การออกแบบโครงสร้างการควบคุมและการเบ็ดเสร็จพลังงานของโรงงานอะชีโตน

นางสาวสิริกร จึงธนากรกุล

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต
สาขาวิชาวิศวกรรมเคมี ภาควิชาวิศวกรรมเคมี
คณะวิศวกรรมศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
ปีการศึกษา 2551

DESIGN OF ENERGY INTEGRATED AND CONTROL STRUCTURES OF ACETONE PLANT

Miss Sirikorn Juengtanakornkul

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering
Department of Chemical Engineering
Faculty of Engineering
Chulalongkorn University
Academic Year 2008

Thesis Title	DESIGN OF ENERGY INTEGRATED AND CONTROL STRUCTURES OF ACETONE PLANT
By	Miss Sirikorn Juengtanakornkul
Field of study	Chemical Engineering
Advisor	Assistant Professor Montree Wongsri, D.Sc.

Accepted by the Faculty of Engineering, Chulalongkorn University in Partial Fulfillment of the Requirements for the Master's Degree.

.... Dean of the Faculty of Engineering

(Associate Professor Boonsom Lerdhirunwong, Dr.Ing.)

THESIS COMMITTEE

.... Chairman

(Associate Professor Sarawut Rimdusit , Ph.D.)

Montree Wongsri

.... Advisor

(Assistant Professor Montree Wongsri, D.Sc.)

Soorathep Kheawhom

.... Examiner

(Soorathep Kheawhom, Ph.D.)

.... External Examiner

(Phisit Jaisathaporn, Ph.D.)

สิริกร จึงธนากรกุล: การออกแบบโครงสร้างการควบคุมและการเบ็ดเสร็จพลังงานของโรงงานอะซีโตน. (DESIGN OF ENERGY INTEGRATED AND CONTROL STRUCTURES OF ACETONE PLANT) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ผู้ช่วยศาสตราจารย์ ดร. มนตรี วงศ์ศรี, 130 หน้า.

ในปัจจุบัน กระบวนการทางเคมีมีความซับซ้อนมากยิ่งขึ้น เนื่องมาจากภายในกระบวนการประกอบไปด้วยสายป้อนกลับ การนำพลังงานมาใช้ใหม่ หรือ อุปกรณ์ชนิดต่างๆที่มีมากขึ้น โดยทั่วไปโรงงานเคมีจะประกอบด้วย 2 ส่วน คือ ส่วนของการทำปฏิกิริยา และส่วนของการแยกสาร ซึ่งทั้งสองส่วนนี้จำเป็นต้องมีการควบคุม เพื่อความปลอดภัยและได้ผลประโยชน์สูงสุด งานวิจัยนี้จึงนำเสนอข่ายงานเครื่องแลกเปลี่ยนความร้อนแบบยืดหยุ่น 3 ทางเลือก และโครงสร้างการควบคุม 3 ทางเลือกสำหรับกระบวนการผลิตอะซีโตน โครงสร้างการควบคุมของกระบวนถูกออกแบบโดยการใช้วิธีการส่งผ่านความแปรปรวนของ (Wongsri, 1990) และเส้นทางการส่งผ่านความร้อนโดย (Wongsri และ Hermawan, 2005) เพื่อให้ได้ซึ่งการนำกลับมวลสารมาใช้ใหม่ในพลวัตสูงสุด งานวิจัยนี้ใช้โปรแกรมไฮซีสในการประเมินสมรรถนะของข่ายงานเครื่องแลกเปลี่ยนความร้อนและโครงสร้างการควบคุม ผลการทดลองพบว่า การเบ็ดเสร็จด้านพลังงานทางเลือกที่ 2 สามารถประหยัดพลังงานได้ 81.49% และโครงสร้างการควบคุมแบบที่ 2 เป็นโครงสร้างที่ดีที่สุดในการจำกัดตัวแปรรบกวน

ภาควิชา........วิศวกรรมเคมี........ ลายมือชื่อนิสิต.......สิริกร จึงธนากรกุล..............................
สาขาวิชา......วิศวกรรมเคมี........ ลายมือชื่ออ.ที่ปรึกษาวิทยานิพนธ์หลัก..................................
ปีการศึกษา.........2551............

##5070422021 : MAJOR CHEMICAL ENGINEERING

KEYWORDS : HEAT INTEGRATED/ACETONE PROCESS / PLANTWIDE CONTROL STRUCTURE

SIRIKORN JUENGTANAKORNKUL: DESIGN OF ENERGY INTEGRATED AND CONTROL STRUCTURES OF ACETONE PLANT. ADVISOR: ASSISTANT PROFESSOR MONTREE WONGSRI, D.Sc., 130 pp.

At present, the chemical processes have very complex flowsheet with recycle stream, energy integration and different unit operations. Generally, a chemical plant consists of reaction sections and separation section. Both sections need to control system for the safety and economical in plant. This work presents the new heat exchanger 3 networks and 3 alternatives of control structure for acetone plant. Heat exchanger network (HEN) are modified in traditional process for energy saving. The plantwide control structures are designed by using the disturbance load propagation method (Wongsri, M., 1990) and heat pathway heuristics (Wongsri, M. and Hermawan Y.D., 2005) to achieve dynamic maximum energy recovery (DMER). In this work, HYSYS is evaluated performances of the heat exchanger networks and control structures. The result shows that alternative 2 can save energy 81.49 % and CS2 is the best control structure for controlling disturbance.

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

Student's Signature Sirikorn Juengtanakornkul
Advisor's Signature M. Wongsri

ACKNOWLEDGEMENTS

Foremost, I would like to express my most sincere thanks to my advisor, Assistant Professor Montri Wongsri, for his guidance and support. Special thanks belong to Associate Professor Sarawut Rimdusit, Dr. Soorathep Kheawhom and Dr. Pisit Jaisathaporn for kindly serving as my committee members.

Many thanks for all of the members in the process control laboratory and friends who have contributed to the contributed to the accomplishment of the work. I would like to express my gratitude to all those who encouraged over the years of my study at Chulalongkorn University.

Finally, I would like to express the highest gratitude to all of family for their love, inspiration, encouragement and financial support throughout this study.

CONTENTS

page

CHAPTER

page

CHAPTER

LIST OF TABLES

LIST OF FIGURES

page

CHAPTER I

INTRODUCTION

This chapter is an introduction of this research. It consists of importance and reasons for research, objectives of the research, scopes of research, contributions of research, research procedures and research contents.

1.1 Importance and Reasons for Research

In the chemical industries, the capital cost of product varies all expenses which come from fixed cost, direct production cost for raw materials, maintenance, labor and utilities. Thus, the operator should think how to safe cost and get high benefit so heat exchanger network is another choice to save energy in many industries. In all processes, the resilient heat exchanger network is usually used because it can support the fluctuation in operating conditions while still maintaining acceptable performance. The problem of control structure of heat exchanger network is how to control process to its target temperature so heat pathways are used to control heat exchanger network when disturbance occurs. To reduce the number of heat exchangers in process, match patterns and disturbance load propagation method (Wongsri, 1990) is used for match streams.

In general, the process in all plants do not have single process or have only single unit operation separated from other process but they are complicated process flowsheet with several recycle streams, energy integration, and many different unit operations. The process should operate under the design condition, use little energy, low waste production and meet the required specification of products. The quality should not higher or lower than the specification of the product. In the real situation, the process will not operate smoothly. All factors do not meet the design conditions. The process always changes due to disturbance from the external factors and the internal factor. It is necessary to have the control system to control the condition and compensate for any deviation occurred. An effective designed structure can achieve the control objective to reduce the cost of production and operate the process within safety and environmental constraints. There are many ways to control process but in this work luyben heuristic design method (1998) and fixture point method are used to solve these problems.

The goal of this work is to use plantwide control strategies to develop the new control structures for the acetone process with energy integration schemes that are designed to achieve the control objective and reduce the cost of production. The performances of control structures are evaluated via commercial software HYSYS.

1.2 Objectives of the research

The objectives of this work are listed below:

1. To simulate acetone process both steady state and dynamics conditions by using hysys simulator.
2. To design heat exchanger networks of acetone plant using disturbance load propagation method (Wongsri, 1990)
3. To design control structures for heat exchanger networks with heat integrated process structures.
4. To evaluate dynamic performance of designed control structures.

1.3 Scopes of the research

The scope of this work are listed below:

1. The simulator of this research is hysys simulators.
2. The description of acetone process is given by Richard Turton (1998).
3. The target for design heat exchanger net work is to achieve maximum energy recovery or the minimum utility requirement.
4. The number of design heat exchanger network in acetone plant is 3 alternatives.
5. The control structures for acetone process are designed by using Luyben's heuristics method for 1 alternative and using fixture point method for 2 alternatives.

1.4 Contributions of the research

The contributions of this work are as follows:

1. The new plantwide control structures for acetone process.
2. The new heat-integrated processes (HIPs) structures for acetone process.

1.5 Research procedures

1. Study of plantwide process control theory, the acetone plant and concerned in formation.
2. Study and design heat exchanger networks of the acetone plant by using HEN heristics.
3. Design heat exchanger networks and control structures.
4. Steady state modeling and simulation of heat exchanger networks of the acetone plant.

5. Study of dynamic modeling and simulation of the heat exchanger network in acetone plant with no energy integation.
6. Design of control structures for heat exchanger network in acetone plant.
7. Dynamic simulation for the energy-integrated acetone plant with control structures design.
8. Assessment of the dynamic performance of the control structure.
9. Analysis of the design and simulation results.
10. Conclusion of the thesis.

1.6 Research Contents

This thesis is divided into six chapters.

Chapter I is an introduction to this research. This chapter consists of research objectives, scopes of the research, contributions of the research, research procedures and research contents.

Chapter II reviews the work carried out on heat exchanger networks (HENs) design, heat integrated processes and plantwide control design.

Chapter III cover some background information of heat exchanger network design, disturbance transfer technique plantwide (Wongsri, 1990) and theory concerning with plantwide control.

Chapter IV describes the process description and the design of heat exchanger networks for the typical of acetone plant.

Chapter V the strategy to design of heat integrated plant (HIP) of acetone process is proposed.

Chapter VI the overall conclusions and recommendations of this thesis are discussed.

CHAPTER II

LITERATURE REVIEW

Our purpose of this chapter is to present a review of the previous work on the conceptual design of chemical process, heat exchanger networks (HENs) and plantwide control design.

2.1 Conceptual Design

A synthesis/analysis procedure for developing first flowsheets and base case designs has been established by Douglas (1985). The procedure is described in terms of a hierarchy of decision levels, as follows:

1. Batch versus continuous
2. Input-output structure of the flowsheet
3. Recycle structure of the flowsheet
4. Separation system specification, including vapor and liquid recovery system
5. Heat exchanger network(HEN)

Douglas (1985) considered a continuous process for producing benzene by hydrodealkylation of toluene (HDA process) to illustrate the procedure. The complete process is always considered at each decision level, but additional fine structure is added to the flowsheet as he proceeds to the later decision level. Each decision level terminates in an economic analysis. Experience indicates that less than one percent of the ideals for new designs are ever commercialized, and therefore it is highly desirable to discard poor projects quickly. Similarly, the later level decisions are guided by the economic analysis of the early level decisions.

