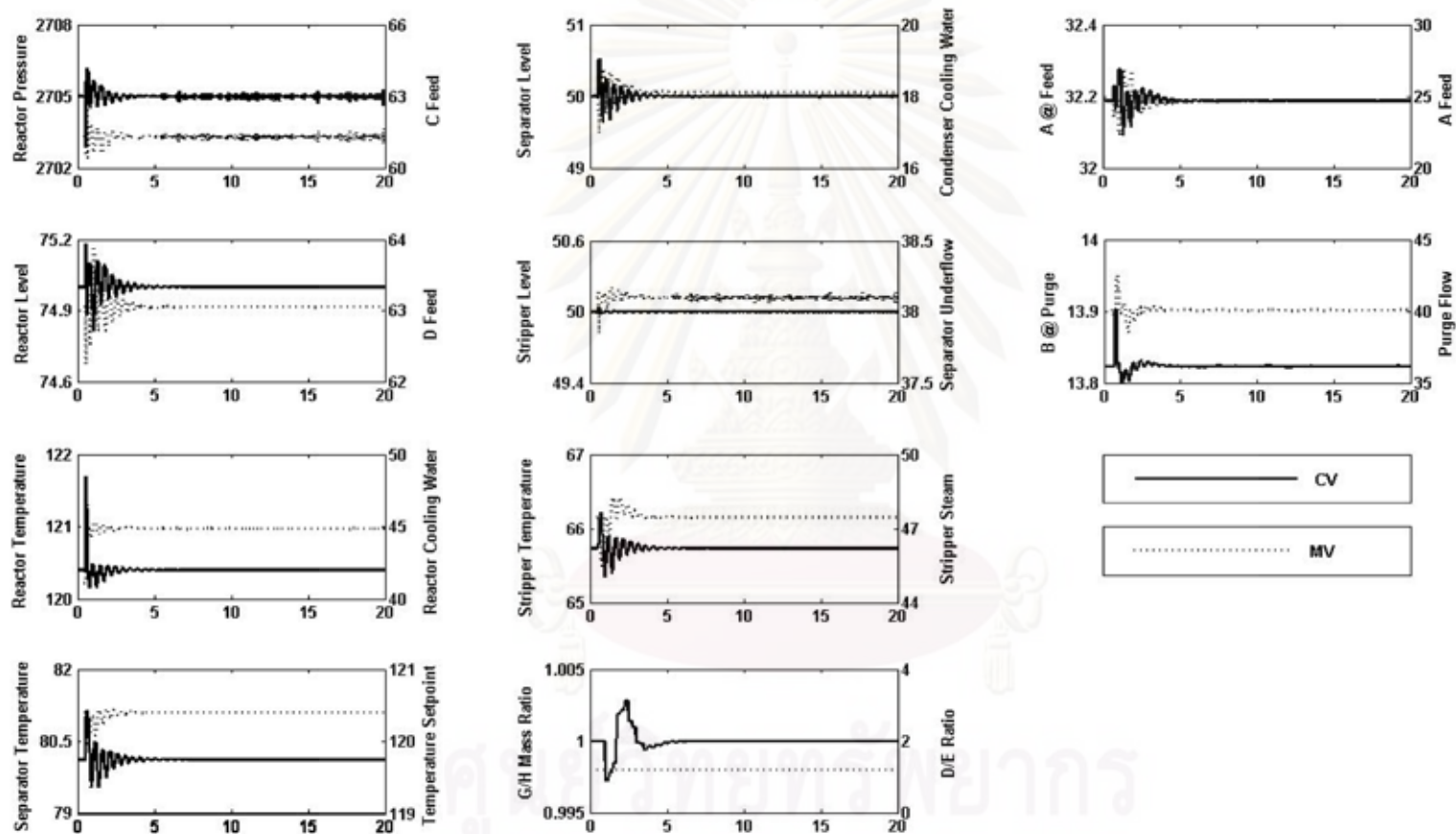


Figure 5.13 Dynamic response of CS0 for IDV4

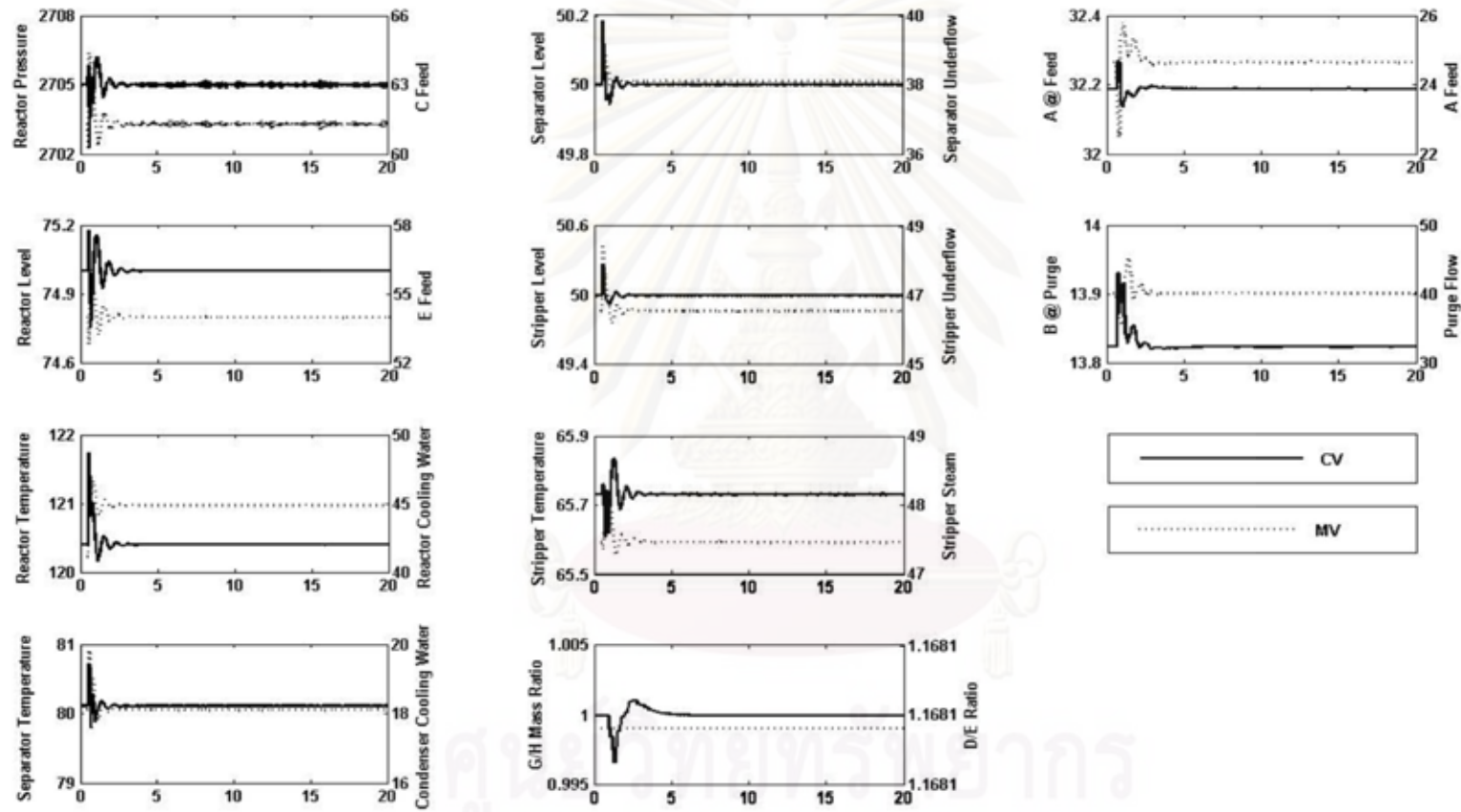


Figure 5.14 Dynamic response of CS1 for IDV4

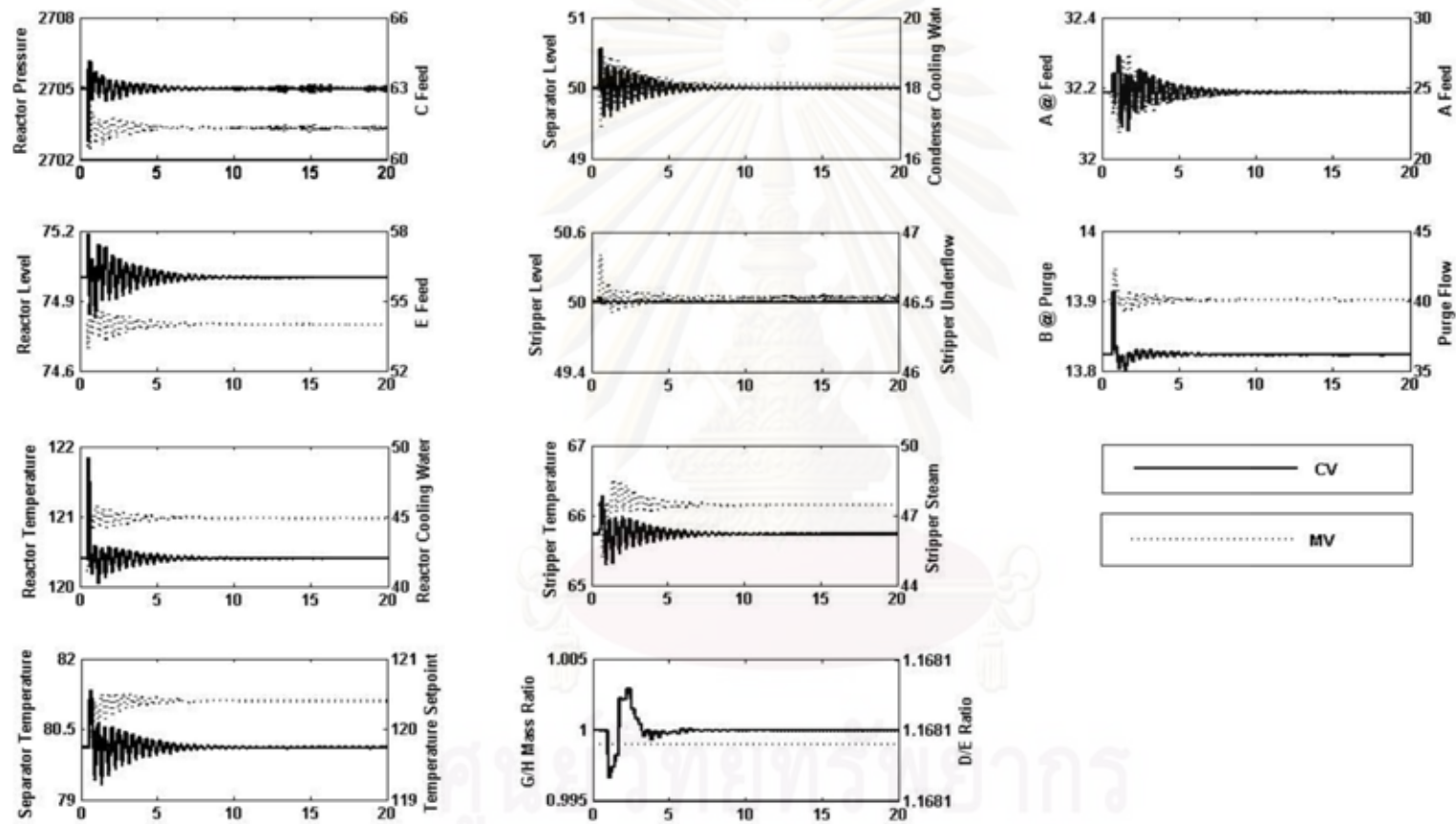


Figure 5.15 Dynamic response of CS2 for IDV4

Table 5.17 and 5.18 show the overall normalized ITAE and IAE of CS0, CS1 and CS2. It can be seen that CS1 give the smallest value of both ITAE and IAE followed by CS0 and CS2 respectively. Table 5.19-5.22 show the IAE and ITAE of the measurements and manipulated variables for all cases.

Table 5.17: Overall Normalized ITAE of CS0, CS1 and CS2

ITAE	CS0	CS1	CS2
Measurements & MVs	207.31	191.69	225.00
All CVs	45.57	28.45	45.97
Important CVs	23.13	13.78	23.08

Table 5.18: Overall Normalized IAE of CS0, CS1 and CS2

IAE	CS0	CS1	CS2
Measurements & MVs	202.98	204.87	216.16
All CVs	43.36	32.06	44.58
Important CVs	21.50	16.52	21.98

## 5.4 Conclusions

In this chapter, a dynamic performance-based optimization for plantwide control structure design is proposed. The proposed methodology conforms to the Class-2 of Stephanopoulos and Ng (2000). The optimization problem is formulated as dynamic mixed integer nonlinear programming. The TE process is selected as the testbed problem. A dynamic optimization (MINLP) technique is applied for establishing a control structure corresponding to the four important CVs that related to shutdown condition directly and the remaining obvious CV-MV pairings are obtained heuristically to save computing time. The performances of obtained control structures are evaluated with dynamic simulation. Our obtained control structures can give the smoother operation compared with Luyben's control structure.