In a series of papers, Fisher et al. (1988 a, b, c) presented a study of the interface between design and control including process controllability, process operability and selecting a set of controlled variables. At the preliminary stages of a process design, most plants are uncontrollable. That is normally there are not enough manipulative variables in the flowsheet to be able to satisfy all of the process constraints and to optimize all of the operating variables as disturbances enter the plant. In order to develop a systematic procedure for controllability analysis, Fisher et al. (1988a) used the design decision hierarchy described by Douglas (1985) as the decomposition procedure and considered HDA process as a case study. Where at some levels, that are level 1, 2 and 3, the process is uncontrollable, but controllable at level 4 and level 5. If the available manipulated variables are compared with the constraints and operating variables introduced at each level, the preliminary controllability criterion can often be satisfied.

Terrill and Douglas (1988) have studied HDA process from a steady state point of view and determined that the process can be held very close to its optimum for a variety of expected load disturbances by using the following strategy: (1) Fix the flow of recycle gas through the compressor at its maximum value, (2) Hold a constant heat input flowrate in the stabilizer, (3) Eliminate the reflux entirely in the recycle column, (4) Maintain a constant hydrogen-to-aromatic ratio in the reactor inlet by adjusting hydrogen fresh feed, (5) Hold the recycle toluene flowrate constant by adjusting fuel to the furnace, (6) Hold the temperature of the cooling water leaving the partial condenser constant.

Downs and Vogel (1993) described a model of an industrial chemical process for the purpose of developing, studying and evaluating process control technology. It consisted of a reactor/separator/recycle arrangement involving two simultaneous gas-liquid exothermic reactions. This process was well suited for a wide variety of studies including both plantwide control and multivariable control problems.

Tyreus and Luyben (1993) considered second order kinetics with two fresh feed makeup streams. Two cases are considered: (1) instantaneous and complete one pass conversion of one of the two components in the reactor so there is an excess of only one component that must be recycled and (2) incomplete conversion per pass so there are two recycle streams. It is shown that the generic liquid-recycle rule proposed by Luyben applies in both of these cases: ”snow-balling” is prevented by fixed the flowrate somewhere in the recycle system. An additional generic rule is proposed fresh feed makeup of any component cannot be fixed unless the component undergoes complete single-pass conversion. In the complete on-pass conversion case, throughput can be set by to fix the flowrate of the limiting reactant. The makeup of the other reactant should be set by level control in the reflux drum of the distillation column.

2.2 Heat Exchanger Networks (HENs)

Marselle et al. (1982) addressed the problem of synthesizing heat recovery networks, where the inlet temperatures vary within given ranges and presented the design procedure for a flexible HEN by finding the optimal network structures for four selected extreme operating conditions separately. The specified worst cases of operating conditions are the maximum heating, the maximum cooling, the maximum total exchange and the minimum total exchange. The network configurations of each worst condition are generated and combined by a designer to obtain the final design. The strategy is to derive similar design in order to have as many common units as possible in order to minimize number of units.

Linhoff and Hindmarsh (1983) presented a novel method for the design of HEN. The method is the first to combine suffcient simplicity to be used by hand with near certainty to identify ”best” designs, even for large problems. Best design features the highest degree of energy recovery possible with a given number of capital items. Moreover, they feature network patterns required for good controllability, plant layout, intrinsic safety, etc. Typically, 20-30 percent energy savings, coupled with capital saving, can be realized in state of the art flowsheets by improved HEN design. The task involves the placement of process and utility heat exchangers to heat and cool process streams from specified supply to specified target temperatures.

Linhoff, Dunford and Smith (1983) studied heat integration of distillation columns into overall process. This study reveals that good integration between distillation and the overall process can result in column operating at effectively zero utility cost. Generally, the good integration is when the integration as column not crossing heat recovery pinches of the process and either the reboiler or the condenser being integrated with the process. If these criteria can be met, energy cost for distillation can effectively be zero.

Saboo and Morari (1983) classified flexible HENs into two classes according to the kind and magnitude of disturbances that effect the pinch location. For the temperature variation, they show that if the MER can be expressed explicitly as a function of stream supply and target conditions the problem belongs to Class I, i.e. the case that small variations in inlet temperatures do not affect the pinch temperature location. If an explicit function for the minimum utility requirement valid over the whole disturbance range does not exist, the problem is of Class II, i.e. the case that large changes in inlet temperature of flowrate variations cause the discrete changes in pinch temperature locations.

Calandranis and Stephanopoulos (1988) proposed a new approach to address the following problems: design the configuration of control loops in a network of heat exchangers and sequence the control action of the loops, to accommodate set point changes and reject load disturbances. The approach proposed exploits the structure characteristics of a HEN by identifying routes through the HEN structure that can allocate load (disturbances, or set point changes) to available sinks (external coolers or heaters). They also discussed several design issues such as the placement of bypass lines and the restrictions imposed by the existence of a process pinch. An online, real-time planning of control actions is the essence of implementation strategies generated by an expert controller, which selects path through the HEN is to be used for each entering disturbance or set point change, and what loops should be activated (and in what sequence) to carry the associated load (disturbance or set point change) to a utility unit.

Ploypaisansang A., (2003) presented to redesign six alternatives for HDA process to be the resiliency networks for maintain the target temperature and also achieve maximum energy recovery (MER). The best resilient network is selected by to trade-off between cost and resiliency. The auxiliary unit should be added in the network for cope safely with the variations and easy to design control structure to the network.

2.3 Design and Control of Heat-Integrated Process

In the last few decades, Douglas, Orcutt, and Berthiaume (1962) studied design and control of feed-effuent heat exchanger - reactor systems. They obtained a simultaneous solution of the steady state heat and material balances for a first order reaction occurring in the system and used it to calculate the values of exchanger and reactor lengths that minimized the equipment cost of the system. A dynamic study indicated that the desired steady state conditions were metsable. However, proportional controller could be used to stabilize the process.

Handogo and Luyben(1987) studied the dynamics and control of a heat-integrated reactor/column system. An exothermic reactor was the heat source, and a distillation column reboiler was the heat sink. Two types of heat-integrated system were examined: indirect and direct heat integration. Both indirect and direct heat-integration systems are found in industry. In the indirect heat-integration system, steam generation was used to cool the reactor, and the steam was used as the heating medium for the reboiler. The direct heat-integration system used the reactor fluid to directly heat the column reboiler. The indirect heat-integration system was found to have several advantages over the direct heat-integration system in terms of its dynamic performance. Both systems were operable for both large and small temperature differences between the reactor and column base. Somewhat unexpectedly, the heat-integration system with a small temperature difference was found to be more controllable than a system with a larger temperature difference. However, the cost of the heat exchanger increased rapidly as the temperature difference decreased. An important thing in this study is how to solve some of control diffculties in the process associated with heat integration schemes. They suggested adding auxiliary utility coolers and reboilers to the process.

Wongsri (1990) studied a resilient HENs design. He presented a simple but effective systematic synthesis procedure for the design of resilient HEN. His heuristic design procedure is used to design or synthesize HENs with pre-specified resiliency. It used physical and heuristic knowledge in finding resilient HEN structures. The design must not only feature minimum cost, but must also be able cope with fluctuation or changers in operating conditions. A resilient HEN synthesis procedure was developed based on the match pattern design and a physical understanding of the disturbances propagation concept. The disturbance load propagation technique was developed from the shift approach and was used in a systematic synthesis method. The design condition was selected to be the minimum heat load condition for easy accounting and interpretation. This is a condition where all process streams are at their minimum heat loads.

Luyben and Luyben (1995) examined the plantwide design and control of a complex process. The plant contains two reactions steps, three distillation columns, two recycle streams, and six chemical components. Two methods, a heuristic design procedure and a nonlinear optimization, have been used to determine an approximate economically optimal steady state design. The designs differ substantially in terms of the purities and flowrates of the recycle streams. The total annual cost of the nonlinear optimization design i2 about 20 percent less than the cost of the heuristic design. An analysis has also been done to examine the sensitivity to design parameters and specifications. Two effect control strategies have been developed using guidelines from previous plantwide control studies; both require reactor composition control as well as flow control of a stream somewhere in each recycle loop. Several alternative control strategies that might initially have seemed obvious do not work.

Jones and Wilson (1997) considered the range ability of flows in the bypass line of heat exchanger through interesting heat exchanger problems. Diffculty is immediately encountered when considering heat exchanger between two process streams; changing the flowrate of one will certainly affect the exit temperature of the other. Unfortunately, interfering with a process stream flowrate immediately upsets the plant mass balance, which is undesirable. The diffculty is overcome by using a bypass that does not affect the total flowrate but changes the proportion actually passing through the heat exchanger and hence the heat transfer. Good engineering practice would maintain a minimum flowrate of 5-10 percent through the bypass. This bypass is expected to be able to handle disturbances.

Chen and Yu (2003) proposed systematic approach to complex FEHE schemes. Because a loss of controllability come the positive feedback loop, several design parameters were studied, and the design heuristic were proposed to give more controllable heat integration schemes. They used two examples, a simple two-FEHE example and an HDA process example to illustrate the assessment of controllability based on process flowsheet. The results showed that, contrary to expectations, some complex heat-integrated reactor design alternatives (e.g., alternative 6 of HDA example) were indeed more controllable than some of the simpler heat-integration schemes (e.g., alternative 1). The increased number of FEHEs allows for a greater number of candidate manipulated inputs and thus provides opportunities for multivariable control.

Wongsri and Hermawan (2005) studied the control strategies for energy-integrated HDA plant (i.e. alternatives 1 and 6) based on the heat pathway heuristics (HPH), i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the dynamic MER can be achieved with some trade-off. In they work, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network. The new control structure with the LSS has been applied in the HDA plant alternatives 1 and 6. The designed control structure is evaluated based on the rigorous dynamic simulation using the commercial software HYSYS. The study reveals that, by selecting an appropriate heat pathway through the network, the utility consumptions can be reduced according to the input heat load disturbances; hence the dynamic MER can be achieved.

Kunajitpimol (2006) presented the resilient heat exchanger networks to achieve dynamic maximum energy recovery, plantwide control structures, and control strategies are designed for Butane Isomerization plant. The control difficulties associated with heat integration are solved by adding auxiliary utilities which is kept minimal. Four alternatives of heat exchanger networks (HEN) designs of the Butane Isomerization plant are proposed. They used the heat from the reactor effluent stream to provide the heat for the column reboiler. The energy saved is 24.88 % from the design without heat integration, but the additional capital is 0.67% due to adding of a process to process exchanger and an auxiliary utility exchanger to the process. The plantwide control configuration of heat-integrated plant is designed following Luyben's heuristic method. Various heat pathways throughout the network designed using Wongsri's disturbance propagation method to achieve DMER.

CHAPTER III

THEORY

A typical chemical plant flowsheet has a mixture of multiple units connected both in series and parallel that consist of reaction sections, separation sections and heat exchanger network. So plantwide process control involves the system and strategies required to control entire plant consisting of many interconnected unit operations.