Table 5.19: Normalized ITAE of all measurements for all cases

ITAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
CVs												
A Feed	1.81	0.21	0.99	1.00	1.00	1.00	0.95	1.03	1.01	0.74	0.36	1.90
D Feed	1.60	1.23	0.17	0.40	1.33	1.27	0.81	1.13	1.06	0.49	0.60	1.91
E Feed	1.06	0.94	1.00	0.40	1.33	1.27	0.81	1.13	1.06	0.49	0.60	1.91
C Feed	0.20	1.79	1.01	1.02	0.99	0.99	0.87	1.09	1.04	1.14	0.99	0.86
Recy Flow	1.46	0.55	0.99	1.35	0.70	0.95	0.61	1.27	1.12	1.01	0.94	1.05
Reac Feed	0.88	1.12	1.00	1.27	0.88	0.85	0.93	1.05	1.02	0.89	0.76	1.35
Reac Press	1.05	0.93	1.02	1.09	1.09	0.82	1.22	0.96	0.81	1.09	0.97	0.94
Reac Lev	0.99	0.86	1.15	1.35	0.71	0.94	1.43	0.38	1.19	0.68	0.40	1.92
Reac Temp	0.81	1.14	1.05	0.94	1.15	0.92	0.85	0.96	1.19	0.55	0.52	1.93
Purge Flow	0.68	1.33	0.99	1.01	1.00	0.99	1.00	1.00	1.00	0.86	1.15	0.99
Sep Temp	1.53	0.23	1.24	1.63	0.17	1.19	1.82	0.30	0.87	0.66	0.13	2.21
Sep Lev	1.98	0.09	0.93	1.59	0.12	1.29	1.85	0.09	1.06	0.67	0.14	2.19
Sep Press	1.67	0.95	0.38	1.20	1.00	0.80	0.80	1.14	1.07	1.04	0.85	1.11
Sep U Flow	1.98	0.14	0.89	2.10	0.51	0.39	1.88	0.41	0.71	1.85	0.95	0.20
Str Lev	0.98	1.03	0.99	1.36	0.76	0.88	1.43	0.64	0.94	1.22	0.84	0.94
Str Press	1.69	0.97	0.34	1.50	0.83	0.67	0.81	1.13	1.06	1.08	0.95	0.97
Str U Flow	0.76	1.73	0.51	0.27	1.39	1.34	0.46	1.37	1.17	0.09	1.49	1.42
Str Temp	1.23	0.65	1.12	1.37	0.67	0.95	1.05	1.01	0.94	0.71	0.21	2.07
Str Stm Flow	1.33	0.68	0.99	1.02	0.99	0.99	0.67	1.26	1.07	0.73	0.34	1.94
Comp Work	1.01	1.00	0.99	1.02	0.98	1.00	0.98	1.01	1.01	0.74	0.60	1.65
RCW Temp	1.08	0.92	1.00	1.18	0.92	0.90	1.05	0.97	0.99	0.61	0.43	1.96
CCW Temp	1.48	0.54	0.98	0.56	1.13	1.30	1.18	0.88	0.94	0.62	0.34	2.04
A @ Feed	0.89	0.98	1.14	0.99	1.02	1.00	0.88	1.05	1.07	0.73	0.39	1.89
B @ Feed	1.15	0.95	0.90	1.40	0.60	1.00	1.01	1.00	0.99	0.83	1.23	0.94
C @ Feed	0.99	1.01	0.99	1.09	0.89	1.02	0.97	1.02	1.01	0.67	1.03	1.30
D @ Feed	0.95	1.05	1.00	0.73	1.08	1.19	0.88	1.08	1.04	0.62	0.64	1.74
E @ Feed	0.93	1.07	1.00	1.13	0.96	0.91	0.85	1.10	1.05	0.93	0.59	1.47
F @ Feed	1.41	0.61	0.98	0.83	0.89	1.28	1.02	0.98	0.99	0.14	2.58	0.28
A @ Pur	1.13	0.88	1.00	1.00	1.01	0.99	1.02	0.98	1.00	0.71	0.51	1.78
B @ Pur	1.65	1.14	0.21	0.77	0.97	1.25	1.82	0.71	0.46	0.81	1.16	1.03
C @ Pur	1.03	0.98	0.99	1.04	0.93	1.03	0.99	1.01	1.00	0.58	1.11	1.31
D @ Pur	1.22	0.78	1.00	1.55	0.80	0.64	1.63	0.57	0.80	0.66	0.42	1.93
E @ Pur	0.90	1.10	1.00	1.14	0.96	0.90	0.78	1.15	1.07	0.93	0.59	1.49
F @ Pur	1.45	0.58	0.98	0.80	0.91	1.30	1.03	0.98	0.99	0.15	2.49	0.37
G @ Pur	1.00	1.00	1.00	1.01	1.01	0.97	1.00	1.00	1.00	0.65	0.18	2.17
H @ Pur	1.00	0.99	1.00	0.93	0.99	1.07	1.07	0.95	0.98	0.68	0.17	2.16
D @ Prod	1.29	0.71	1.01	1.06	0.98	0.96	0.44	1.38	1.17	0.83	0.71	1.46
E @ Prod	0.92	1.08	1.00	1.01	1.00	0.99	0.94	1.04	1.02	0.96	0.50	1.53
F @ Prod	1.37	0.65	0.98	0.96	0.98	1.06	1.02	0.98	0.99	0.30	2.16	0.54
G @ Prod	0.98	1.02	1.00	0.85	1.20	0.95	1.01	0.99	1.00	1.04	0.71	1.26
H @ Prod	1.03	0.96	1.01	0.82	1.21	0.97	1.01	0.99	1.00	1.01	0.70	1.29

Table 5.20: Normalized ITAE of all manipulated variables for all cases

ITAE MVs	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
D feed	1.60	1.23	0.17	0.40	1.33	1.27	0.81	1.13	1.06	0.48	0.59	1.93
E feed	1.60	1.23	0.17	0.40	1.33	1.27	0.81	1.13	1.06	0.48	0.59	1.93
A feed	1.81	0.20	0.99	1.00	1.00	1.00	0.95	1.03	1.01	0.73	0.36	1.91
C feed	0.20	1.79	1.01	1.02	0.99	0.99	0.87	1.09	1.04	1.09	0.97	0.94
Recycle	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Purge	0.33	1.71	0.96	1.01	1.00	0.99	1.00	1.00	1.00	0.85	1.19	0.96
Sep Liq	1.54	1.46	0.00	2.49	0.51	0.00	2.35	0.65	0.00	1.79	1.21	0.00
Str Liq	0.00	1.99	1.01	0.00	1.51	1.49	0.00	1.68	1.32	0.00	1.51	1.49
Str Stm	1.33	0.68	0.99	1.02	0.99	0.99	0.67	1.26	1.07	0.78	0.38	1.84
RCWF	0.81	1.19	1.00	0.23	1.45	1.32	0.81	1.13	1.06	1.00	1.00	1.00
CCWF	1.83	0.21	0.96	1.05	0.81	1.13	1.39	0.74	0.88	0.63	0.30	2.07
Agi Spd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 5.21: Normalized IAE of all measurements for all cases

IAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
CVs												
A Feed	1.33	0.64	1.02	1.00	1.00	1.00	0.96	1.03	1.01	0.87	0.46	1.67
D Feed	1.48	1.21	0.31	0.42	1.56	1.02	0.84	1.12	1.04	0.56	1.00	1.44
E Feed	1.05	0.95	1.00	0.42	1.56	1.02	0.84	1.12	1.04	0.56	1.00	1.44
C Feed	0.28	1.71	1.01	1.01	1.01	0.98	0.88	1.09	1.03	0.96	1.07	0.97
Recy Flow	1.43	0.57	1.00	1.13	0.81	1.06	0.74	1.20	1.06	0.79	1.19	1.02
Reac Feed	0.88	1.13	1.00	1.04	1.02	0.94	0.93	1.05	1.02	0.82	0.84	1.34
Reac Press	0.92	1.04	1.03	0.94	1.15	0.91	1.11	1.00	0.89	0.92	1.01	1.07
Reac Lev	1.17	0.81	1.01	1.48	0.67	0.85	1.55	0.39	1.06	0.83	0.69	1.48
Reac Temp	0.73	1.18	1.09	0.92	1.16	0.92	0.88	1.00	1.12	0.70	0.84	1.46
Purge Flow	0.69	1.28	1.03	1.00	1.01	0.99	1.00	1.00	1.00	0.68	1.55	0.77
Sep Temp	1.15	0.39	1.47	1.66	0.13	1.21	1.63	0.30	1.07	0.92	0.21	1.87
Sep Lev	1.55	0.11	1.35	1.62	0.06	1.31	1.79	0.07	1.14	0.93	0.13	1.94
Sep Press	1.38	0.95	0.67	0.99	1.12	0.88	0.84	1.12	1.04	0.91	0.80	1.29
Sep U Flow	1.95	0.16	0.88	1.50	1.19	0.31	1.85	0.42	0.73	0.95	1.69	0.37
Str Lev	0.61	1.60	0.79	0.95	1.25	0.80	1.23	0.87	0.90	0.68	1.47	0.84
Str Press	1.60	0.99	0.41	1.25	1.01	0.73	0.84	1.12	1.04	0.88	0.98	1.14
Str U Flow	0.75	1.73	0.53	0.28	1.62	1.09	0.51	1.37	1.12	0.13	2.00	0.87
Str Temp	0.94	0.79	1.27	1.30	0.82	0.88	1.03	1.05	0.92	0.95	0.23	1.82
Str Stm Flow	1.32	0.68	1.00	1.01	1.01	0.98	0.78	1.19	1.03	1.01	0.30	1.69
Comp Work	1.00	1.01	1.00	1.01	0.99	1.00	0.98	1.01	1.01	0.91	0.52	1.57
RCW Temp	1.08	0.93	1.00	1.10	0.91	0.98	1.04	0.97	0.99	0.74	0.69	1.56
CCW Temp	1.45	0.57	0.99	0.93	0.92	1.16	1.17	0.88	0.95	0.83	0.50	1.67
A @ Feed	0.92	0.99	1.09	1.00	1.00	1.00	0.96	1.02	1.02	0.87	0.48	1.65
B @ Feed	0.76	1.20	1.04	1.34	0.68	0.98	1.00	1.00	1.00	0.67	1.62	0.71
C @ Feed	0.98	1.03	0.99	1.06	0.92	1.02	0.97	1.02	1.01	0.83	0.82	1.35
D @ Feed	0.95	1.05	1.00	0.91	0.92	1.17	0.90	1.07	1.02	0.71	0.96	1.33
E @ Feed	0.94	1.06	1.00	1.04	1.04	0.92	0.86	1.11	1.03	1.03	0.62	1.34
F @ Feed	1.40	0.62	0.98	0.93	0.78	1.29	1.02	0.98	1.00	0.28	2.24	0.47
A @ Pur	1.06	0.92	1.02	1.00	1.00	1.00	1.01	0.99	1.00	0.87	0.54	1.59
B @ Pur	1.55	1.19	0.26	1.05	0.71	1.24	1.25	0.95	0.80	0.72	1.43	0.84
C @ Pur	1.02	0.99	0.99	1.03	0.95	1.02	0.99	1.01	1.00	0.87	0.75	1.38
D @ Pur	1.21	0.79	1.00	1.26	1.09	0.65	1.48	0.64	0.88	0.76	0.65	1.59
E @ Pur	0.91	1.09	1.00	1.05	1.04	0.92	0.80	1.15	1.05	1.02	0.66	1.32
F @ Pur	1.45	0.58	0.98	0.91	0.78	1.30	1.02	0.98	0.99	0.32	2.07	0.61
G @ Pur	1.00	1.00	1.00	1.02	1.00	0.98	1.00	1.00	1.00	0.91	0.26	1.83
H @ Pur	1.01	0.99	1.00	1.16	0.76	1.08	1.04	0.97	0.99	0.94	0.24	1.82
D @ Prod	1.29	0.71	1.00	1.03	1.02	0.95	0.47	1.39	1.14	0.92	0.82	1.26
E @ Prod	0.93	1.08	1.00	1.01	1.01	0.99	0.95	1.04	1.01	1.15	0.40	1.45
F @ Prod	1.35	0.67	0.98	0.99	0.95	1.06	1.02	0.98	1.00	0.59	1.59	0.83
G @ Prod	0.98	1.02	1.00	0.90	1.15	0.95	1.01	0.99	1.00	1.06	0.72	1.22
H @ Prod	0.99	1.01	1.00	0.89	1.15	0.96	1.01	0.99	1.00	1.06	0.69	1.24



Table 5.22: Normalized IAE of all manipulated variables for all cases

IAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
MVs												
D feed	1.48	1.21	0.31	0.42	1.56	1.02	0.84	1.12	1.04	0.56	1.01	1.44
E feed	1.48	1.21	0.31	0.42	1.56	1.02	0.84	1.12	1.04	0.56	1.01	1.44
A feed	1.33	0.64	1.02	1.00	1.00	1.00	0.96	1.03	1.01	0.87	0.46	1.67
C feed	0.28	1.71	1.01	1.01	1.01	0.98	0.88	1.09	1.03	0.89	1.05	1.06
Recycle	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Purge	0.50	1.46	1.04	1.00	1.01	0.99	1.00	1.00	1.00	0.67	1.61	0.72
Sep Liq	1.54	1.46	0.00	1.72	1.28	0.00	2.15	0.85	0.00	0.89	2.11	0.00
Str Liq	0.00	1.99	1.01	0.00	1.76	1.24	0.00	1.74	1.26	0.00	2.13	0.87
Str Stm	1.32	0.68	1.00	1.01	1.01	0.98	0.78	1.19	1.03	1.05	0.31	1.63
RCWF	0.82	1.18	1.00	0.52	1.45	1.03	0.83	1.13	1.04	1.00	1.00	1.00
CCWF	1.79	0.24	0.97	1.16	0.65	1.19	1.38	0.73	0.89	0.81	0.49	1.69
Agi Spd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

# CHAPTER VI

## COMBINED MATHEMATIC AND HEURISTIC APPROACH FOR PLANTWIDE CONTROL STRUCTURE DESIGN

This chapter illustrates the benefit of the combined mathematic and heuristic approach for designing the control structure of TE process. The approach can be divide into two main parts: 1) heuristic and 2) mathematic. Especially in mathematic part, the dynamic performance-based optimization is applied for establishing the plantwide control structure.

### 6.1 Introduction

A combined mathematic and heuristic approach is proposed for plantwide control structure design. Heuristic rules are used for selecting controlled variables (CVs) and manipulated variables (MVs) sets and establishing obvious control loops to save computing time. Consequently, a dynamic performance-based optimization is adopted to establish control structure of the plant. The approach assumes that the process dynamic model is available. The optimization problem can be formulated in the form of Mixed Integer Nonlinear Programming (MINLP). The objective function reflects the dynamic control performance of CVs and MVs under the influence of time (ITAE of CVs and MVs). The approach is investigated on the Tennessee Eastman (TE) process. The obtained control structures are evaluated with the nonlinear TE process in the face of various disturbances and setpoint changing.

The works discussed above raise some issues that need to be studied further. For the lack or incomplete knowledge, the methodologies are heuristic-based; while the systematic or mathematical programming approach has been developed and

gained interests recently. To gain advantages of two main approaches, the combined mathematic and heuristic approach is presented in this work. The heuristic rules are used for controlled variables (CVs) and manipulated variables (MVs) selection. To save computing time, some obvious control loops are assigned heuristically. The dynamic performance-based optimization is developed for CV-MV pairings. It is worthwhile to point out our main contributions. First, our objective function is accounted on the dynamic performances of the controlled process explicitly. The real-time performance evaluation is applied to get more realistic. Second, our process model used in the optimization is more rigorous and accurate than some works discussed above. Third, our optimization problem is comprehensive and easy to solve with commercial optimization solver. Our optimization is formulated as the Mixed Integer Nonlinear Programming (MINLP) to establish the CVs-MVs pairing. The process disturbances are included in the optimization problem as the treatment of uncertainties while the model uncertainties are not considered in this work. Our proposed methodology could be categorized as the Class-2 of Stephanopoulos and Ng (2000). The control structures design results are illustrated and evaluated by dynamic simulation and compared with the control structure proposed by Luyben (1999).

## 6.2 Plantwide Control Structure Design of the TE Process

Our proposed methodology, the combined mathematic and heuristic plantwide control structure design procedure, is applied on the TE process. The design procedure is shown in table 6.1 and described step by step as follows.

### Step 1: Controlled Variable Selection

In this paper, a set of CVs is selected heuristically. Luyben's nine steps procedure is the famous heuristic procedure for design control structure. However, once we consider the procedure deeply, it gives the guideline for selecting CVs implicitly. So that, a CVs set proposed by Luyben et.al. (1999) is adopted in this work. It is not only the good guideline but it is also a reasonable way to compare our obtained control structure with theirs. The CVs are reactor temperature,

Table 6.1: Combined mathematic and heuristic plantwide control structure design procedure

Step	Comments
Heuristic Part	
1. Controlled Variable Selection	<ul style="list-style-type: none"> <li>• Select the CVs set</li> </ul>
2. Manipulated Variable Selection	<ul style="list-style-type: none"> <li>• Select the MVs set</li> </ul>
3. Finding the CV-MV pairings	<ul style="list-style-type: none"> <li>• Determine the possible CV-MV pairings</li> <li>• Close the obvious control loops</li> <li>• Eliminate the unreasonable CV-MV pairings</li> </ul>
Mathematic Part	
4. Finding tuning parameters for all candidate control loops	<ul style="list-style-type: none"> <li>• Determine tuning parameters for candidate CV-MV pairings using relay-feedback testing</li> </ul>
5. Establishing plantwide control structure via dynamic performance-based optimization	<ul style="list-style-type: none"> <li>• Determine control structure corresponding to the rest of CVs using optimization technique</li> <li>• The optimization problem is formulated as the MINLP</li> </ul>

reactor pressure, reactor level, separator level, stripper level, separator temperature, stripper temperature, product  $G/H$  ratio, component  $A$  and component  $B$ . In this set, there are five CVs related directly to process shutdown criteria given by Downs and Vogel (1993): reactor temperature, reactor pressure, reactor level, separator level, and stripper level.