3.1 Integrated Process

Three basic features of integrated chemical process lie at the root of our need to consider the entire plant's control system: the effect of material recycle, the effect of energy integration, and the need to account for chemical component inventories.

3.1.1 Material Recycles

Material is recycled for six basic and important reasons.

1. 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.

2. 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. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

3. Improve yields

   In reaction system such as A → B → C, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much of the undesirable product C. Therefore the concentration of B is kept fairly low in the reactor and a large recycle of A is required.

4. 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 (an excess of one reactant or a product) so that the reactor temperature increase will not be too large. High temperature can potentially create several unpleasant events: it can lead to thermal runaways, it can deactivate catalysts, it can cause undesirable side reactions, it can cause mechanical failure of equipment, etc. So the heat of reaction is absorbed by the sensible heat required to rise the temperature of the excess material in the stream flowing through the reactor.

5. Prevent side reactions

   A large excess of one of the reactants is often used so 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 product components in the reactor effluent stream and recycled back to the reactor.

6. Control properties

   In many polymerization reactors, conversion of monomer is limited to achieve the desired polymer properties. These include average molecular weight, 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.

3.1.2 Energy Integration

The fundamental reason for the use of energy integration is to improve the thermodynamics efficiency of the process. This translates into a reduction in utility cost.

3.1.3 Chemical Component Inventories

In chemical processes can characterize a plant's chemical species into three types: reactants, products, and inert. The real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every molecule of reactants fed into the plant must either be consumed or leave as impurity or purge. Because of their value so we prevent reactants from leaving. This means we must ensure that every mole of reactant fed to the process is consumed by the reactions.

This is an important, from the viewpoint of individual unit, chemical component balancing is not a problem because exit streams from the unit automatically adjust their flows and composition. However, when we connect units together with recycle streams, the entire system behaves almost like a pure integrator in terms of reactants. If additional reactant is fed into the system without changing reactor conditions to consume the reactants, this component will build up gradually within the plant because it has no place to leave the system.

3.2 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex. Two basic effect of recycle is:

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 time constants of the individual units. 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.

3.2.1 Snowball Effect

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.

3.3 Step of Plantwide Process Control Design Procedure

Step1: Establish control objectives

Assess the steady-state design and dynamic control objects for the process. This is probably the most important aspect of the problem because different control objectives lead to different control structures. The ”best” control structure for a plant depends upon the design and control criteria established.

These objectives include reactor and separation yields, product quality specification, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine control degrees of freedom

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to set point. The placement of these control valves can sometimes be made to improve dynamic performance, but often there is no choice in their location.

Most of these valves will be used to achieve basic regulatory control of the process: set production rate, maintain gas and liquid inventories, control product qualities, and avoid safety and environmental constraints. Any valves that remain after these vital tasks have been accomplished can be utilized to enhance steady-state economic objectives or dynamic controllability (e.g. minimizes energy consumption, maximize yield, or reject disturbances).

Step 3: Establish energy management system

Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system. Thus, we use the term energy management to describe two functions.

1. We must provide a control system that removes 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.
2. If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensure 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.

Heat integration of a distillation column with other columns or with reactors is widely used in chemical plants to reduce energy consumption. While these designs look great in terms of steady-state economics, they can lead to complex dynamic behavior and poor performance due to recycling of disturbances. If not already included in the design, trim heater/cooler or heat exchanger bypass line 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.

Step 4: Set production rate

Establish the variable that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate. To obtain higher production rate, we must increase overall reaction rates. This can be accomplished by raising temperature, increasing reactant concentrations, increasing reactor holdup, or increasing reactor pressure. The variable we select must be dominant for the reactor

We often want to select a 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 hitting an operational constraint.

Step 5: Control product quality and handle safety, operational, and environmental constraints

We should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times and large steady-state gains.It should be note that, since product quality considerations have become more important, so it should be establish the product-quality loops first, before the material balance control structure.

Step 6: Fix a flow in every recycle loop and control inventories (pressure and level)

In most process 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 the recycle loop are controlled by level. We have to determine what valve should be used to control each inventory variable. Inventories include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should be controlled with the manipulate variable that has the largest effect on it within that unit (Richardson rule).

Gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields (Douglas doctrine)

Proportional-only control should be used in non-reactive level loops for cascade units in series. Even in reactor level control, proportional control should be considered to help filter flowrate disturbances to the downstream separation system.

Step 7: Check component balances

Component balances are particularly important in process with recycle streams because of their integrating effect. We must identify the specific mechanism or control loop to guarantee that there will be no uncontrollable buildup of any chemical component within the process (Downs drill).

In process, we don't want reactant components to leave in the product streams because of the yield loss and the desired product purity specification. Hence we are limited to the use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. The purge rate is adjusted to control the inert composition in the recycle stream so that an economic balance is maintained between capital and operating costs.

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations. A tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor.

Step 9: Optimize economics or improve dynamic controllability

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 process performance (e.g. minimize energy, maximize selectivity) or improve dynamic response.

3.4 Plantwide Energy Management

3.4.1 Heat Exchanger Dynamics

Heat exchangers have fat dynamics compared to other unit operations in a process. Normally the time constant is measured in second but could be up to a few minutes for large exchangers. Process-to-process exchangers should be modeled rigorously by partial differential equations since they are distributed systems. This introduces the correct amount of dead time and time constant in exit stream temperatures, but the models are inconvenient to solve.

For propose of plantwide control studies it is not necessary to have such detailed descriptions of the exchanger dynamics, since these units rarely dominate the process response. Instead, it is often possible to construct useful models by letting two sets of well-stirred tanks in series heat exchanger.

3.4.2 Heat Pathways

The most of energy required for heating certain streams within the process is matched by similar amount required for cooling other streams. Heat recover from cooling a stream could be recycled back into the process and used to heat another stream. This is the purpose of heat integration and heat exchanger networks (HENs).

From a plantwide perspective we can now discern three different ”heat pathways” in the process. See Figure 3.1 for an illustration. The first pathway dissipates to the environment heat generated by exothermic reaction and by degradation of mechanical work (e.g. compression, pressure drop, and friction). This pathway is from inside the process and flow out. It is of course possible to convert some of the heat to work as it is removed from high temperature in the process.

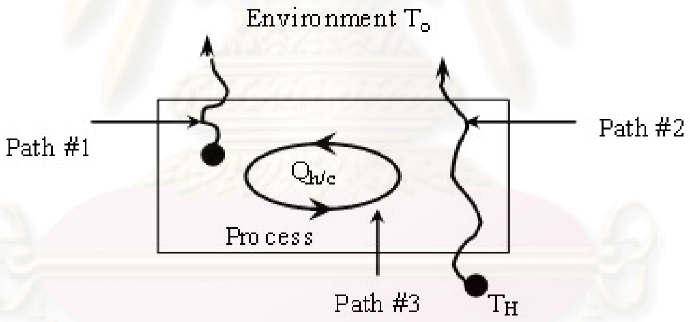


Figure 3.1 Heat Pathways

A second pathway carries heat from utilities into the process. Mechanical work is extracted from the heat as it flows from a high supply way goes through the process and is needed to satisfy the thermodynamic work requirements of separation. Work is also extracted from the heat stream to overcome process inefficiencies with stream mixing and heat transfer.

The third pathway is internal to process. Here heat flows back and forth between different unit operations. The magnitude of this energy path depends upon the heating and cooling needs and the amount of heat integration implemented.

Whenever the internal path is missing, and there is a heating requirement, the heat has to be supplied from utilities. The same amount of heat must eventually be rejected to the environment elsewhere in the process.

3.4.3 Heat Recovery

We can make great improvements in the plant's thermal efficiency by recycling much of the energy needed for heating and cooling process streams. There is of course a capital expense associated with improved efficiency but it can usually be justified when the energy savings are accounted for during the lifetime of the project. Of more interest to us in the current context is how heat integration affects the dynamics and control of a plant and how we can manage energy in plants with a high degree of heat recovery.

3.4.4 Control of Utility Exchangers

The purpose of unit operation controls is to regulate the amount of energy supplied or removed. This is typically done by measuring a temperature in the process and manipulating the flowrate of utility. A PI-controller is adequate in most instances. The location of the temperature measurement depends upon the purpose of the heat exchange. The control point should be located where the effects of the added energy are felt the most. When the utility exchanger is used for stream heating and cooling, the control point is on the stream being heated or cooled.

3.4.5 Control of Process-to-Process Exchangers

Process-to-process (P/P) exchangers are used for heat recovery within a process. Most heat exchanger network are not operable at the optimum steady state design conditions; i.e., normally they can tolerate disturbances that decrease the loads but not those that increase loads and there not an adequate number of manipulative variables to be able to satisfy the process constraints and to optimize all of the significant operating variables. These types of operability limitations can be identified by using steady state considerations, and normally these operability limitations can be overcome by installing an appropriate utility exchanger and by installing bypass around the exchangers.

3.6.5.1 Use of Auxiliary Exchangers

When the P/P exchanger is combined with a utility exchanger, we also have a few design decisions to make. The utility exchanger can be installed to P/P exchanger either in series or parallel. Figure 3.2 shows the combination of P/P exchanger with a utility exchanger. Generally, the utility system of a complex energy-integrated plant is designed to absorb large disturbances in the process, and making process-to-utility exchangers relatively easy to control.

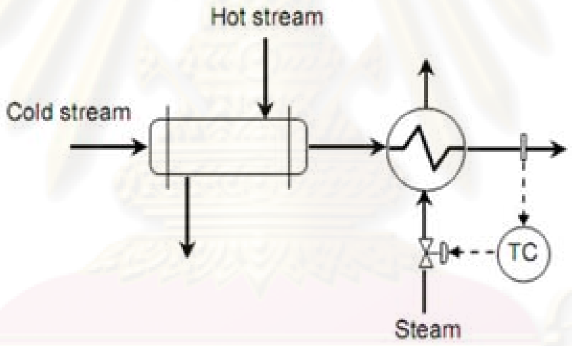


Figure 3.2 Control of process-to-process heat exchanger using the auxiliary utility

The relative sizes between the recovery and the utility exchangers must be established. From a design standpoint we would like to make the recovery exchanger large and utility exchanger small. This gives the most heat recovery, and it is also the least expensive alternative from an investment standpoint.

3.6.5.2 Use of Auxiliary Exchangers

When the bypass method is used for unit operation control, we have several choices about the bypass location and the control point. Figure 3.3 shows the most common alternatives. For choosing the best option, it depends on how we define the best. Design consideration might suggest, we measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high-temperature service. Cost consideration would also suggest a small bypass flow to minimize the exchanger and control valve sizes.

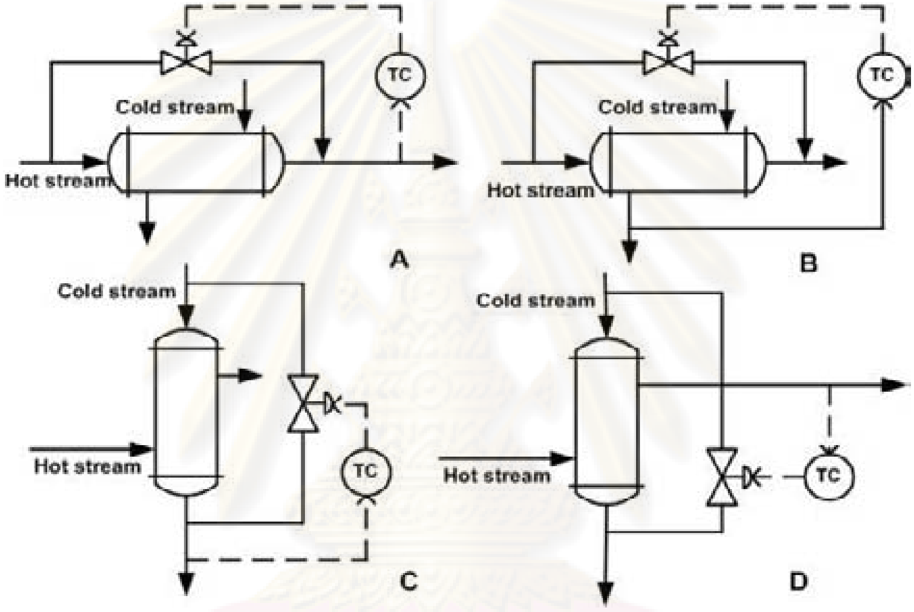


Figure 3.3 Bypass controls of process to process heat exchangers where: (a) controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing cold stream

From a control standpoint, we should measure the most important stream, regardless of temperature, and bypass on the same side as well we control (see Figure 3.3 a and c). This minimizes the effects of exchanger dynamics in the loop. We should also want to bypass a large fraction of the controlled stream since it improves the control range. This requires a large heat exchanger. There are several general heuristic guidelines for heat exchanger bypass streams. We typically want to bypass the flow of the stream whose temperature we want to control. The bypass should be about 5 to 10 percent of the flow to be able to handle disturbances. Finally, we must carefully consider the fluid mechanics of the bypass design for the pressure drops through the control valves and heat exchanger.

3.5 Heat Exchanger Network

It is generally accepted that an optimal network must feature a minimum number of units that reflects on a capital cost and minimum utility consumption that reflects on operating costs. A good engineering design must exhibit minimum capital and operating costs. For Heat Exchanger Network (HEN) synthesis, other features that are usually considered in design are operability, reliability, safety, etc. in recent years the attention in HEN synthesis has been focused on the operability features of a HEN, e.g. the ability of a HEN to tolerate unwanted changes in operating conditions. It has been learned that considering only a cost objective in synthesis may lead to a worse network, i.e. a minimum cost network may not be operable at some neighboring operating conditions. The design must not only feature minimum cost, but also be able cope with a fluctuation or changes in operating conditions. The ability of a HEN to tolerate unwanted changes is called resiliency. It should be note that the ability of a HEN to tolerate wanted changes is called flexibility.

The resiliency property of a design becomes an important feature to be accounted for when the extent of integration of a design introduces significant interactions among process components. The energy integration of a HEN generates a quite complex interaction of process streams, despite the fact that transfer of heat from hot to cold process streams is the only activity of the network. The goal of a network is to deliver the process streams to their target temperatures by using most of their heating and cooling availability and a minimum of heating and cooling utilities. The process streams are coupled through a net of heat exchangers. Changes in conditions of one stream in the network may affect the performances of many heat exchanges and the conditions of several process streams. Since resiliency is a property of a network structure.

3.5.1 Definition of HEN Resiliency

In the literature, resiliency and flexibility have been used synonymously to describe the property of HEN to satisfactorily handle variations in operating conditions. These two terms have difference in meaning.

The resiliency of a HEN is defined as the ability of a network to tolerate or remain feasible for disturbances in operating conditions (e.g. fluctuations of input temperatures, heat capacity flowrate, etc.). As mentioned before, HEN flexibility is closed in meaning to HEN resiliency, but HEN flexibility usually refers to the wanted changes of process conditions, e.g. different nominal operating conditions, different feed stocks, etc. That is, HEN flexibility refers to the preservation of satisfactory performance despite varying conditions, while flexibility is the capability to handle alternate (desirable) operating conditions.

A further distinction between resiliency and flexibility is suggested by Colberg el al. (1989). Flexibility deals with planed, desirable changes that often have a discrete set of values, resilience deal with unplanned, undesirable changes that naturally are continuous values. Thus a flexibility is a 'multiple period' type of problem. A resilience problem should be a problem with a continuous range of operating conditions in the neighborhood of nominal operating points.

Wongsri (1990) developed the heuristic and procedures for resilient heat exchanger network synthesis. The heuristics are used to develop basic and derived match patterns which were classified according to their (1) resiliency (2) chances that they are in solution and (3) the matching rules like the pinch method, and the thermodynamics law etc. Furthermore the same author developed for synthesize heat exchanger network called "The Disturbance Propagation Method". This method will find a resiliency network structure directly from the resiliency requirement and also feature minimum number of units and maximum energy recovery.

3.5.2 Design Conditions

There are several design conditions for resilient HEN synthesis. Usually, these are specified at extreme operating conditions. The following conditions (Wongsri, 1990) are:

1. *Nominal Operating Condition.* This is an operating condition that is obtained from a steady state heat and mass balance of a process. In a good design, a network must be operated at this condition most of the time. In general, a fluctuation in operating condition is plus and minus from this point.

2. *Maximum Heat Load Condition.* This is a condition where all process stream are at their maximum heat loads. For example inlet temperatures of hot streams are the highest and of cold streams are the lowest. This is also known as the largest maximum energy recovery condition.

3. *Maximum Cooling Condition.* This is a condition where hot process streams are at their maximum heat loads whereas cold process streams are at their minimum heat loads. For example inlet temperatures of hot and cold streams are the highest.

4. *Minimum Heating Condition.* This is a condition where hot process streams are at their minimum heat loads whereas cold process streams are at their maximum heat loads. For example inlet temperatures of hot and cold streams are the lowest.

5. *Minimum Heat Load Condition.*This is a condition where all process streams are at their minimum heat loads. For example inlet temperatures of hot streams are the lowest and of cold streams are the highest. This is also known as the lowest maximum energy recovery condition.

The worst case condition of this work is the condition that minimum heat supplies by hot process stream and maximum heat demand by cold process stream. This viewpoint is shown in Figure. 3.4.

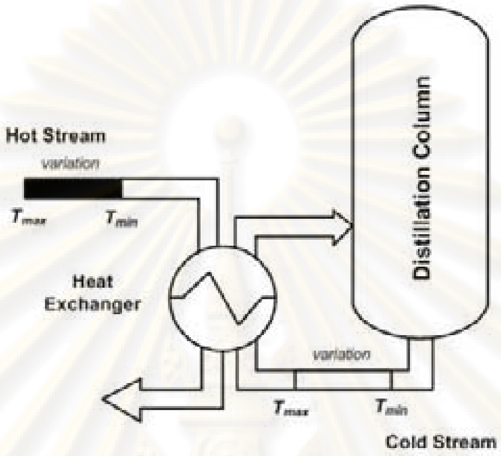


Figure 3.4 A viewpoint of worst case condition

3.5.3 Match Patterns

HEN synthesis is usually considered as a combinatorial matching problem. For a HEN in which a design property is regarded as a network property, or a structure property, we need to look beyond the match level to a higher level where such a property exists, e.g. to a match structure or match pattern. Match patterns are the descriptions of the match configuration of two, possibly more process streams and their properties that are thermally connected with heat exchangers. Not only the match description, e.g. heat duty of an exchanger and inlet and outlet temperatures is required but also the position of a match, e.g. upstream or downstream, the magnitude of the residual heat load and the heat capacity flowrates between a pair of matched streams. So, we regard the resilient HEN synthesis problem as a match pattern combinatorial problem where more higher - level design qualities are required.

By using the 'tick off rule' there are four match patterns for a pair of hot and cold streams according to the match position and the length of streams. The four patterns are considered to the basic match pattern classes. The members of these classes are the patterns where other configurations and properties are specified. The four match pattern classes are simply called A, B, C and D and are shown in Figure 3.5 to 3.8 respectively.

1. *Class A Match Pattern:* The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the cold end of the cold stream. The residual heat load is on the hot portion of the cold stream(See Figure 3.5). A match of this class is a first type match at cold end position and the heat load of the cold stream is greater than that of the hot stream. This is a upstream match. For a heating subproblem, a Class A match is favored, because it leaves a cold process stream at the pinch heuristics.

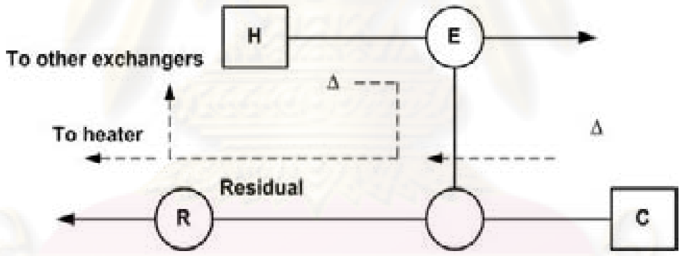


Figure 3.5 Class A Match Pattern

2. *Class B Match Pattern:* The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the hot end of the hot stream. The residual heat load is on the cold portion of the hot stream (See Figure 3.6). A match of this class is a second type match; a hot end match and the heat load of the hot stream are greater than that of the cold stream. This is an upstream match. For a cooling subproblem, a Class B match is favored, because it leaves a hot process stream at the cold end also follows the pinch heuristics.

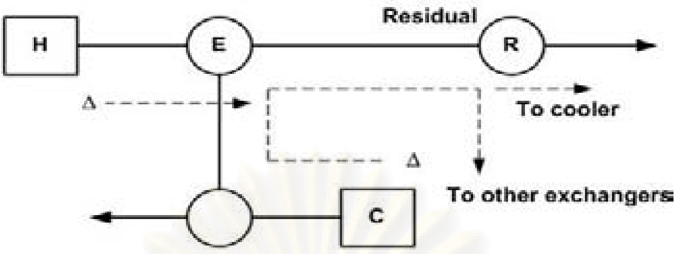


Figure 3.6 Class B Match Pattern

3. *Class C Match Pattern:*The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the cold end of the hot stream. The residual heat load is on the hot portion of the hot stream (See Figure 3.7). A match of this class is a first type match; a cold end match and the heat load of the hot stream are greater than that of the cold stream. This is a downstream match.

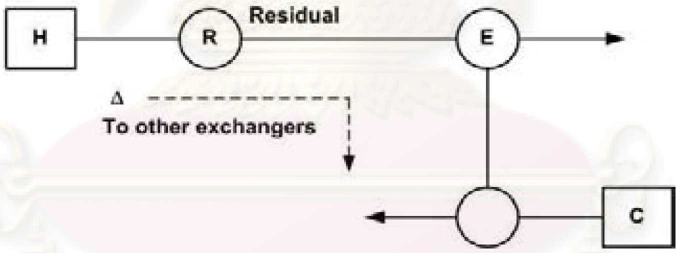


Figure 3.7 Class C Match Pattern

4. *Class D Match Pattern:*The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the hot end of the cold stream. The residual heat load is on the cold portion of the cold stream (See Figure 3.8). A match of this class is a second type match; a hot end match and the heat load f the cold stream is greater than that of the hot stream. This is a downstream match.