### Step 2: Manipulated Variable Selection

There are 12 manipulators in the TE process. Agitator speed is fixed at the constant speed then we do not include it in the set of MVs. Hence, the remains of MVs are  $D$  feed,  $E$  feed,  $C$  feed, recycle, purge, separator liquid, stripper liquid, stripper steam, reactor cooling water, and condenser cooling water.

### Step 3: Finding of the candidate CV-MV pairings

Before finding of candidate CV-MV pairings, obvious control loops will be established. First, due to instability arises in the reactor; reactor temperature

must be controlled tightly. The reactor cooling water flow is selected as MV of this loop because it has strong and direct effect on reactor temperature. Second, product  $G/H$  ratio could be controlled easily by ratio control of  $D/E$  feed. By Richardson Rule (Luyben et. al., 1999),  $D$  feed is selected as MV of this loop. It will be calculated proportional to  $E$  feed.  $E$  feed which has the larger flowrate is still included in MVs set.

There are 8 CVs and 9 MVs for establishing the control structure. The overall number of CV-MV pairings is 72. To save computing time, unreasonable CV-MV pairings are eliminated from the overall combination. The possible candidate CV-MV pairings are listed in Table 6.2.

Table 6.2: Candidate CV-MV pairings

CVs	Candidate MVs				
Reactor Pressure	$E$ Feed	$C$ Feed	Recycle	Purge	CCW
Reactor Level	$E$ Feed	Recycle	CCW		
Separator Level	$C$ Feed	Recycle	Purge	Sep. Liq. F.	CCW
Separator Temperature	$C$ Feed	Recycle	Purge	Sep. Liq. F.	CCW
Stripper Level	$C$ Feed	Sep. Liq. V.	Str. Liq. V.	Str. Stm. V.	
Striper Temperature	$C$ Feed	Str. Liq. F.	Str. Stm. F.		
$A$ in Feed	$A$ Feed	$C$ Feed	Recycle	Purge	
$B$ in Purge	Recycle	Purge			

#### Step 4: Finding of tuning parameters for all candidate pairing

Tuning parameters of all candidate CV-MV pairings are determined in this step. The discrete proportional-integral (PI) control is used on all control loops. As seen in the optimization problem,  $\tilde{K}^P$  is the proportional gain matrix and  $\tilde{K}^I$  is the integral gain matrix. Elements in these matrices are obtained using relay feedback testing technique and Tyreus-Luyben tuning method. Relay feedback testing technique is used for determining of ultimate gain and ultimate period, while Tyreus-Luyben tuning method is used for calculating of the PI tuning parameters.

#### Step 5: Establishing of plantwide control structure via dynamic performance-based optimization

Dynamic performance-based optimization is used for establishing the plantwide control structure. Parameters in the optimization problem (Eq.4.5) are set as followed. For the weighting factor  $w_y$  and  $w_u$ , the important of CVs and MVs is weighted equally. The number of tested disturbance  $n$  is 4 (IDV-1, 2, 4 and 6). The details of disturbances are presented in the paper (Downs and Vogel, 1993). There are 8 CVs to be optimized shown in table 6.2 so the number of control loops  $N$  is 8. The number of measurements  $N_y$  and  $N_u$  manipulated variables are 41 and 12, respectively. The time period  $T$  for the dynamic model is 20 hours with sampling time  $\Delta T$  is 1/100 hours.

The Tomlab-MINLP commercial optimization package is used to carry out an optimization result. Each optimization batch takes about 1-1.5 hours. Due to the nonlinear problem, a global optimum is not guaranteed. The optimization is solved about 30 times by the result of previous step is set to be the starting point of the next step. All results are ranked to find the best control structure corresponding to the selected CVs. The three best CV-MV pairings established by optimization are presented in the table 6.3. In this work, the best and second best control structures will be implemented and evaluated via dynamic simulation.

Table 6.3: Optimization Results

	Reac	Reac	Reac	Sep	Sep
Best	Press	Lev	Temp	Temp	Lev
1	$C$ Feed	Recycle	RCW	CCW	Sep Liq
2	$C$ Feed	$E$ Feed	RCW	CCW	Sep Liq
3	$C$ Feed	$E$ Feed	RCW	Purge	CCW

Table 6.3:(Cont)

	Str	Str	Comp A	Comp B	Value of
Best	Lev	Temp	Feed	Purge	Obj. Func.
1	Str Liq	Str Stm	$A$ Feed	Purge	54643.90
2	Str Liq	Str Stm	$A$ Feed	Purge	65306.01
3	Str Liq	Str Stm	$A$ Feed	Recycle	78967.28

The control structure of TE process proposed by Luyben et al (1999) was used to compare with our control structures. Luyben et al. (1999) proposed two control structures for TE process: 1) on supply structure and 2) on demand

structure. We select the On Supply control structure as the reference. Table 6.4 compares among our control structures, the best result (CS1) and the second result (CS2), and Luyben's control structure (CS0). The reactor temperature and product G/H ratio loops are also shown in the table. It can be seen that most of control loops are familiar. The differences are in the reactor level, separator temperature, separator level and stripper level. The plantwide control structures presented in table 6.4 are illustrated in the figure 6.1-6.3.

Table 6.4: Comparison between CS0, CS1 and CS2

CVs	CS0	CS1	CS2
	MVs	MVs	MVs
React. Press.	<i>C</i> Feed	<i>C</i> Feed	<i>C</i> Feed
React. Level	<i>D</i> Feed	Recycle	<i>E</i> Feed
React. Temp.	RCWF	RCWF	RCWF
Sep. Temp.	React. Temp. Setp.	CCWF	CCWF
Sep. Level	CCWF	Sep. Liquid Flow	Sep. Liquid Flow
Strip. Level	Sep. Liquid Flow	Strip. Liquid Flow	Strip. Liquid Flow
Strip. Temp.	Strip. Steam Flow	Strip. Steam Flow	Strip. Steam Flow
Comp <i>A</i> in Feed	<i>A</i> Feed	<i>A</i> Feed	<i>A</i> Feed
Comp <i>B</i> in Purge	Purge Valve	Purge Valve	Purge Valve
<i>G/H</i> ratio	<i>D/E</i> ratio	<i>D/E</i> ratio	<i>D/E</i> ratio

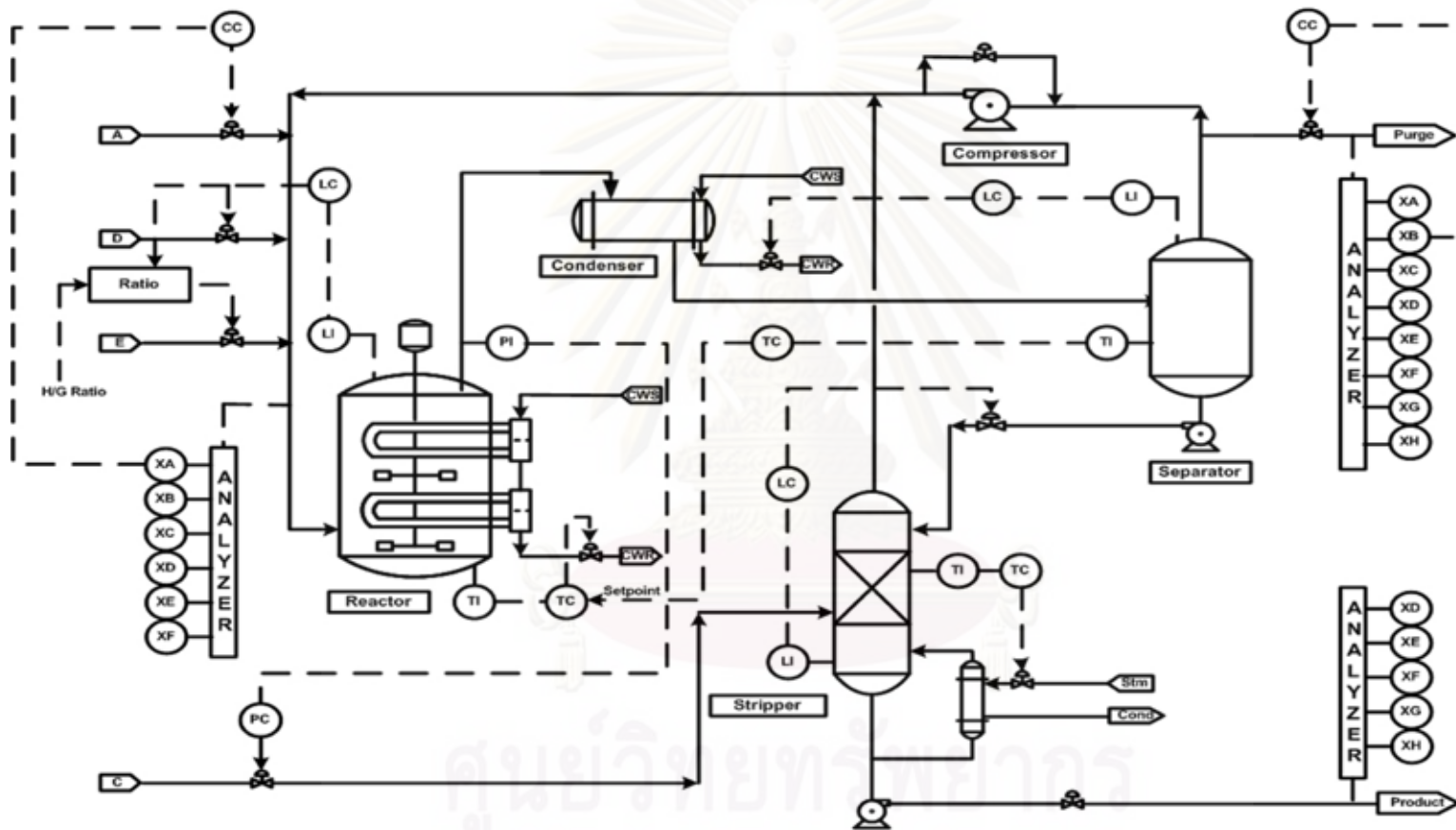


Figure 6.1 Luyben's Control structure (CS0)



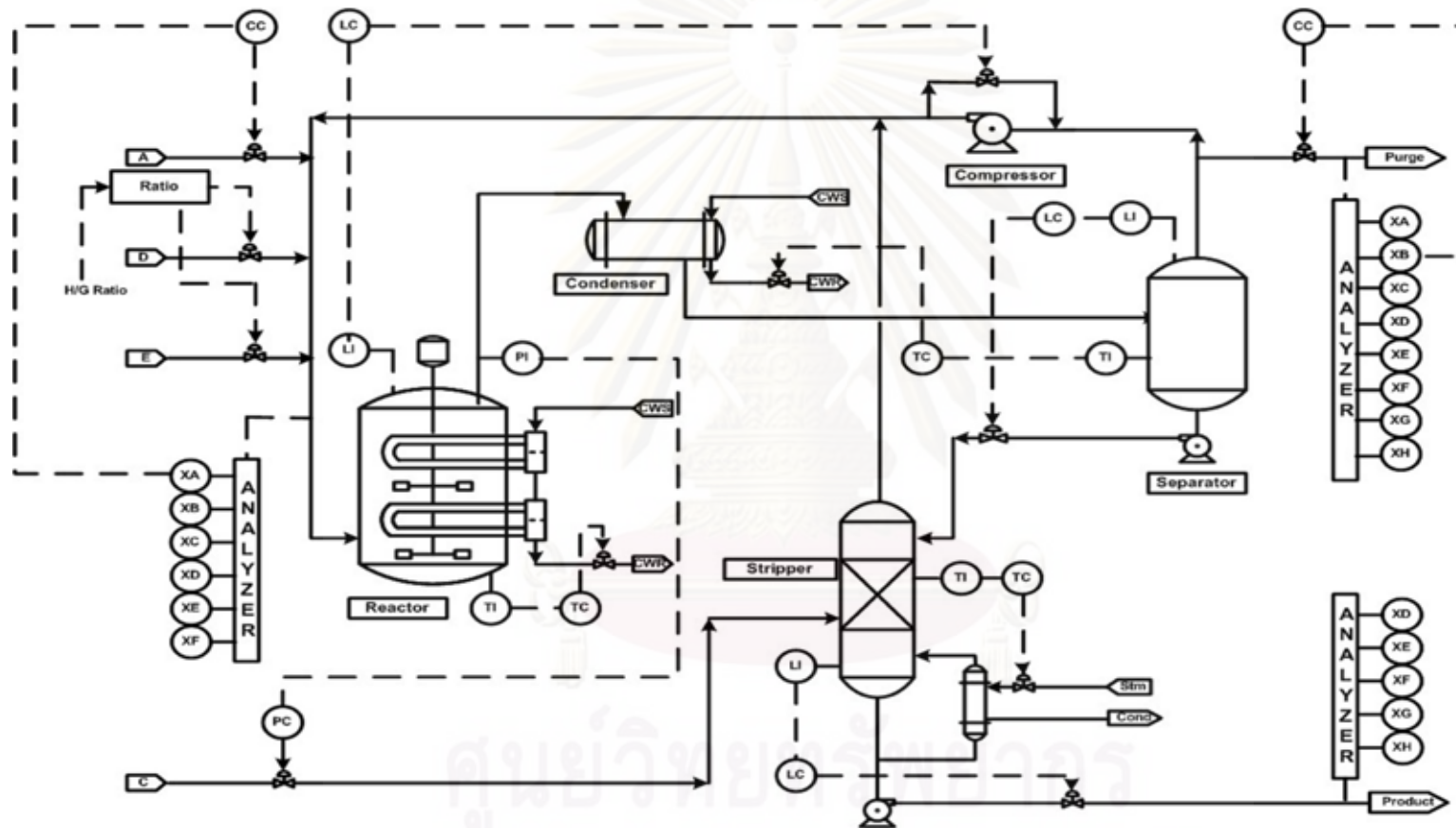


Figure 6.2 The First Best Control structure (CS1)