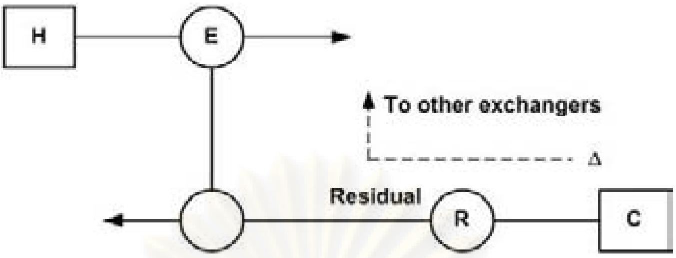


Figure 3.8 Class D Match Pattern

When the residual heat load in a match pattern is matched to a utility stream, it is closed or completed pattern. Otherwise, it is an open or incomplete pattern. It can be seen that if the heat load of the residual stream is lea than the minimum heating or cooling requirement then the chances that the match pattern will be matched to a utility stream is high.

3.6 Design of Heat Pathways for Dynamic MER

For the plantwide energy management, the heat pathways through the network are designed so that the dynamic MER can always be achieved. In this work, the heat pathways are designed based on the match patterns design and disturbance propagation technique (Wongsri, 1990)

A simplified HEN as shown in Figure 3.9 is used to explain how an appropriate heat pathway should be activated to carry associated load to the utility unit. For instance, when the inlet temperature of a disturbed cold stream decreases, path 1 (Figure 3.9a) should be activated by controlling the cold outlet temperature of FEHE. This will have the effect of shifting the positive disturbance load to the cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty. Consider the case when the inlet temperature of a disturbed cold stream increases, path 2 (Figure 3.9b) should be activated by controlling the hot outlet temperature of FEHE to shift its negative disturbance load to heater. Thus, the negative disturbance load of a cold stream will result in decrease of the heater duty.

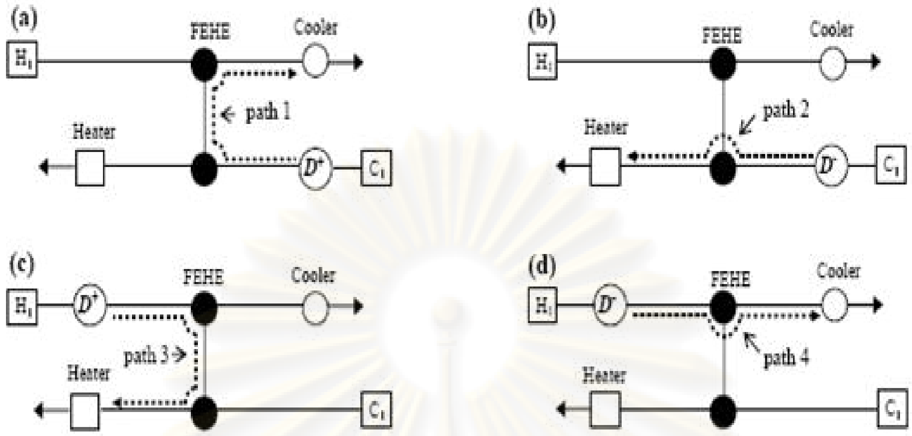


Figure 3.9 Heat pathways in the simplified HEN to achieve the highest possible dynamic MER, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C1 to the cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream C1 to the heater, (c) path 3 is used to shift the positive disturbance load of the hot stream H1 to the heater, and (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to the cooler

On the other hand, when the inlet temperature of a disturbed hot stream increases, path 3 (Figure 3.9c) should be activated by controlling the hot outlet temperature of FEHE to shift its positive disturbance load to heater. As a result, the heater duty will be decreased. Consider the case when the inlet temperature of a disturbed hot stream decreases, path 4 (Figure 3.9d) should be activated by controlling the cold outlet temperature of FEHE to shift its negative disturbance load to cooler. As a result, the cooler duty will be decreased.

3.7 Design and Control of Heat Pathways for Heat Exchanger Networks

The LSS can be used to select an appropriate heat pathway to carry associated load to a utility unit. In this chapter, we figure out the heuristics of selection and manipulation of heat pathways for some typical HEN examples that widely used in the petroleum and chemical industries (e.g. HEN alternatives of HDA process given by Terril and Douglas, 1987). We also show where the LSS should be placed on a heat exchanger unit so that it can be used to direct the disturbance load to a specified utility unit.

For all of the examples of HENs, we assume that:

- The utility exchangers can handle all variations of heat load.
- The path for disturbance loads is co-current with all of the process streams.
- Any heat exchanger will have enough heat transfer area to accommodate increases in heat loads of disturbed process stream.
- Bypass lines are provided to all heat exchangers as a standard feature to adjust heat load

CHAPTER IV

ACETONE PROCESS

4.1 Process Description

Acetone also known as dimethyl ketone (CH_3COCH_3)is colourless, mobile, flammable liquid with mildly pungent and somewhat aromatic odour. It is widely as a solvent for vast majority of resins, nitrocellulose, cellulose acetate and pharmaceuticals. It derivatives are ketenes, methyl methacrylate, bisphenol A, diacetone alcohol, mesityl oxide, methyl isobutyl ketone, hexylene glycol and isophorone.

There are 2 important technologies to produce acetone. First, production of acetone is as a by-product of the manufacture of phenol. Benzene is alkylated to cumene which is further oxidized to cumene hydroperoxide and finally cleaved to yield phenol and acetone. Catalyst can be chosen as an alternative synthetic route when high-purity acetone is required, such as in biomedical applications. Second, isopropyl alcohol is used as the raw material. This is a viable commercial alternative and a few plants continue to operate using the process. The primary advantage of this process is that the acetone produced is free from trace aromatic compounds, particularly benzene. For this reason acetone produces from IPA may be favored by the pharmaceutical industry due to the very tight restrictions placed on solvents by the Food and Drug Administration (FDA).

Acetone is produced by isopropyl alcohol (IPA) which feed is near an azeotropic mixture with 88 wt% isopropyl alcohol and 12 wt% water at 25^0C and 1 atm. The feed is fed into a tank where it is mixed with the recycled unreacted IPA/water mixture stream from IPA column. This material is pumped and vaporized before entering the reactor. The reaction to produce acetone is given below:

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$$

isopropyl alcohol   actone   hydrogen

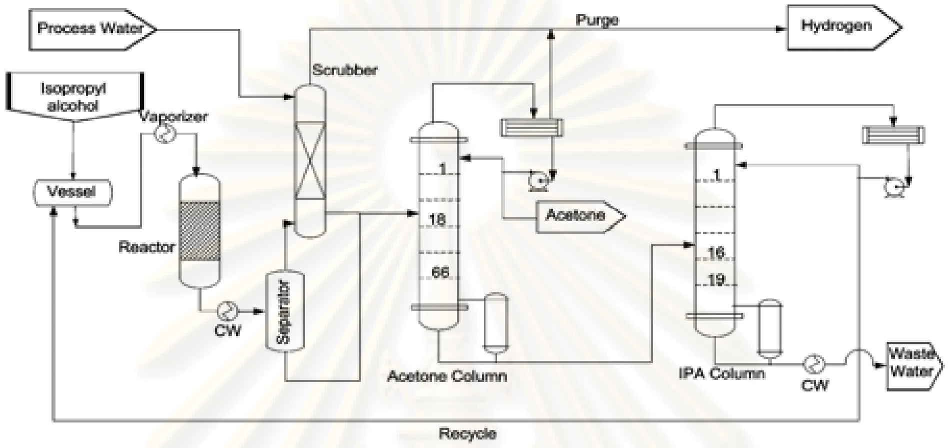


Figure 4.1 Basic unit operations in the reaction section of acetone process.

The reaction conditions are typically 2 bars and 350^0C, giving single-pass conversion of 85-92%. The reaction is endothermic with a standard heat of reaction of 62.9 kJ/mol. The reaction is kinetically controlled and occurs in the vapor phase over a catalyst. The reaction kinetics are the first order with respect to the concentration of alcohol and can be estimated from the following equation:

$$-r_{IPA} = k_0\big[\tfrac{E_a}{RT}\big]C_{IPA}\tfrac{kmol}{m^3reactors}$$

with E_a = 72.38 Mj/kmol, $k_0 = 3.51\times10^5 \; \frac{m^3gas}{m^3reactors}$, $C_{IPA} = \frac{kmol}{m^3gas}$

Where r_{IPA} has units of moles of kilomoles of isopropyl alcohol per m^3 of reactor per second.

The reactor effluent, containing acetone, hydrogen, water and unreacted IPA, is cooled and partially condensed in a heat exchanger and sent to the phase separator. The vapor leaving the phase separator is scrubbered with water to recover additional acetone, and the liquid is combined with the liquid from the separator and sent to the separations section. Two distillation columns are used to separated the acetone product (99.9 mole %) and to remove the excess water from the unused IPA, which is then recycled back to the surge vessel.

In practice, several side reactions can occur to a small extent. Thus, trace quantities of propylene, diisopropyl ether, acetaldehyde and other hydrocarbons and oxides of carbon can be formed. The non-condesables are removed with the hydrogen while the aldehydes and ethers may be removed with acid washing or adsorption. These side reactions are not accounted for in this preliminary design.

For the design presented, the reactor was simulated with catalyst in 2 inch (50.4 mm) diameter tubes each 20 feet (6.096 m) long and with a concurrent flow of a heat transfer medium on the shell side of the shell and tube reactor. The resulting arrangement gives 90% conversion of IPA per psia.

4.2 Design of heat exchanger networks

In this chapter, the heat exchanger network design method provided by Wongsri (1990) is used to design the resilient heat exchanger networks for acetone process. The design procedures and definitions from previous chapters will be an accessory to design in conceptual design. The problem table method is applied to find pinch temperature and reach maximum energy recovery (MER). The information for used in design is shown in the following table.

Table 4.1 The information of acetone process

Stream Name	Tin^0C	$Tout^0C$	W ($kW/^0C$)	Duty (kW)
H1 : H1: Reactor Product Stream	350	20	3.2	1055.84
H2 : IPA Column Condenser	83.8	82.71	184.55	201.98
C1 : Reactor Feed Stream	31.27	234	4.9	994.08
C2 : Product Column Reboiler	106.73	106.77	6292.71	208.34

4.2.1 Acetone Process Alternative 1

There are only two streams in the network. So we can find pinch temperature by using problem table method as following: See Table 4.2. At the minimum heat load condition, the pinch temperature occurs at $41.27/31.27^0C$. The minimum utility requirements have been predicted 6.48 kW of hot utilities and 68.04 kW of cold utilities.

Table 4.2 Problem table for alternative 1

W ($kW/^0C$)		T hot (^0C)	T cold (^0C)	ΣW ($kW/^oC$)	ΔT (^0C)	Required Heat(kW)	Interval (kW)	Cascade Heat(kW)	Sum Interval(kW)
H1	C1								
		350.00	340.00			Qh			
3.20	0.00	244.00	234.00	3.20	106.00	6.48	339.07	345.56	339.07
3.20	4.9	41.27	31.27	-1.7	202.73	345.56	-345.56	0	-6.48
3.20	0	20	10.00	3.20	21.27	0	68.04	68.04	61.56
								Qc	

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.3. Figure 4.2 shows a design of resilient heat exchanger network for acetone process alternative 1. In our case, the minimum temperature difference in the process-to-process-heat-exchangers is set to 10^0C.

Table 4.3 Synthesis table for alternative 1

Hot end synthesis table							
Stream	Load	W	T1	T2	D1	D2	Action
a) Stage 1							
H1	955.62	3.2	345	46.27	31.99	31.99	Selected A[H]
C1	969.56	4.9	234.00	231.57	0.00	98.07	Selected
b) Stage 2							
H1	0.00	0.00	0.00	0.00	0.00	0.00	
C1	13.94	4.90	234.00	231.16	0.00	98.07	To Heater
Cold end synthesis table							
H1	52.05	3.20	36.27	20	31.99	0.00	To cooler

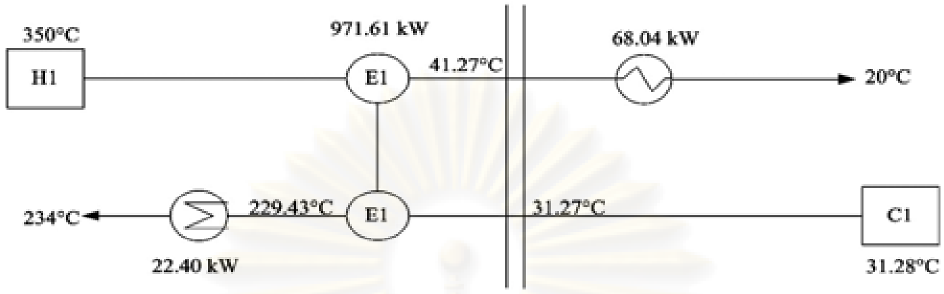


Figure 4.2 Resilient Heat Exchanger Network of Alternative 1.

4.2.2 Acetone Process Alternative 2

There are three streams in the network. So we can find pinch temperature by using Problem Table Method as following: See Table 4.4. At the minimum heat load condition, the pinch temperature occurs at $41.27/31.27^0C$. The minimum utility requirements have been predicted 214.64 kW of hot utilities and 68.04 kW of cold utilities.

Table 4.4 Problem table for alternative 2

W ($kW/^0C$)			T hot (^0C)	T cold (^0C)	ΣW (kW/^oC)	ΔT (^0C)	Required Heat(kW)	Interval (kW)	Cascade Heat(kW)	Sum Interval(kW)
H1	C1	C2								
			350.00	340.00			Qh			
3.20	0.00	0.00	244.00	234.00	3.20	106.00	214.64	339.07	553.71	339.07
3.20	4.90	0.00	116.77	106.77	-1.7	127.23	553.71	-216.75	336.96	122.33
3.20	4.90	6292.71	116.73	106.73	-6294.42	0.03	336.96	-208.40	128.56	-86.07
3.20	4.90	0.00	41.27	31.27	-1.70	75.47	128.56	-128.56	0.00	-214.64
3.20	0.00	0.00	20.00	10.00	3.20	21.27	0.00	68.04	68.04	-146.60
									Qc	

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.5. Figure 4.3 shows a design of resilient heat exchanger network for acetone process alternative 2. In our case, the minimum temperature difference in the process-to-process-heat-exchangers is set to 10^0C.

Table 4.5 Synthesis table for alternative 2

Hot end synthesis table							
Stream	Load	W	T1	T2	D1	D2	Action
a) Stage 1							
H1	955.62	3.20	345.00	46.27	31.99	31.99	Selected
C1	969.38	4.90	234.00	36.27	0.00	49.02	
C2	145.42	6292.71	106.77	106.74	0.00	125.85	selected
b) Stage 2							
H1	684.35	3.20	318.14	46.27	31.99	31.99	Selected
C1	969.38	4.90	234.00	36.27	0.00	49.02	Selected
C2	72.71	6292.71	106.77	106.76	0.00	125.85	To heater
c) Stage 3							
C1	285.03	4.90	234.00	94.41	0.00	49.02	Selected
Cold end synthesis table							
H1	52.05	3.20	36.27	20.00	31.99	0.00	To cooler

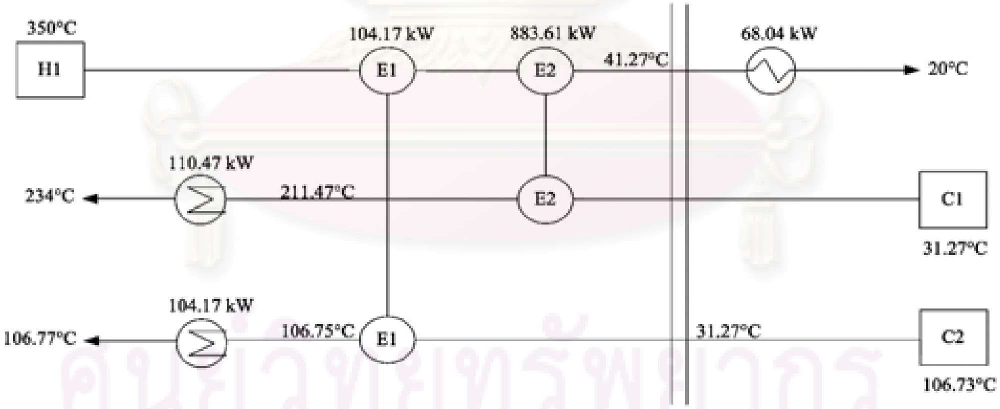


Figure 4.3 Resilient Heat Exchanger Network of Alternative 2.

4.2.3 Acetone Process Alternative 3

There are three streams in the network. We can not find pinch temperature by using Problem Table Method.

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.6. Figure 4.4 shows a design of resilient heat exchanger network for acetone process alternative 3. In our case, the minimum temperature difference in the process-to-process-heat-exchangers is set to 10^0C.

Table 4.6 Synthesis table for alternative 3

Stream	Load	W	T1	T2	D1	D2	Action
a) Stage 1							
H1	1055.64	3.20	350.00	20.00	31.99	0.00	
H2	201.98	184.35	83.80	82.71	3.69	0.00	Selected
C1	994.08	4.90	234.00	31.27	0.00	49.03	Selected
b) Stage 2							
H1	1055.64	3.20	350.00	20.00	31.99	0.00	Selected
H2	146.59	184.35	83.50	82.71	3.69	0.00	to Heater
C1	938.70	4.90	234.00	42.56	0.00	49.03	Selected
c) Stage 3							
H1	410.64	3.20	148.37	20.00	31.99	0.00	To cooler
C1	293.70	4.90	234.00	174.10	0.00	49.03	To heater

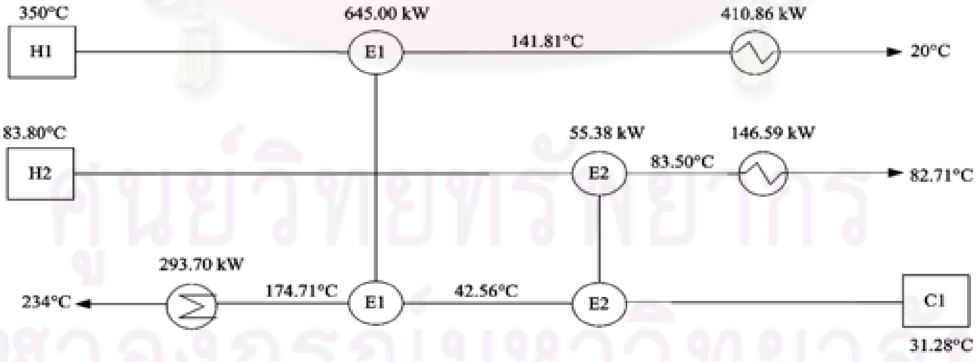


Figure 4.4 Resilient Heat Exchanger Network of Alternative 3.

4.3 The acetone Alternatives

Three alternatives of heat exchanger networks (HEN) designs of acetone plant are proposed. In alternative 1 has one heat exchanger for exchange duty between reactor inlet stream and reactor outlet stream as in figure 4.5.

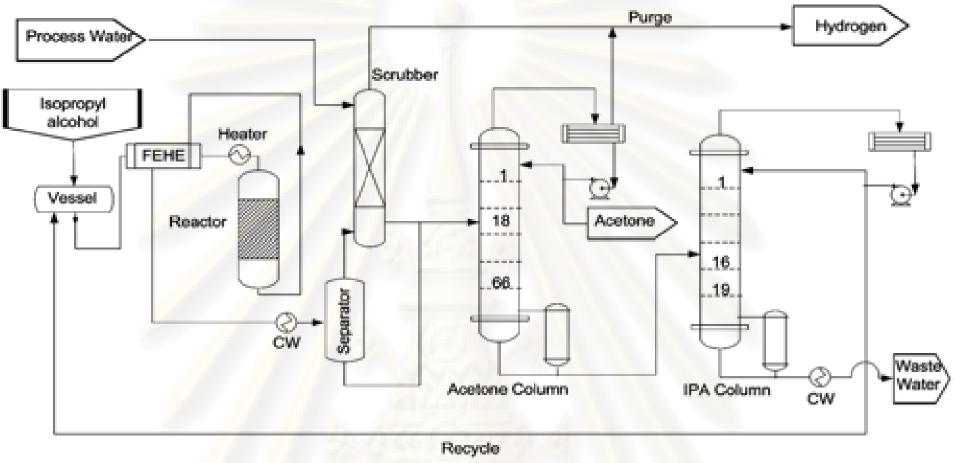


Figure 4.5 Acetone process alternative 1.

In alternative 2 has two heat exchangers for preheating inlet reactor stream and the reboiler in IPA column is driven by reactor effluent stream. In this work, the IPA column is added an auxiliary reboiler to supply the heat because the total heat from the reactor isn't enough to reboil the column as in figure 4.6.

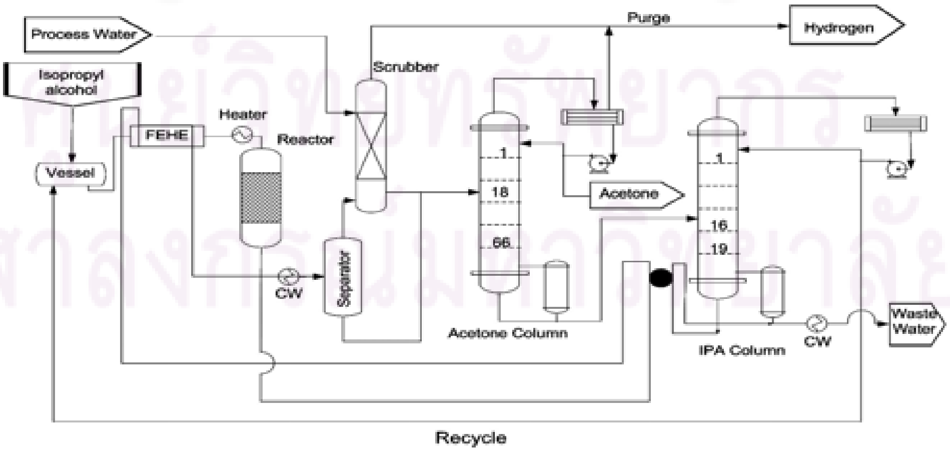


Figure 4.6 Acetone process alternative 2.