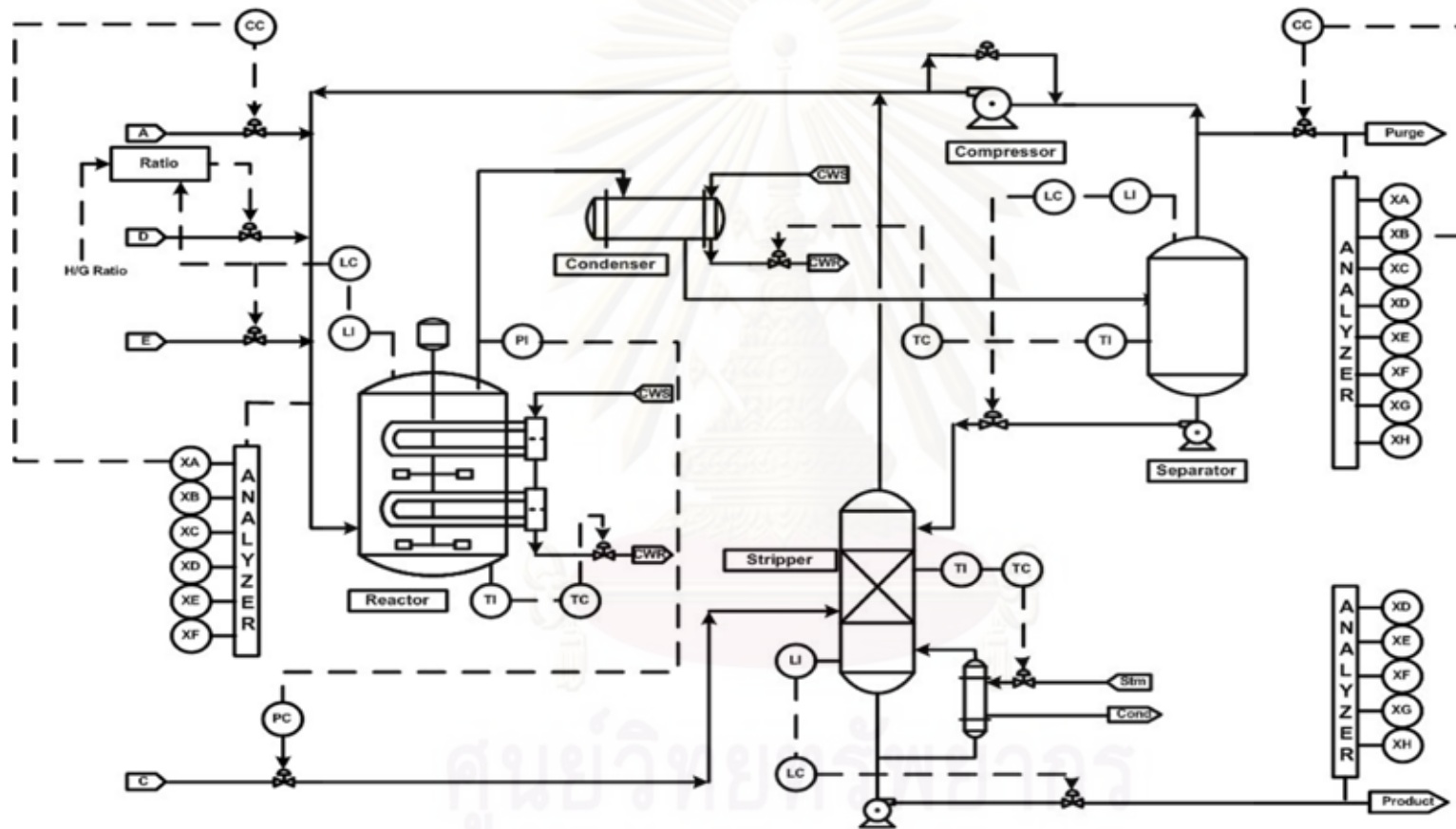


Figure 6.3 The Second Best Control structure (CS2)

### 6.3 Dynamic Simulation and Discussions

To evaluate dynamic performances of plantwide control structures, our control structures and Luyben's control structure are implemented on the nonlinear model of TE process. PI controllers in each loop are re-tuned by relay feedback testing and some trial and error. The tuning parameters for CS0 (Luyben's Cs), CS1 and CS2 are shown in table 6.5-6.7. In dynamic simulation, situations of change in operation condition and presence of disturbances are set to occur in the TE process. The performance index (ITAE and IAE) and responses of TE process controlled by each control structure are shown and discussed case by case.

Table 6.5: CS0's tuning parameters

Controlled Variable	Manipulated Variable	$K_C$	$\tau_I$
Reactor Pressure	$C$ Feed	1	0.3
Reactor Level	$D$ Feed	4	0.3
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Reactor Temp Setpoint	0.3	0.2
Separator Level	Condenser Cooling Water Flow	2	1
Stripper Level	Separator Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp $A$ in Feed	$A$ Feed	25	1.5
Comp $B$ in Purge	Purge Valve	100	1.5

Table 6.6: CS1's tuning parameters

Controlled Variable	Manipulated Variable	$K_C$	$\tau_I$
Reactor Pressure	$C$ Feed	1	0.3
Reactor Level	Recycle	20	0.1
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Condenser Cooling Water Flow	2	0.1
Separator Level	Separator Liquid Flow	5	0.1
Stripper Level	Stripper Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp $A$ in Feed	$A$ Feed	25	1.5
Comp $B$ in Purge	Purge Valve	100	1.5

Table 6.7: CS2's tuning parameters

Controlled Variable	Manipulated Variable	$K_C$	$\tau_I$
Reactor Pressure	$C$ Feed	1	0.3
Reactor Level	$E$ Feed	5	0.1
Reactor Temperature	Reactor Cooling Water Flow	3.5	0.2
Separator Temperature	Condenser Cooling Water Flow	2	0.1
Separator Level	Separator Liquid Flow	5	0.1
Stripper Level	Stripper Liquid Flow	5	0.1
Stripper Temperature	Stripper Steam Flow	2	0.1
Comp $A$ in Feed	$A$ Feed	25	1.5
Comp $B$ in Purge	Purge Valve	100	1.5

### 6.3.1 Change in operation condition

The  $G/H$  ratio setpoint is changed from 50/50  $G/H$  to 1/3  $G/H$ . The normalized ITAE and IAE values are shown in table 6.8 and 6.9. It can be seen that CS1 and CS2 give better ITAE and IAE value than CS0. The responses of CS0, CS1 and CS2 are shown in figure 6.4-6.6. All control structures can track  $G/H$  ratio in a monotonic manner within 5 hours. As can be seen from figures, CS1 gives more smooth results than other control structures for other control loops.

Table 6.8: Normalized ITAE of CS0, CS1 and CS2 for change in  $G/H$  ratio

ITAE	CS0	CS1	CS2
Measurements & MVs	62.10	47.15	49.75
All CVs	14.21	7.05	8.74
Important CVs	7.17	3.17	4.66

Table 6.9: Normalized IAE of CS0, CS1 and CS2 for change in  $G/H$  ratio

IAE	CS0	CS1	CS2
Measurements & MVs	59.36	48.52	51.13
All CVs	12.95	7.50	9.54
Important CVs	6.54	3.54	4.91