In alternative 3 has two heat exchangers for preheat inlet reactor stream and the condenser in IPA column is driven by reactor effluent stream. In this work, the IPA column is added an auxiliary cooler to supply the heat because the total heat from the reactor isn't enough to condense the column as in figure 4.7.

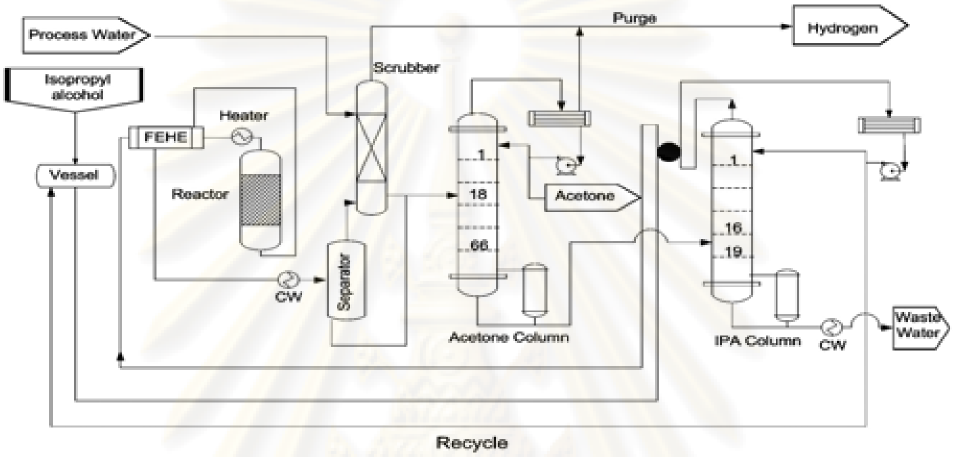


Figure 4.7 Acetone process alternative 3.

4.4 Steady State Modeling

First, a steady state model is built in HYSYS using the flowsheet equipment design information taken from Turton (1998). For the simulation, the UniquacPeng-Robinson model is selected for physical property calculation. The reaction kinetics are modeled with standard Arrhenius kinetic expressions available in HYSYS which the kinetic data is taken from Turton (1998).

4.4.1 Steady State Simulation of Acetone Process (Base Case)

All of two columns are simulated using the 'distillation column' module. When columns are modeled in steady state, besides the specification of inlet stream, pressure profiles, number of trays and feed tray, two additional variables should be additionally specified for column with condenser or reboiler. These could be the duties, reflux rate, draw stream rates, composition fraction, etc. We chose to specify a priori overhead and bottom component mole fraction for all columns. Although the tray diameter and spacing, weir length and hight are not required for steady state modeling, they are required for dynamic simulation.

4.4.2 Steady State Simulation for Alternatives 1, 2 and 3

In alternative 1, there are one FEHE between reactor inlet stream and reactor outlet stream for preheat raw material before entering reactor.

In alternative 2, there are two FEHEs and additionally the reboiler in the IPA column is driven by the reactor effluent stream, whereas in alternative 3, the condenser in the IPA column is driven by the reactor effluent stream

Several RECYCLE modules should be inserted in the streams for these alternatives in simulations. The numbers of RECYLE modules are 2 for alternative1 and 3 for alternative 2 and 3.

All process-to-process heat exchanger are simulated using a heat exchanger a hot stream on shell side and cold stream in tube side. A minimum ΔT of about 10^0C is assumed for all process to process heat exchangers.

In all alternatives, the IPA column is simulated using the "distillation column" module. For alternative 2, The IPA column is simulated using a 'refluxed absorber' that it doesn't not include a reboiler. A tank needs to accommodate liquid from the bottom of IPA column. Since a "reflux absorber" module is used, only one variable need to be specified for the columns with condenser. The overhead mole fraction is chosen to be specified for a "refluxed absorber" module. For alternative 3, The IPA column is simulated using a 'reboiled absorber' that it doesn't not include a condenser. A tank needs to accommodate stream from the top of IPA column. Since a "reboiled absorber" module is used, only one variable need to be specified for the columns with condenser. The bottom mole fraction is chosen to be specified for a "refluxed absorber" module.

Energy saving from steady state which simulated by HYSYS is shown in table 4.7. Duty in this table comes from two columns which differences from others unit. The result showed that alternative 2 can save energy more than other alternatives.

Table 4.7 Energy integration for acetone process (steady state simulation)

	Base case	Alternatives		
		1	2	3
1. Utilities usage (kW)				
Heater	994.61	58.64	125.81	295.54
effluent cooler	1055.79	119.73	124.34	411.12
IPA column condenser	202.13	202.08	205.24	-
Auxiliary IPA condenser	-	-	-	148.29
IPA column reboiler	208.30	208.29	-	208.37
Auxiliary IPA reboiler	-	-	149.22	-
Total hot utilities	1202.90	266.93	125.81	503.91
Total cold utilities	1257.91	321.81	329.58	411.12
2. Energy saving %	-	76.08	81.49	62.82

CHAPTER V

CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION

5.1 Plantwide control design procedure

In this work, we design control structure by using Luyben heuristic design method (1997) for control structure 1 and 2 and fixture point method (Wongsri, 2008) for control structure 3 and 4.

5.1.1 Nine-step approach of Luyben

Step 1. Establish Control Objectives

For this process, we want to achieve the acetone product at 99.9 mole%. Feed is near an azeotropic mixture with 88 wt% isopropyl alcohol and 12 wt% water at 25^0C and 1 atm. Due to selectivity considerations, the maximum temperature should not exceed 375^0C and maximum single pass conversion should not exceed 95% are used. The reactor effluent gas must be quenched to 20^0C.

Step 2. Determine Control Degree of Freedom

There are 12 control degrees of freedom. They include; two fresh feed valves for isopropyl alcohol and water, vaporizer valve, furnace fuel valve, acetone column steam, bottoms, reflux, distillate, cooling water, and vapor product valves; IPA column steam, bottoms, reflux, distillate, and cooling water valves.

Step 3. Establish Energy management system

In this process, the reactor uses fluidized bed reactor but HYSYS doesn't have this equipment. We use isothermal plug flow reactor instead. So the reactor feed must be heated equal the reactor exit temperature (350^0C). The acetone product is produced from the endothermic reaction. We choose to control reactor exit temperature with reactor heating flow because of its direct effect.

In all alternatives, we design a feed-effluent heat exchanger (FEHE) to reduce the amount of heat in heater. So form a steady-state view point, the economic trade off between utility and capital costs would produces a fairly large heat exchanger and a small heater. However, the heat of vaporization supplied in heater must be dissipated to utilities at the reactor effluent cooler.

Step 4. Set Production Rate

There are not constrained to set production either by supply or demand, then the production rate can be set by acetone production. Considering of the kinetics equation is found that the two variables alter the reaction rate; temperature and isopropyl alcohol concentration.

Step 5. Control Product Quality and Address Safety, Operational, and Environmental Concerns

Acetone purity must be maintained at 99.9% for this research. We can control by manipulating IPA column reboiler duty to maintain temperature in the column or use reflux to manipulate purity.

In distillation, to avoid the high pressure safety constraint, we must control pressure by flooded condenser cooling water valve. In part of level, we use distillate and bottom valves to control level in condenser and reboiler, respectively.

Step 6. Control Inventories and Fix a Flow in Every Recycle Loop

Three pressures must be controlled: acetone stripper, acetone column and IPA column. In acetone stripper, the stripper overhead valve is opened. In acetone column and IPA column, pressure control can be achieved by manipulating cooling water flow to overhead consideration rate.

For liquid loops, there are six liquid levels in the process: tank, phase separator and two (base and overhead receiver) in each column. In the tank, level is controlled by inlet valve. In two columns, distillate flow controls overhead receiver level and bottoms flow controls base level

In most processes a flow control should be present in all recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows, while the process is perturbed by small disturbance. We call this high sensitivity of the recycle flowrates to small disturbances the "snowball effect". There are two recycle control loops in this research; reference control structure and the first control structure.

Step 7. Check Component Balances

Component balances consists of:

- Hydrogen is purged from the gas recycle loop to prevent it from accumulating.
- Water is removed in the bottoms stream from the IPA column, where steam flow controls base level.
- The inventory of acetone is accounted for by temperature and overhead receiver level control in the acetone column.
- Isopropyl alcohol inventory is accounted for by level control in tank.
- Flow control accounts for water inventory.

Step 8. Control Individual Unit Operations

The rest degrees of freedom are assigned for control loops within individual units. These include:

- Cooling water flow to the cooler controls process temperature to the separator.
- Refluxes to the acetone and IPA columns are flow controlled.

Step 9. Optimize Economics or Improve Dynamic Controllability

For this step isn't considered in this work.

5.1.2 Fixture Point Theorem

The fixture point theorem is proposed by Wongsri, 2008 to define the most sensitive control variable. The method is as follows:

1. Consideration process in dynamic mode (we run the process until the process responses are steady state.).

2. To find all control variables (CV) and manipulate variables (MV).

3. Test the dynamic process response by step change one MV (other MVs are set at manual mode). Calculation all IAE control variables which deviate from steady state).

4. Math the high CV IAE with MV. MV should be direct effect near MV. Then, we consider next CV with other MVs.

5.2 Design of plantwide control structures

In all control structures of this work, the same loops are as follows:

- Valve V1 is manipulated to control IPA fresh feed flowrate.
- Valve V2 is manipulated to control water fresh feed flowrate.
- Valve V3 is manipulated to control pressure in acetone stripper.
- Valve V4 is manipulated to control phase separator level.
- Heater duty is manipulated to control the reactor inlet temperatue.
- Reactor duty is manipulated to control the reactor exit temperatue.
- Waste water cooler duty is manipulated to control the waste water temperatue.
- Heater duty is manipulated to control the reactor inlet temperatue.

Four control structures are presented in this work. Control structure 1 and 2 (CS1 and CS2) are design following Luyben's heuristic method. Control structure 3 and 4 are used Fixture point which proposed by Wongsri, 2008. The control parameters are given in Appendix B.

5.2.1 Design of control structure 1 (CS1)

This control structure is shown in Figure 1. This control structure follow: the fresh flowrate is controlled by valve. All utilities controlled stream exit temperature. In separation section, the temprature of IPA column on tray 64 is controlled by hot utilities of reboiler, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser and reboiler are controlled by distillate valve and bottom valve, respectively. The temperature of IPA column on tray 11 is controlled by hot utilities of reboiler, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser and reboiler are controlled by distillate valve and bottom valve, respectively.

5.2.2 Design of control structure 2 (CS2)

This control structure follow: the fresh flowrate is control by valve. All utilities controlled stream exit temperature. In separation section, the temprature of IPA column on tray 64 is controlled by hot utilities of reboiler, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser and reboiler are controlled by distillate valve and bottom valve, respectively. The Acetone composition is controlled bt reflux valve. In IPA column, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser is controlle by reboiler duty. Liquid level in reboiler is controlled by bottom valve. Recycle stream is fixed by recycle valve.

5.2.3 Design of control structure 3 (CS3)

This control structure follow: the fresh flowrate is controlled by valve. All utilities controlled stream exit temperature. In separation section, the temprature of IPA column on tray 64 is controlled by hot utilities of reboiler, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser and reboiler are controlled by distillate valve and bottom valve, respectively. The temperature of IPA column on tray 11 is controlled by bottom valve, pressure is controlled by cold utilities of condenser, the reflux flow in distillation is fixed with reflux valve. Liquid level in condenser is controlled by distillate valve. Liquid level in reboiler is controlled by reboiler duty.

5.2.4 Design of control structure 4 (CS4)

This control structure follow: the fresh flowrate is controlled by valve. All utilities controlled stream exit temperature. In IPA column, pressure is controlled by cold utilities of condenser. Liquid level in condenser and reboiler are controlled by distillate valve and reboiler duty, respectively. Bottom flowrate is controlled by bottom valve. The Acetone composition is controlled bt reflux valve. In IPA column, the temperature of IPA column on tray 11 is controlled by hot utilities of reboiler. Pressure is controlled by cold utilities of condenser. Liquid level in condenser and reboiler is controlled by reflux valve and bottom valve, respectively. Liquid level in reboiler is controlled by bottom valve. Recycle stream is fixed by recycle valve.

5.3 Energy Management of Heat-Integrated Process

As the operating conditions the designed control system must regulate the entrie process to meet the desired condition. On the other hand, changes in the load disturbance of the cold or hot stream affect energy consumption of the utility units. Therefore, for a complex energy-integrated plant, it is important to study the heat pathway control in order to mange the heat load disturbance in such a way that the maximum energy recovery (MER) can always be achieved.

We now look at the plantwide control issues around energy management. The control configurations of RHEN are determined using the Heat Pathway Heuristics (HPH) (Wongsri and Hermawan, 2005). The objective of HPH design is to find proper heat pathways to achieve the dynamic HEN operation objective which is desired target variables and maximum energy recovery. As the operating conditions change or heat load disturbances enter, the designed control system must regulate the heat flow within the network to meet the desired goal.

HPH is used in design and operation of RHEN. HPH is about how to properly direct heat load disturbance throughout the network to heat sinks or heat sources in order to achieve MER at all time. First two kinds of disturbances is needed to be introduced: Positive disturbance load, D+, an entering disturbance resulting in increasing heat load of a stream; Negative disturbance load, D-, an entering disturbance resulting in decreasing heat load of a stream. The heat pathway should be short to minimize the input and propagated disturbances, simply a path with minimized upsets.

5.3.1 Design of Heat Pathways and HEN Control Configuration for Alternative 1

The design of the heat pathways for alternative 1 is shown in figure 5.1. Both the positive and negative disturbance loads of C1 are directed to heater and cooler (figure 5.2 a) and b)). The positive and the negative disturbance loads of H1 are shifted to heater and cooler (figure 5.2 c) and d)). So FEHE1 should be controlling.

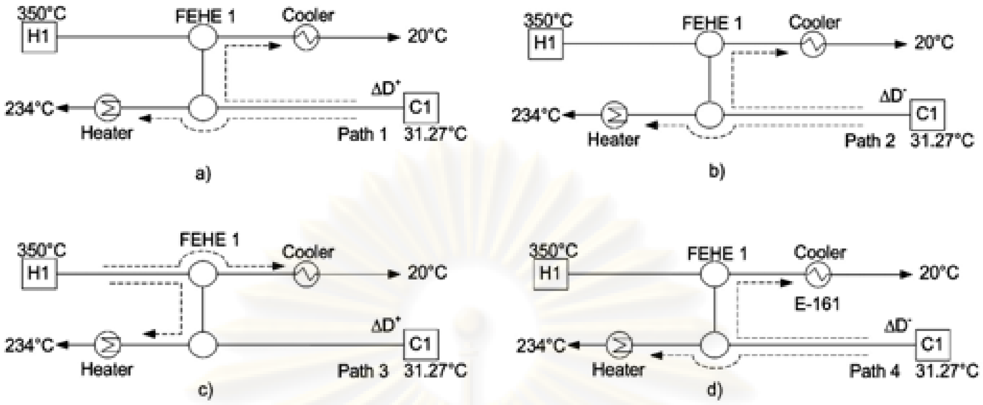


Figure 5.1 Heat pathways through alternative 1, where: (a) path 1 is used to shift the both positive disturbance load of the cold stream C1 to heater or cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream C1 to heater or cooler (c) path 3 is used to shift the positive disturbance load of the hot stream H1 to heater or cooler and (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to heater or cooler.

The control systems for alternative 1 work as follows: figure 5.2 shows the hot and cold outlet temperatures of FEHE1 are controlled at their nominal set point by manipulating the valve on the bypass line (VBP1). Whenever the hot outlet temperature of FEHE1 above the allowable limit due to, for example, a positive disturbance load entering the hot stream H1 (figure 5.2 c)), the control action to the hot temperature control (TC1) close the valve VBP1.

As a result, the hot outlet temperature of FEHE1 will drop to its normal temperature and the cold outlet temperature of FEHE1 will be further increased. If the hot outlet temperature of FEHE1 drops below the allowable limit, i.e., a desired-condition during operation, due to the negative disturbance load entering the hot stream H1 (figure 5.2 d)), the control action to TC2 out open the valve VBP1. Consequently, the hot outlet temperature of FEHE1 will rise to its normal temperature and the cold outlet temperature of FEHE1 will be increased. In the case of cold stream, disturbances (figure 5.2 a) and d)) can transfer to heater or cooler like path 3 and path 4 so a selector controller with low selector switch (LSS) for FEHE1 is employed to select an appropriate heat pathway.

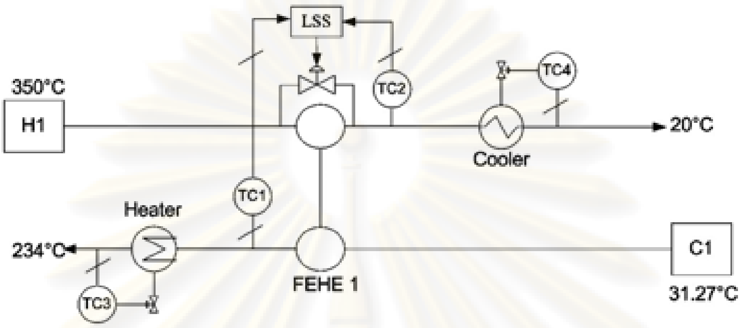


Figure 5.2 Control configurations of alternative 1

5.3.2 Design of Heat Pathways and HEN Control Configuration for Alternative 2

The design of the heat pathways for alternative 2 is shown in Figure 5.3. The controller of FEHE1 between H1 and C1 is like alternative 1. Consideration in other streams, when cold inlet (C2) temperature decreases (figure 5.5 c)) should be activated by controlling the cold outlet temperature of FEHE2 (VBP2). This will have the effect of shifting the positive disturbance load to heater2. Thus, heater2 duty will be increase. When the inlet cold temperature increases (figure 5.5 d)) should be activated by controlling the cold outlet temperature of FEHE2 to shift its negative disturbance load to heater2. Thus, heater2 duty will be increase. Consideration the case when disturbance in hot inlet (H1) temperature occurs (figure 5.5 e) and f)) should be activated by controlling the hot outlet temperature of FEHE2 (VBP2).

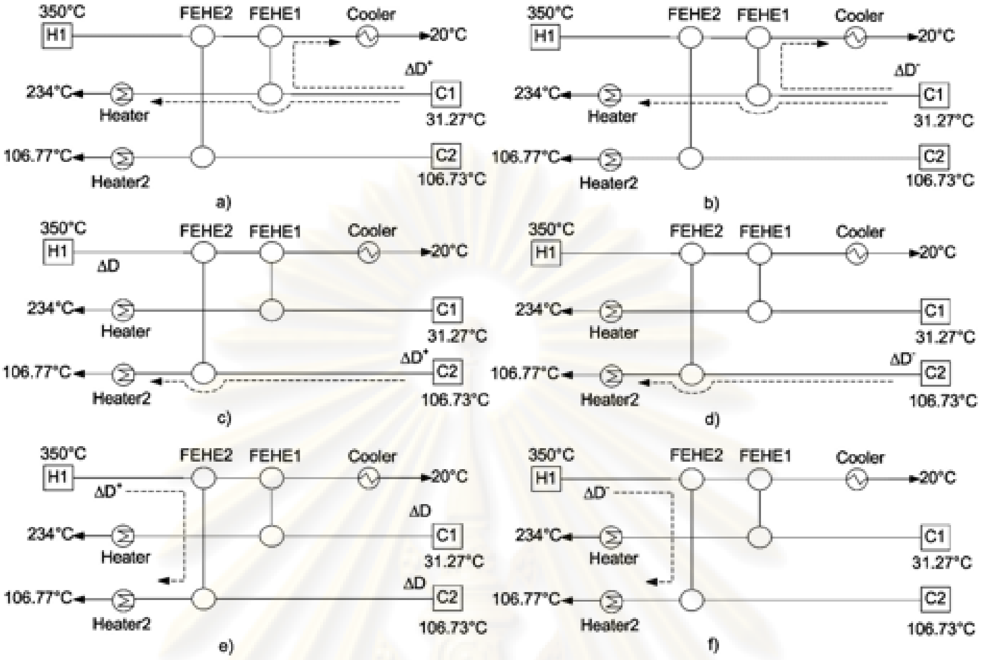
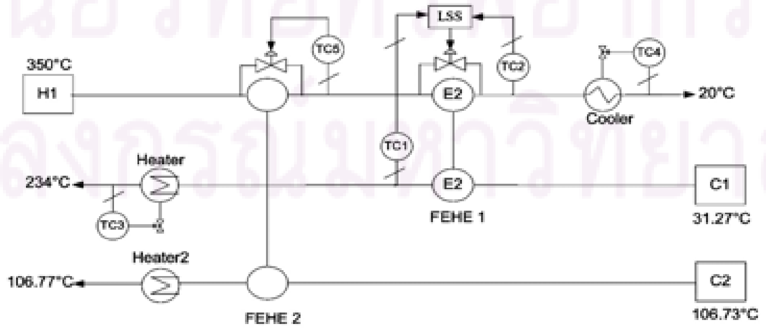


Figure 5.3 Heat pathways through alternative 2, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C1 to heater or cooler,(b) path 2 is used to shift the negative disturbance load of the cold stream C1 to heater or cooler, (c) path 3 is used to shift the positive disturbance load of the cold stream C2 to heater2, (d) path 4 is used to shift the negative disturbance load of the cold stream C2 to heater2, (e) path 5 is used to shift the positive disturbance load of the hot stream H1 to heater2, (f) path 6 is used to shift the negative disturbance load of the hot stream H1 to heater2



Figyre 5.4 Control configurations of alternative 2

5.3.3 Design of Heat Pathways and HEN Control Configuration for Alternative 3