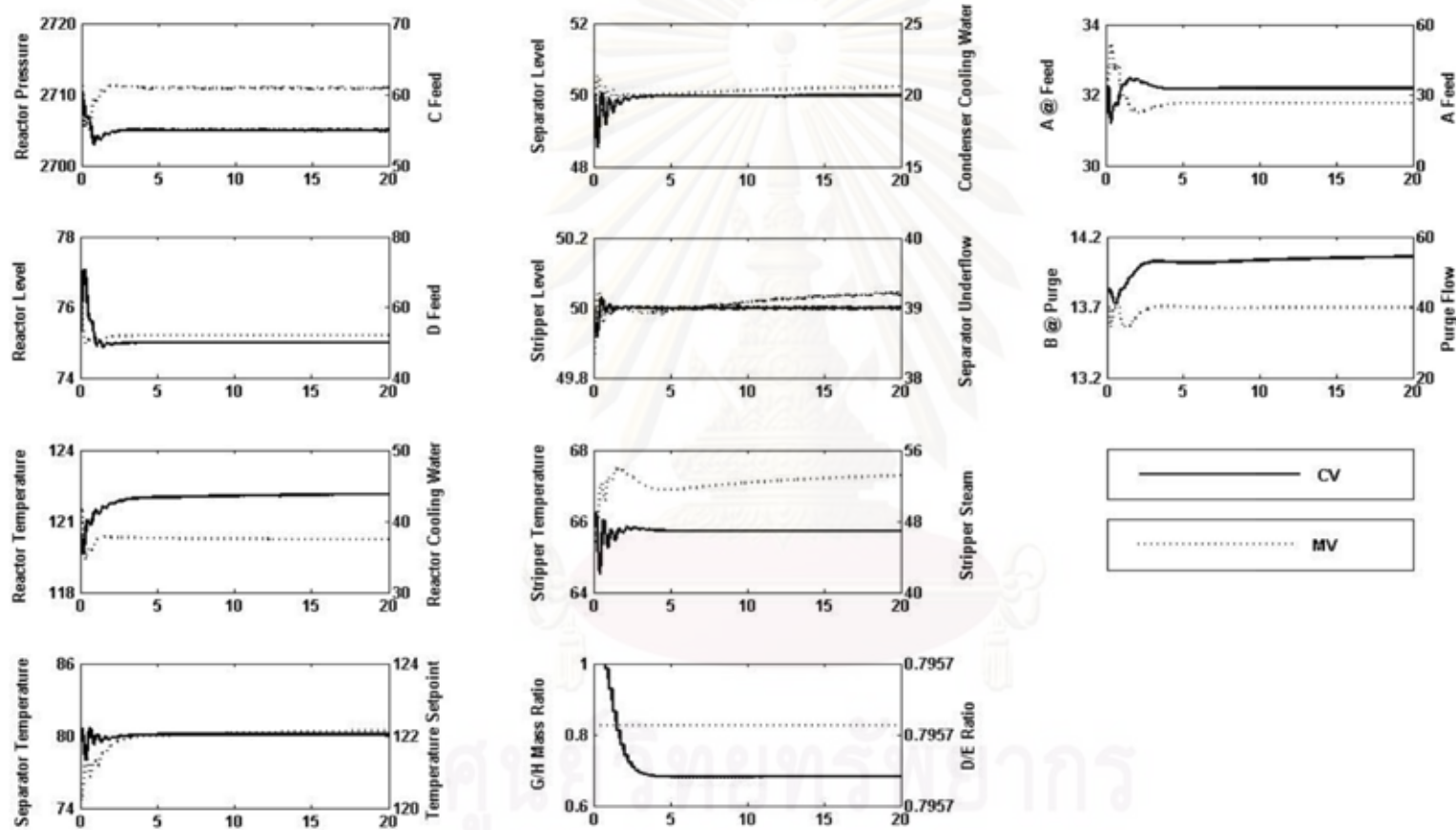


Figure 6.4 Dynamic response of CS0 for change in G/H ratio

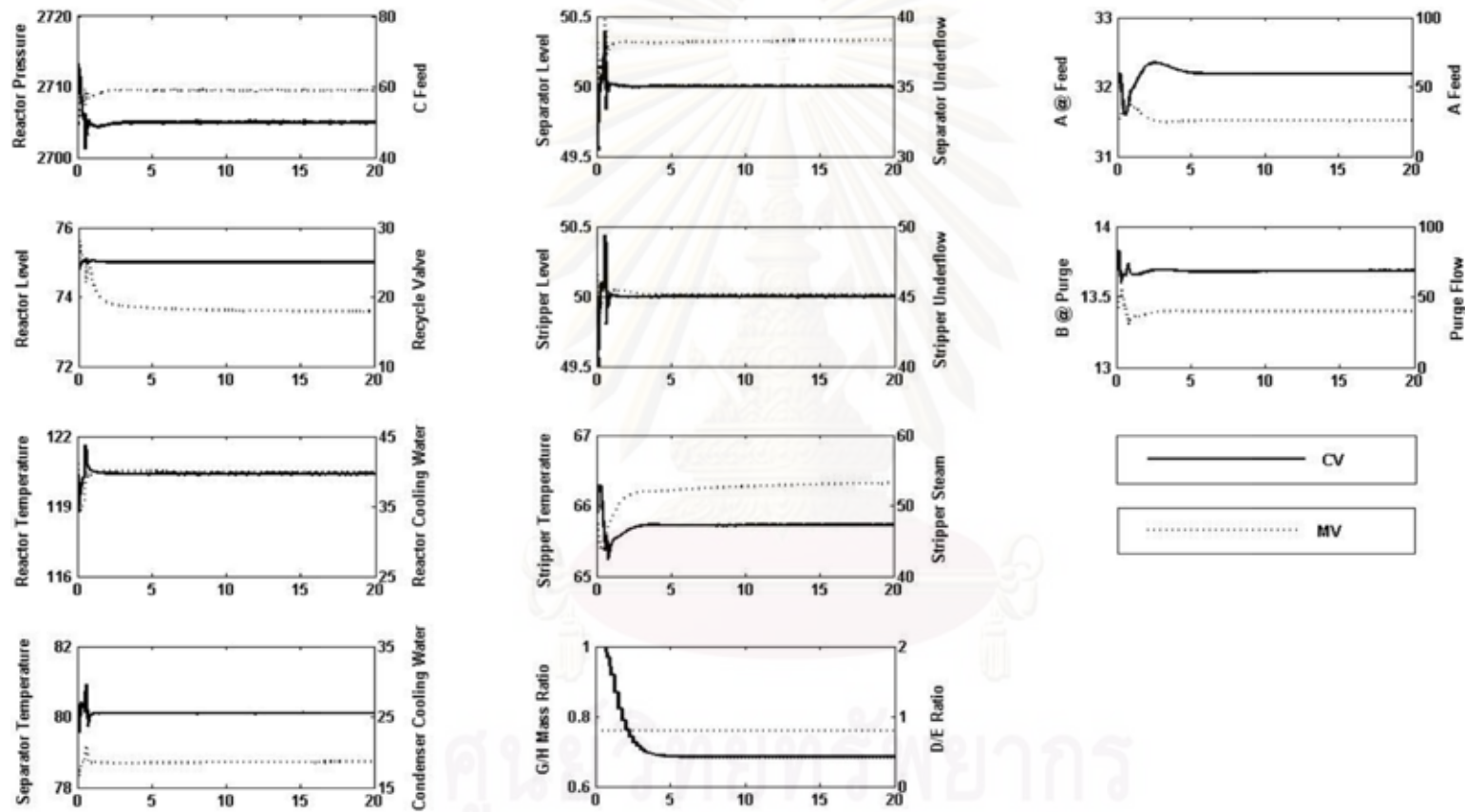


Figure 6.5 Dynamic response of CS1 for change in G/H ratio

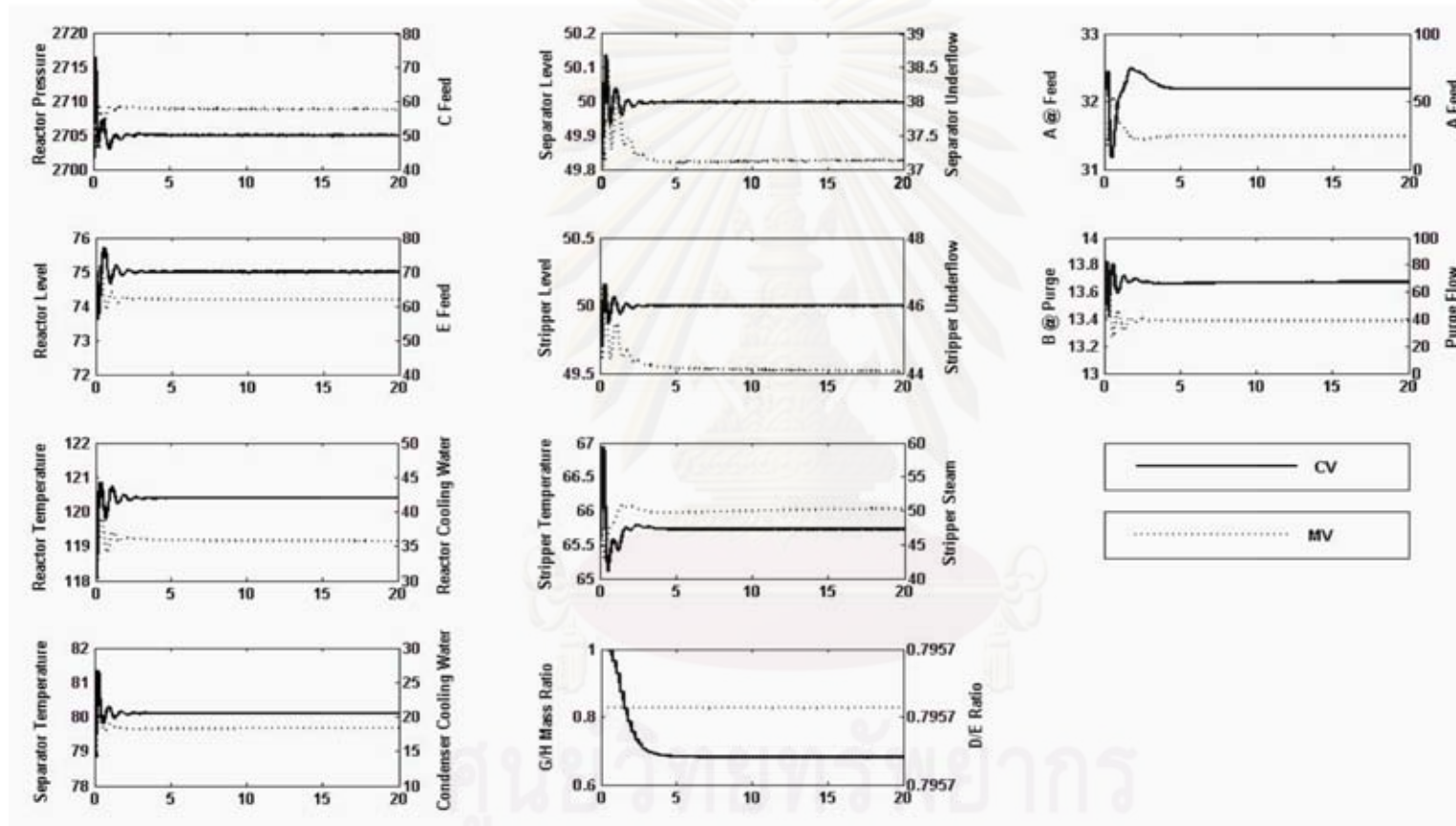


Figure 6.6 Dynamic response of CS2 for change in G/H ratio

### 6.3.2 Presence of disturbances IDV1

A change of  $A/C$  ratio in  $C$  feed (IDV1) occurs at 0.5 hour. The normalized ITAE and IAE values are shown in table 6.10 and 6.11. It can be seen that CS1 give the best ITAE and IAE in most case except that ITAE of all CVs. Figure 6.7-6.9 give the response of CS0, CS1 and CS2. As can be seen from figures, the effects of IDV1 on the  $G/H$  ratio take about 7-8 hours to die out in all control structures. In other loops, CS1 and CS2 can achieve a smooth results compared with CS0 except for product flow.

Table 6.10: Normalized ITAE of CS0, CS1 and CS2 for IDV1

ITAE	CS0	CS1	CS2
Measurements & MVs	52.20	51.89	54.91
All CVs	13.42	8.59	8.00
Important CVs	7.30	3.63	4.07

Table 6.11: Normalized IAE of CS0, CS1 and CS2 for IDV1

IAE	CS0	CS1	CS2
Measurements & MVs	52.95	50.27	55.77
All CVs	13.95	7.96	8.09
Important CVs	7.19	3.46	4.35



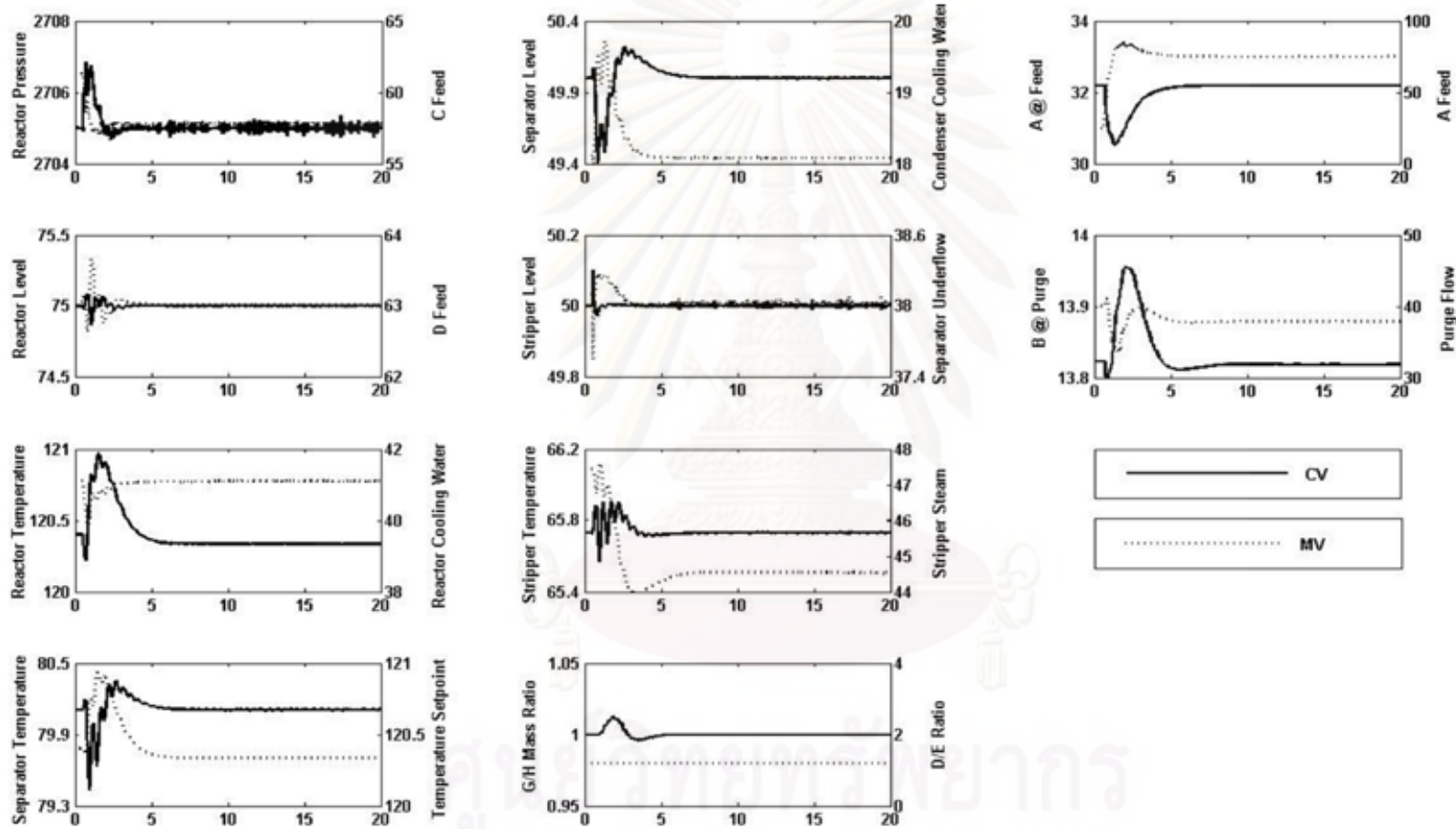


Figure 6.7 Dynamic response of CS0 for IDV1

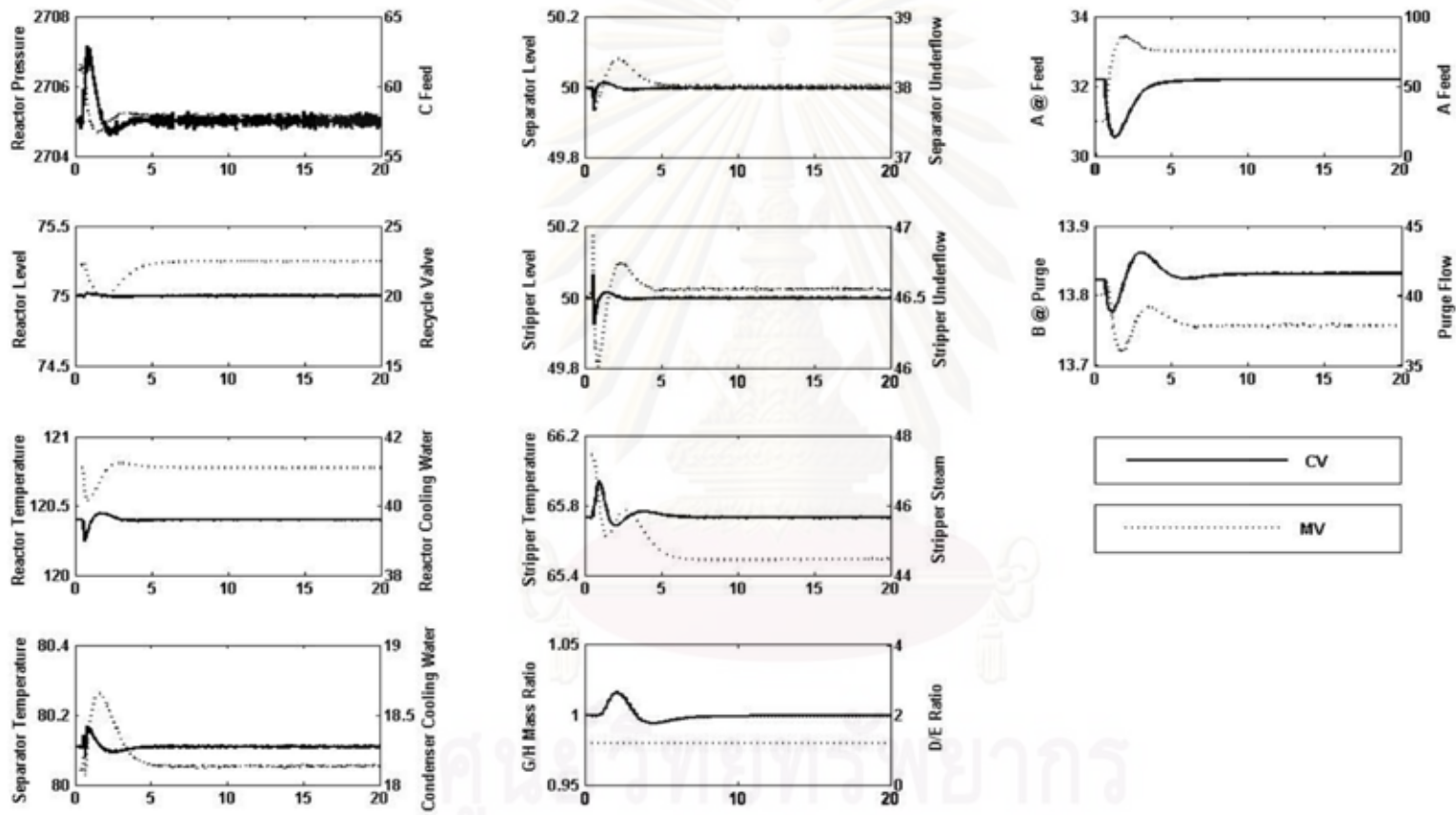


Figure 6.8 Dynamic response of CS1 for IDV1

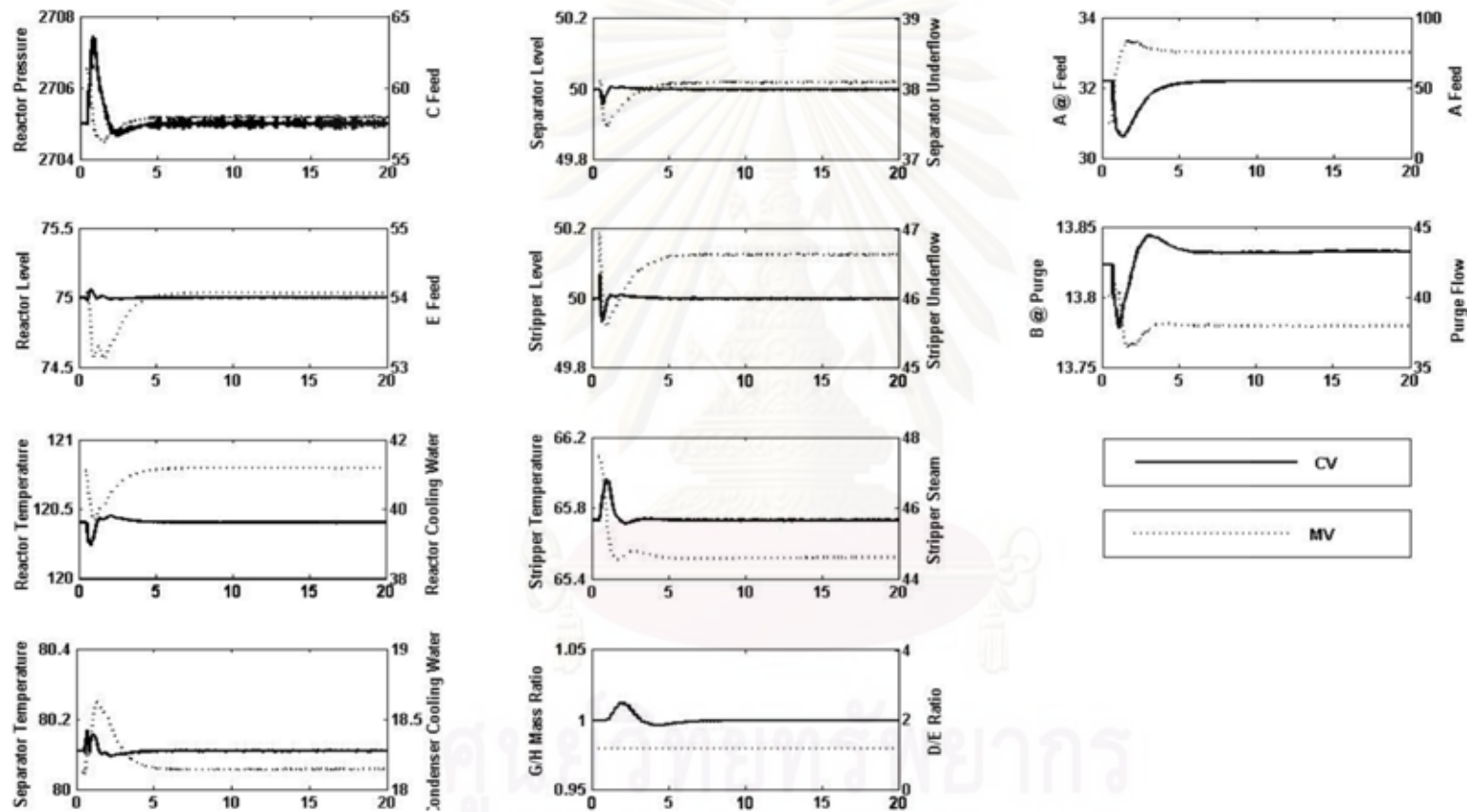


Figure 6.9 Dynamic response of CS2 for IDV1

### 6.3.3 Presence of disturbances IDV2

A change of  $B$  composition in  $C$  feed stream (IDV2) occurs at 0.5 hour. The normalized ITAE and IAE values are shown in table 6.12 and 6.13. It can be seen that CS1 give quite large IAE and ITAE in case of all measurement and MVs. However, in other cases, CS1 and CS2 give better ITAE and IAE than CS0. Figure 6.10-6.12 give the response of CS0, CS1 and CS2. When IDV2 occurs, all control structures cannot keep  $G/H$  ratio at its setpoint. CS0 gives a large change in reactor temperature while the other control structures can achieve a setpoint. This is due to using of cascade control on reactor temperature.

Table 6.12: Normalized ITAE of CS0, CS1 and CS2 for IDV2

ITAE	CS0	CS1	CS2
Measurements & MVs	50.68	61.65	46.67
All CVs	15.27	7.39	7.34
Important CVs	8.44	3.25	3.31

Table 6.13: Normalized IAE of CS0, CS1 and CS2 for IDV2

IAE	CS0	CS1	CS2
Measurements & MVs	50.30	61.17	47.53
All CVs	14.43	7.56	8.01
Important CVs	7.98	3.45	3.57

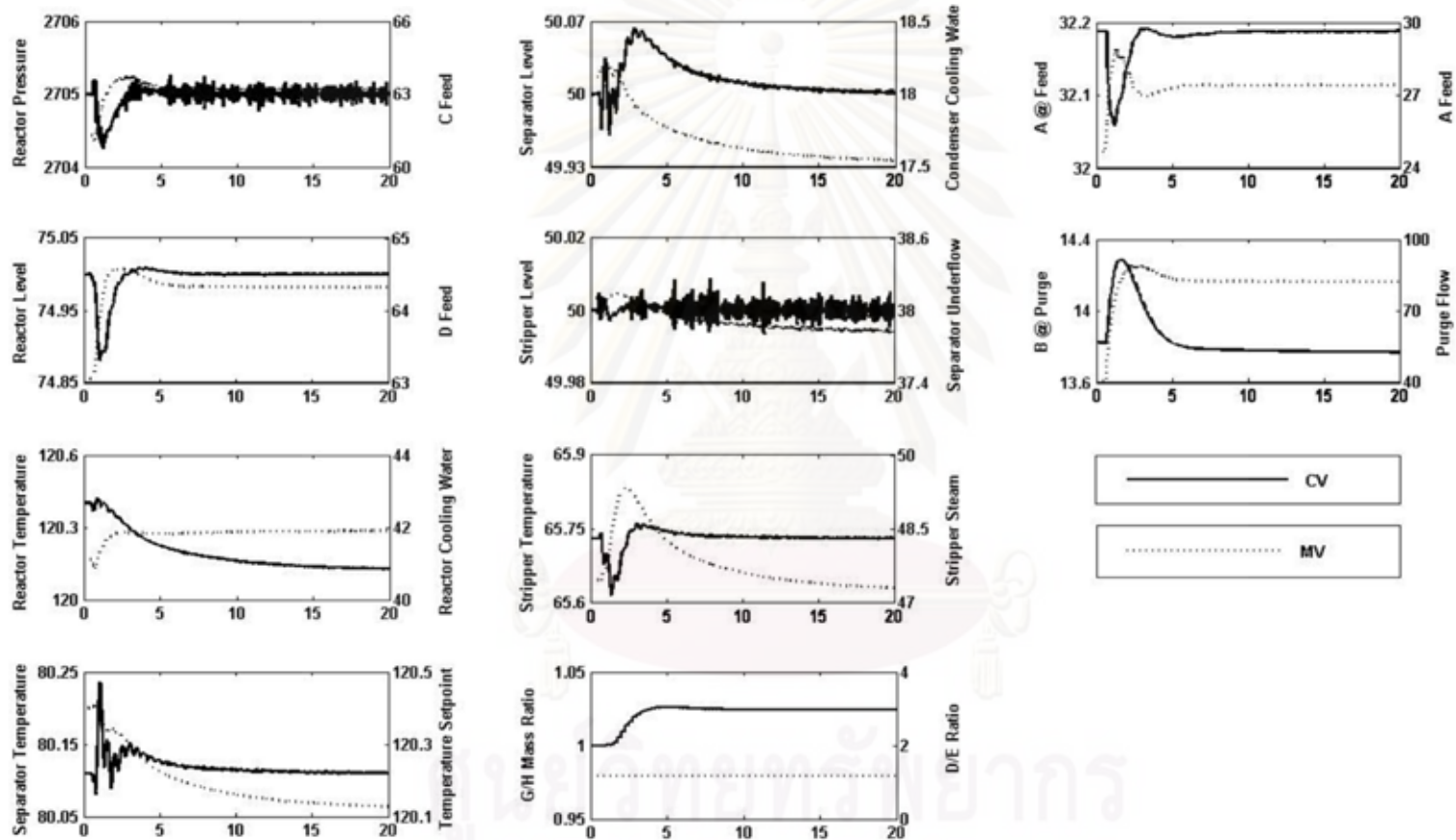


Figure 6.10 Dynamic response of CS0 for IDV2

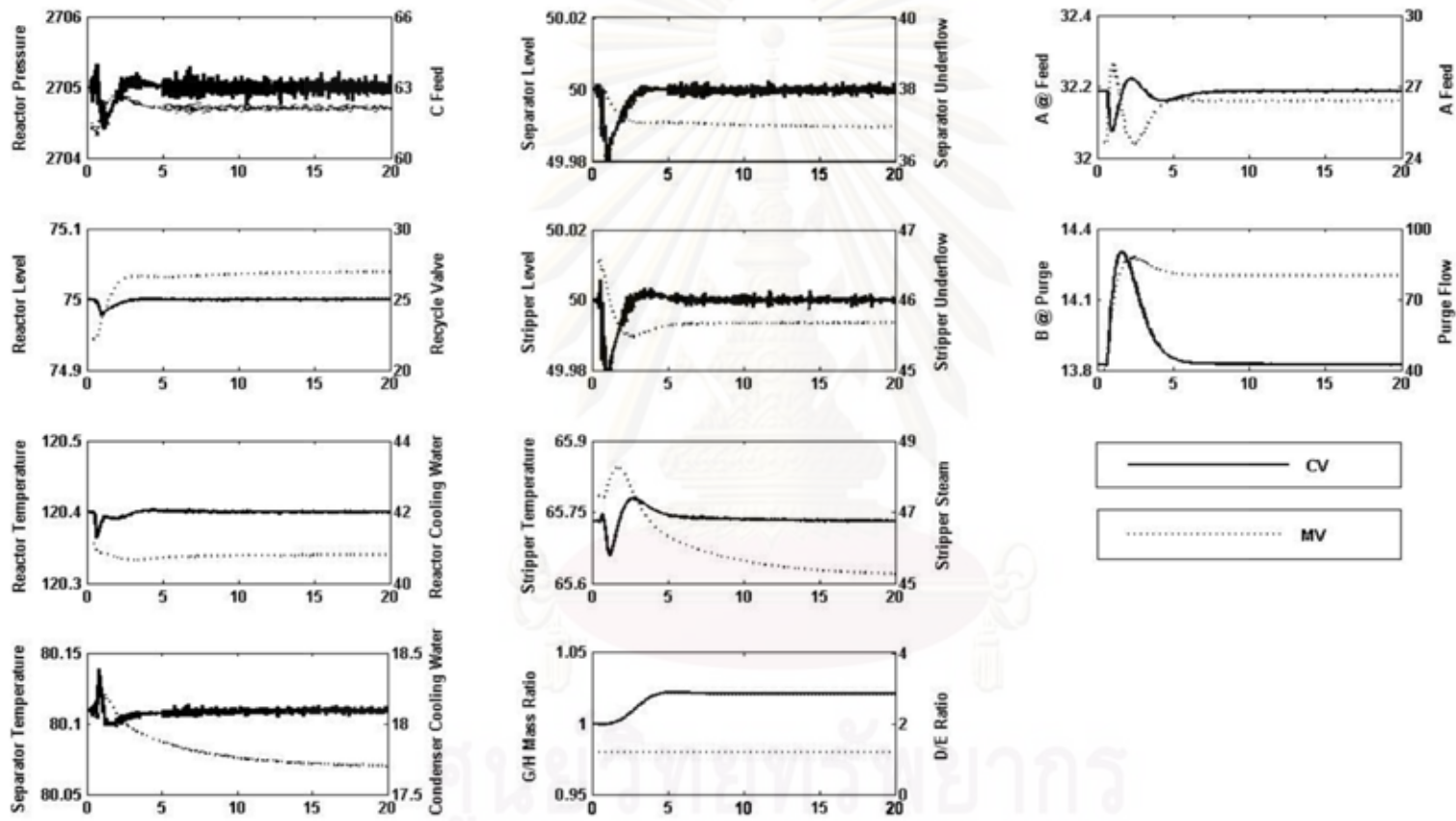


Figure 6.11 Dynamic response of CS1 for IDV2

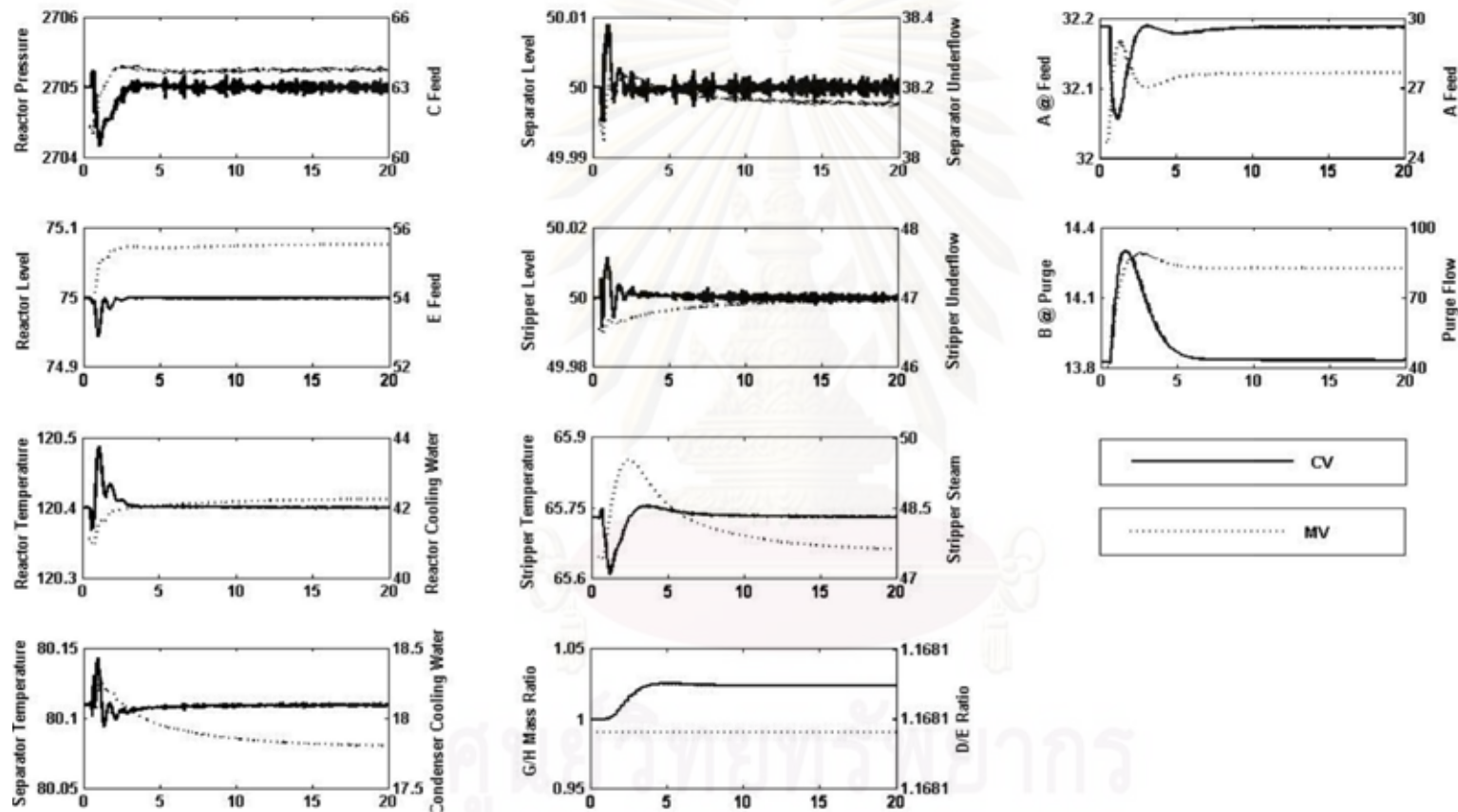


Figure 6.12 Dynamic response of CS2 for IDV2

### 6.3.4 Presence of disturbances IDV4

A change of reactor cooling water temperature (IDV4) occurs at 0.5 hour. The normalized ITAE and IAE values are shown in table 6.14 and 6.15. It can be seen that CS1 and CS2 give better ITAE and IAE than CS0 in most case. Figure 6.13-6.15 give the response of CS0, CS1 and CS2. Figures show that the effects of IDV4 take about 5-6 hours to die out in CS0 while take less than 5 hours in other control structures. Moreover, it can be noted that CS0 give more oscillation than others.

Table 6.14: Normalized ITAE of CS0, CS1 and CS2 for IDV4

ITAE	CS0	CS1	CS2
Measurements & MVs	58.06	53.62	47.32
All CVs	14.65	7.87	7.48
Important CVs	7.56	3.25	4.19

Table 6.15: Normalized IAE of CS0, CS1 and CS2 for IDV4

IAE	CS0	CS1	CS2
Measurements & MVs	52.96	55.32	50.72
All CVs	13.55	7.98	8.47
Important CVs	6.49	3.54	4.97



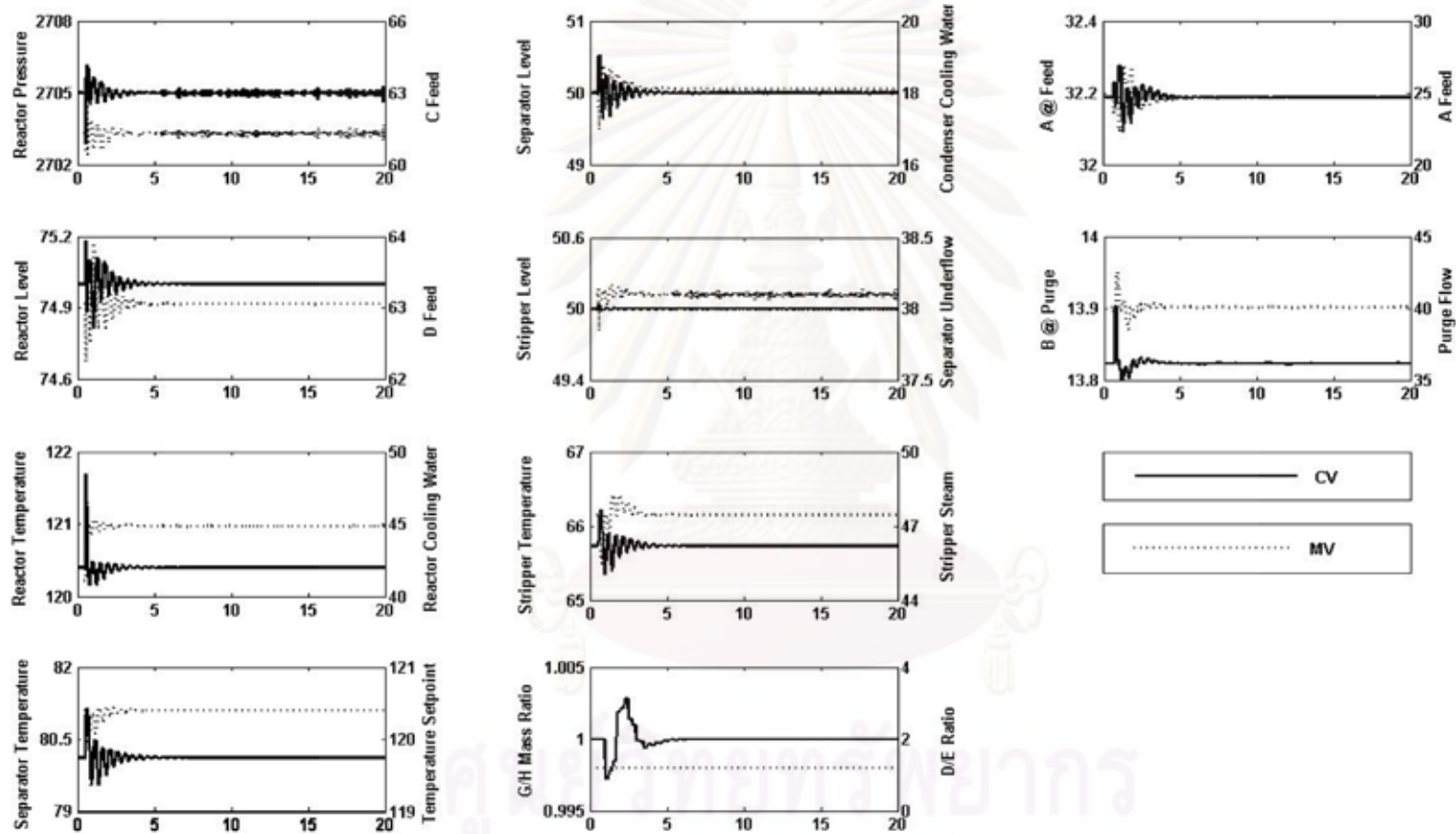


Figure 6.13 Dynamic response of CS0 for IDV4

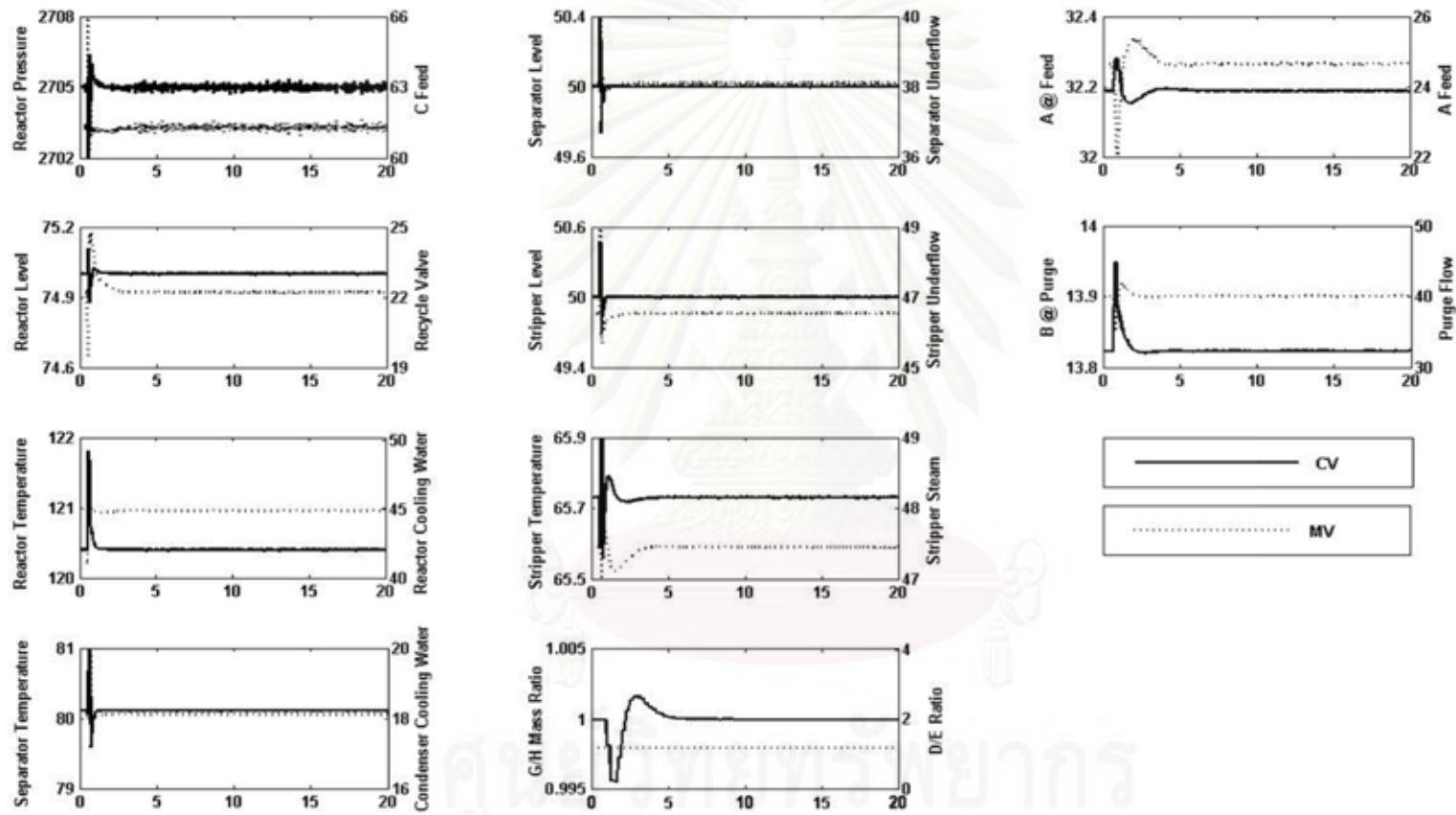


Figure 6.14 Dynamic response of CS1 for IDV4

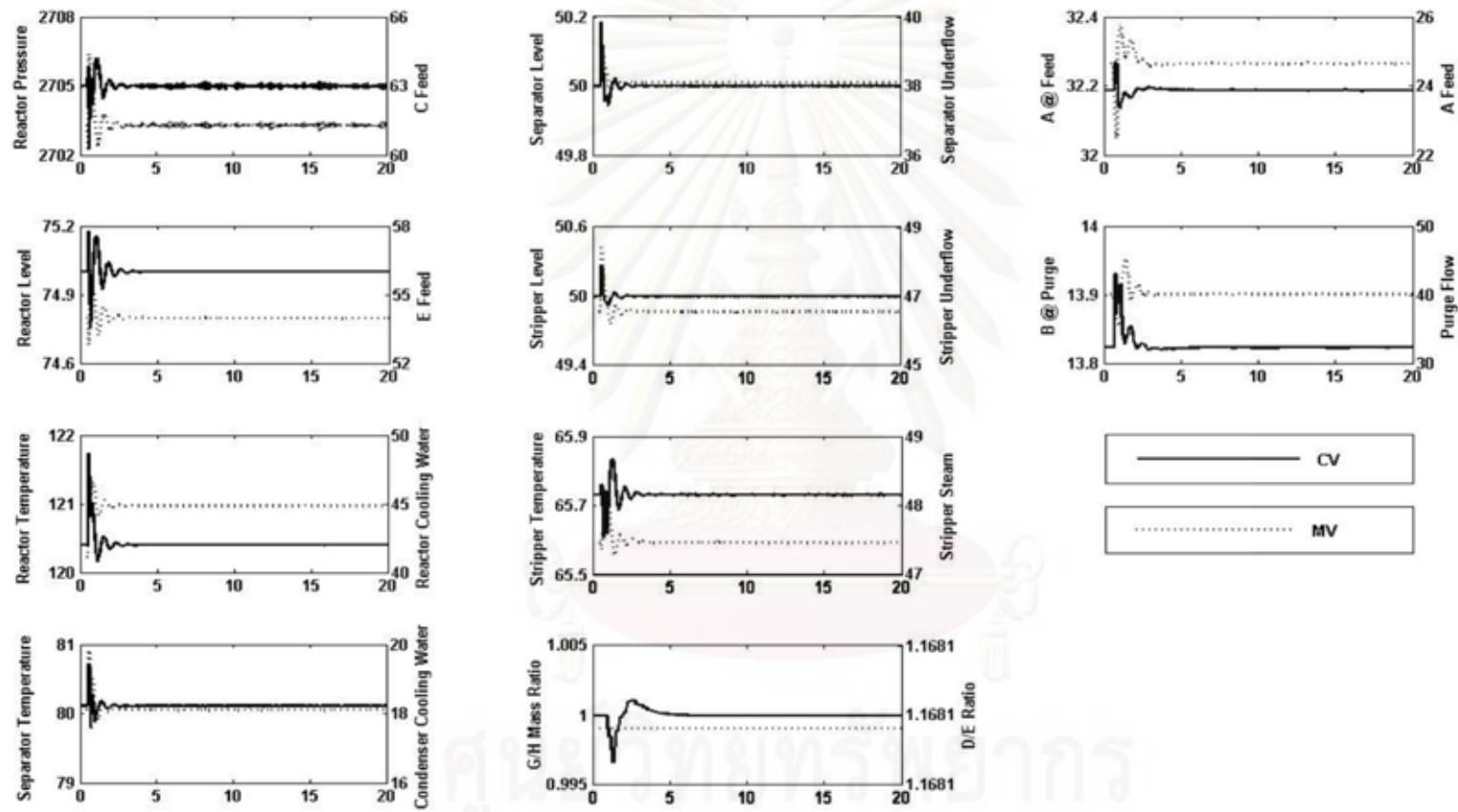


Figure 6.15 Dynamic response of CS2 for IDV4

The overall normalized ITAE and IAE re shown in table 6.16 and 6.17. It can be seen that in overall cases CS1 and CS2 give better ITAE and IAE than CS0. CS2 give the best ITAE and IAE in case of all measurements and MVs followed by CS1 and CS2 respectively. For other cases, CS1 give the best ITAE and IAE followed by CS2 and CS0. Table 6.18-6.21 show the IAE and ITAE of the measurements and manipulated variables for all cases.

Table 6.16: Overall Normalized ITAE of CS0, CS1 and CS2

ITAE	CS0	CS1	CS2
Measurements & MVs	223.04	214.32	198.64
All CVs	57.54	30.91	31.55
Important CVs	30.46	13.30	16.23

Table 6.17: Overall Normalized IAE of CS0, CS1 and CS2

IAE	CS0	CS1	CS2
Measurements & MVs	215.57	215.28	205.15
All CVs	54.89	31.00	34.11
Important CVs	28.21	13.99	17.80

## 6.4 Conclusions

In this chapter, a combined mathematic and heuristic approach for plantwide control structure design is proposed. The approach is divided into two part, 1) heuristic part and 2) mathematic part. The heuristic rules are used to select the set of CVs and MVs. The obvious control loops are also obtained by heuristic. In mathematic part, dynamic performance-based optimization is used for establishing the plantwide control structures for the remaining CVs. The optimization problem is formulated as mixed integer nonlinear programming (MINLP). The optimization conforms to the Class-2 of Stephanopoulos and Ng (2000). The TE process is selected as the testbed problem. The performances of obtained control structures are evaluated with dynamic simulation compared with Luyben's control structure. It can be seen from the dynamic response, our obtained control structures can achieve appropriate results.

Table 6.18: Normalized ITAE of all measurements for all cases

ITAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
CVs												
A Feed	1.79	1.00	0.20	1.00	1.00	1.00	1.11	0.70	1.20	1.26	1.17	0.57
D Feed	1.70	0.00	1.30	0.69	0.00	2.31	1.25	0.00	1.75	1.43	0.00	1.57
E Feed	1.06	0.99	0.95	0.69	0.00	2.31	1.25	0.00	1.75	1.43	0.00	1.57
C Feed	0.19	1.11	1.70	1.01	1.00	0.98	1.11	0.49	1.40	1.10	0.99	0.91
Recy Flow	1.81	0.51	0.68	0.97	1.53	0.50	0.21	2.37	0.43	0.83	1.44	0.73
Reac Feed	1.28	0.08	1.64	0.73	1.76	0.50	0.63	1.66	0.71	0.97	1.26	0.77
Reac Press	0.94	1.18	0.89	0.88	1.10	1.01	1.09	1.08	0.83	1.00	1.16	0.84
Reac Lev	1.46	0.29	1.24	1.47	0.74	0.78	1.95	0.53	0.52	1.73	0.37	0.91
Reac Temp	0.89	0.89	1.22	0.90	0.92	1.18	1.08	0.76	1.16	1.24	0.66	1.10
Purge Flow	0.72	0.87	1.41	1.00	1.01	1.00	1.01	0.97	1.02	0.80	1.14	1.06
Sep Temp	2.33	0.33	0.34	2.36	0.39	0.26	2.14	0.51	0.36	2.14	0.47	0.39
Sep Lev	2.76	0.12	0.12	2.61	0.19	0.19	2.68	0.18	0.13	2.17	0.41	0.41
Sep Press	0.25	2.61	0.14	0.41	2.22	0.37	0.14	2.67	0.19	0.97	1.28	0.76
Sep U Flow	1.85	1.02	0.13	1.31	1.37	0.32	0.63	2.24	0.14	1.55	0.67	0.78
Str Lev	1.12	0.69	1.19	1.43	0.67	0.90	1.63	0.70	0.67	1.42	0.65	0.94
Str Press	0.24	2.62	0.14	0.31	2.51	0.18	0.14	2.67	0.19	0.92	1.31	0.77
Str U Flow	0.72	0.67	1.62	0.42	0.38	2.20	0.41	1.39	1.20	0.11	0.98	1.91
Str Temp	1.36	0.94	0.70	1.27	1.09	0.64	0.99	1.07	0.95	1.92	0.55	0.53
Str Stm Flow	1.17	1.23	0.60	1.01	1.01	0.98	0.26	2.26	0.48	1.45	0.93	0.63
Comp Work	0.76	1.49	0.75	1.11	0.82	1.07	0.57	1.84	0.59	0.86	1.49	0.65
RCW Temp	1.18	0.82	1.00	1.58	0.19	1.23	1.36	0.38	1.26	1.43	0.64	0.93
CCW Temp	2.10	0.12	0.78	0.49	1.51	0.99	1.20	0.90	0.90	1.50	0.75	0.75
A @ Feed	0.94	1.03	1.03	0.99	1.00	1.02	0.82	1.21	0.97	1.21	1.20	0.59
B @ Feed	1.04	1.11	0.85	1.27	1.18	0.56	1.03	0.95	1.02	0.76	1.15	1.10
C @ Feed	0.90	1.18	0.92	1.36	0.53	1.11	0.79	1.38	0.83	0.60	1.49	0.91
D @ Feed	0.94	1.02	1.04	0.79	1.04	1.17	0.96	0.85	1.18	1.21	0.65	1.14
E @ Feed	0.86	1.16	0.98	1.21	0.76	1.03	0.51	1.82	0.67	0.89	1.55	0.56
F @ Feed	1.58	0.74	0.69	0.95	1.03	1.02	1.02	0.99	0.99	0.11	1.38	1.52
A @ Pur	1.08	1.08	0.84	0.99	1.01	1.00	0.90	1.23	0.87	1.05	1.27	0.68
B @ Pur	1.29	0.82	0.89	0.87	1.03	1.10	1.83	0.45	0.72	0.87	0.97	1.15
C @ Pur	0.94	1.16	0.89	1.24	0.64	1.12	0.80	1.38	0.82	0.49	1.55	0.96
D @ Pur	1.39	0.72	0.89	1.62	0.55	0.84	1.35	1.17	0.47	1.36	0.82	0.83
E @ Pur	0.80	1.22	0.98	1.22	0.74	1.03	0.41	1.99	0.60	0.89	1.55	0.56
F @ Pur	1.64	0.70	0.65	0.92	1.04	1.04	1.03	0.99	0.98	0.11	1.37	1.51
G @ Pur	0.99	1.02	0.99	1.01	0.97	1.01	0.95	1.09	0.96	1.97	0.55	0.49
H @ Pur	1.03	0.96	1.01	0.74	1.48	0.79	1.40	0.37	1.24	1.98	0.57	0.45
D @ Prod	1.58	0.55	0.87	1.06	0.95	0.99	0.25	1.97	0.78	1.00	1.14	0.86
E @ Prod	0.82	1.21	0.97	1.02	0.97	1.00	0.74	1.44	0.82	1.12	1.31	0.58
F @ Prod	1.49	0.80	0.71	0.99	1.00	1.01	1.02	1.00	0.98	0.22	1.31	1.47
G @ Prod	1.01	0.93	1.06	0.66	1.41	0.93	1.04	0.94	1.03	0.93	1.44	0.64
H @ Prod	1.22	0.63	1.15	0.62	1.47	0.91	1.07	0.89	1.05	0.94	1.41	0.65

Table 6.19: Normalized ITAE of all manipulated variables for all cases

ITAE MVs	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
D feed	1.70	0.00	1.30	0.69	0.00	2.31	1.25	0.00	1.75	1.42	0.00	1.58
E feed	1.70	0.00	1.30	0.69	0.00	2.31	1.25	0.00	1.75	1.42	0.00	1.58
A feed	1.79	1.00	0.20	1.00	1.00	1.00	1.11	0.70	1.20	1.26	1.17	0.56
C feed	0.19	1.11	1.70	1.01	1.00	0.98	1.11	0.49	1.40	0.99	1.16	0.84
Recycle	0.00	3.00	0.00	0.00	3.00	0.00	0.00	3.00	0.00	0.00	3.00	0.00
Purge	0.43	0.28	2.29	1.00	1.01	1.00	1.01	0.96	1.02	0.79	1.15	1.07
Sep Liq	1.44	0.21	1.35	1.37	1.35	0.28	0.48	2.38	0.13	1.30	0.87	0.84
Str Liq	0.00	1.11	1.89	0.00	0.68	2.32	0.00	2.09	0.91	0.00	1.21	1.79
Str Stm	1.17	1.23	0.60	1.01	1.01	0.98	0.26	2.26	0.49	1.39	0.97	0.64
RCWF	1.08	0.34	1.58	0.37	0.35	2.28	1.07	0.45	1.49	1.00	1.00	1.00
CCWF	2.26	0.48	0.26	1.24	0.80	0.96	1.33	0.96	0.71	1.62	0.68	0.69
Agi Spd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 6.20: Normalized IAE of all measurements for all cases

IAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
CVs												
A Feed	1.38	0.96	0.66	1.00	1.00	1.00	1.13	0.67	1.20	1.29	1.06	0.65
D Feed	1.65	0.01	1.35	0.65	0.00	2.35	1.28	0.00	1.72	1.12	0.00	1.88
E Feed	1.06	0.99	0.95	0.65	0.00	2.35	1.28	0.00	1.72	1.12	0.00	1.88
C Feed	0.26	1.13	1.61	1.00	1.00	1.00	1.12	0.50	1.38	1.00	0.93	1.06
Recy Flow	1.74	0.55	0.70	1.28	0.80	0.92	0.30	2.23	0.48	0.61	1.55	0.85
Reac Feed	1.22	0.22	1.56	1.02	0.97	1.00	0.60	1.72	0.68	0.53	1.95	0.52
Reac Press	0.96	0.96	1.08	0.86	1.05	1.09	1.09	0.94	0.97	0.97	1.01	1.01
Reac Lev	1.71	0.12	1.17	1.73	0.51	0.76	2.08	0.41	0.52	1.52	0.29	1.19
Reac Temp	0.77	1.02	1.21	0.94	0.87	1.18	1.13	0.61	1.26	1.05	0.73	1.22
Purge Flow	0.72	0.95	1.33	1.00	0.99	1.00	1.01	0.97	1.02	0.64	0.91	1.45
Sep Temp	1.99	0.36	0.65	2.55	0.25	0.20	2.16	0.44	0.40	2.11	0.43	0.46
Sep Lev	2.60	0.22	0.18	2.78	0.12	0.11	2.65	0.25	0.11	2.36	0.34	0.31
Sep Press	0.32	2.47	0.22	0.48	1.95	0.56	0.16	2.62	0.22	0.90	1.35	0.75
Sep U Flow	1.84	1.01	0.15	0.97	1.25	0.78	0.57	2.30	0.13	0.68	1.12	1.20
Str Lev	0.51	1.22	1.27	0.88	0.91	1.21	1.05	1.24	0.71	0.60	1.17	1.23
Str Press	0.25	2.60	0.15	0.25	2.54	0.21	0.15	2.66	0.19	0.46	2.05	0.49
Str U Flow	0.69	0.73	1.59	0.36	0.56	2.08	0.42	1.43	1.15	0.11	1.15	1.73
Str Temp	1.18	0.89	0.93	1.23	1.00	0.77	1.00	0.98	1.02	2.05	0.48	0.47
Str Stm Flow	1.19	1.19	0.62	1.01	0.99	1.00	0.48	1.79	0.73	1.75	0.75	0.50
Comp Work	0.77	1.46	0.77	0.95	1.10	0.94	0.54	1.90	0.56	0.76	1.82	0.42
RCW Temp	1.16	0.84	1.00	1.41	0.42	1.17	1.34	0.42	1.24	1.21	0.71	1.08
CCW Temp	2.03	0.18	0.79	1.03	0.94	1.03	1.11	1.05	0.83	1.29	0.97	0.74
A @ Feed	1.04	0.86	1.10	1.00	1.00	1.00	0.98	0.99	1.03	1.27	1.07	0.66
B @ Feed	0.75	1.09	1.17	1.32	1.01	0.67	1.02	0.97	1.01	0.61	0.93	1.46
C @ Feed	0.89	1.17	0.93	1.23	0.70	1.07	0.78	1.40	0.82	0.70	1.61	0.69
D @ Feed	0.94	1.02	1.04	0.99	1.02	1.00	0.98	0.84	1.17	1.04	0.60	1.35
E @ Feed	0.87	1.14	0.99	0.98	1.05	0.97	0.50	1.85	0.65	0.90	1.56	0.54
F @ Feed	1.57	0.74	0.69	1.11	0.96	0.93	1.02	0.99	0.99	0.20	1.34	1.46
A @ Pur	1.06	1.02	0.92	1.00	1.00	1.00	0.92	1.18	0.90	1.06	1.29	0.65
B @ Pur	1.21	0.85	0.93	1.27	0.88	0.85	1.24	0.81	0.95	0.64	1.09	1.27
C @ Pur	0.94	1.15	0.91	1.17	0.75	1.08	0.79	1.40	0.81	0.74	1.61	0.65
D @ Pur	1.37	0.74	0.89	1.08	1.00	0.93	1.36	1.05	0.59	1.15	0.88	0.97
E @ Pur	0.82	1.19	0.99	0.98	1.05	0.97	0.40	2.02	0.58	0.87	1.57	0.56
F @ Pur	1.64	0.70	0.65	1.10	0.96	0.94	1.03	0.99	0.98	0.24	1.33	1.43
G @ Pur	1.00	1.01	0.99	1.01	1.01	0.98	0.96	1.08	0.96	1.90	0.58	0.52
H @ Pur	1.03	0.96	1.01	1.12	1.15	0.73	1.37	0.36	1.27	1.97	0.57	0.47
D @ Prod	1.56	0.57	0.86	1.00	1.01	0.99	0.25	2.00	0.75	0.96	1.16	0.88
E @ Prod	0.84	1.19	0.97	1.00	1.01	0.99	0.74	1.45	0.81	1.25	1.31	0.44
F @ Prod	1.46	0.81	0.72	1.02	0.99	0.99	1.02	1.00	0.98	0.52	1.10	1.38
G @ Prod	0.97	1.02	1.01	0.72	1.36	0.92	1.05	0.92	1.03	0.96	1.39	0.65
H @ Prod	1.01	0.97	1.02	0.71	1.38	0.91	1.08	0.87	1.05	1.00	1.35	0.66



Table 6.21: Normalized IAE of all manipulated variables for all cases

IAE	SPChange			IDV1			IDV2			IDV4		
	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2	CS0	CS1	CS2
MVs												
D feed	1.65	0.00	1.35	0.65	0.00	2.35	1.28	0.00	1.72	1.12	0.00	1.88
E feed	1.65	0.00	1.35	0.65	0.00	2.35	1.28	0.00	1.72	1.12	0.00	1.88
A feed	1.38	0.96	0.66	1.00	1.00	1.00	1.13	0.67	1.20	1.30	1.06	0.64
C feed	0.26	1.13	1.61	1.00	1.00	1.00	1.12	0.50	1.38	0.95	0.99	1.05
Recycle	0.00	3.00	0.00	0.00	3.00	0.00	0.00	3.00	0.00	0.00	3.00	0.00
Purge	0.58	0.71	1.71	1.00	0.99	1.01	1.01	0.97	1.02	0.62	0.92	1.47
Sep Liq	1.42	0.23	1.35	1.04	1.19	0.77	0.42	2.41	0.17	0.55	1.19	1.26
Str Liq	0.00	1.14	1.86	0.00	0.82	2.18	0.00	2.17	0.83	0.00	1.27	1.73
Str Stm	1.19	1.19	0.61	1.01	0.99	1.00	0.48	1.79	0.73	1.71	0.79	0.50
RCWF	1.07	0.38	1.55	0.63	0.63	1.74	1.06	0.48	1.45	1.00	1.00	1.00
CCWF	2.22	0.48	0.30	1.41	0.80	0.79	1.33	0.96	0.70	1.50	0.63	0.86
Agi Spd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

## **CHAPTER VII**

### **SUMMARY AND CONCLUSIONS**

The new methodology for synthesizing plantwide control structure is presented in this dissertation. The combined mathematic and heuristic based approach for plantwide control structure design is proposed. The approach takes advantages of both heuristic based and mathematic based approach. Especially in mathematic part, the dynamic performance-based optimization has been proposed to establish the plantwide control structure while the heuristic rules are used for selecting CVs and MVs and for establish the obvious control loops to save computing time. The approach is investigated on the TE process. In this chapter, final summary and overall conclusions for this dissertation are discussed followed by suggestions for the future work on this study.

#### **7.1 The dynamic performance-based optimization for plantwide control structure design**

The dynamic performance-based optimization for plantwide control structure design is proposed in this dissertation. The proposed optimization problem can be categorized as Class-2 problem of uncertainties inclusion (Stephanopoulos and Ng, 2000). The treatment of uncertainties is concerned in the phase of selecting the manipulated variables. The proposed optimization problem is formulated as mixed integer nonlinear programming (MINLP). In this dissertation, the objective function is presented as an integral of the time-weighted absolute error (ITAE) of all measurements and manipulated variables in the face of disturbances. A discrete state-space model is used as the process model in the optimization problem. The integer variables appear in the selection matrix which represents the control structure of the selected process. The problem formulation has been described in

Chapter 4.

It is worthwhile to point out the main contributions of the proposed optimization problem. Firstly, our objective function is accounted on the dynamic performances of the controlled process explicitly. Secondly, our process model used in the optimization is more rigorous and accurate than some works that have been discussed above. Thirdly, our optimization problem is comprehensive and easy to solve using a commercial optimization solver (Tomlab MINLP optimization package).

In chapter 5, the dynamic performance-based optimization is adopted to establish the plantwide control structure of the TE plant. The optimization is limited to establish the control structure only for important CVs of the TE process. The important CVs are defined by those the CVs that relate directly to the process shutdown criteria. While the control structure of the other CVs are established by heuristic. In dynamic simulation, the obtained control structures are compared with Luyben's on supply control structure in the face of various situations. It can be seen that the obtained control structure give appropriate results.

## **7.2 The combined mathematic and heuristic based approach for plantwide control structure design**

This dissertation presents the combined mathematic and heuristic based approach for plantwide control structure design. The approach can be divided into two main parts: 1) heuristic and 2) mathematic. The design procedure consists of five steps as described in chapter 4. The first three steps are heuristic part while the last two steps are mathematic part. The dynamic performance-based optimization which is proposed as the optimization technique for establishing plantwide control structure is used in the fifth step of the proposed procedure. The control structure of the selected plant can be established by following the procedure step by step.

In chapter 6, the combined mathematic and heuristic based approach is used for establishing the plantwide control structure of the TE process. The set of CVs

and MVs are selected by heuristic. Two control loops: 1) reactor temperature and 2) product ratio control are preliminary closed. The remaining CVs are paired with MVs by dynamic performance-based optimization. Number of controlled variables in the optimization problem of this chapter is more than those of the previous chapter hence it take much more time to carry out the results. In dynamic simulation, the obtained control structures are compared with Luyben's on supply control structure in the face of various situations. The obtained control structures give appropriate results compared with those of Luyben.

### **7.3 Recommendation for future works**

1. Application of the combined mathematic and heuristic based approach on the alternative chemical process (e.g. hydrodealkylation (HDA) process, isomerization process)
2. Using the nonlinear process model in the optimization problem in order to increase the accuracy of the process response and the optimization results.

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## VITA

Name : Chaiyapop Siraworakun

Gender : Male

Date of Birth : 24 September 1978

### Education

B.E. in Chemical Engineering, March 2000 King Mongkut's Institute of Technology, North Bangkok



ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย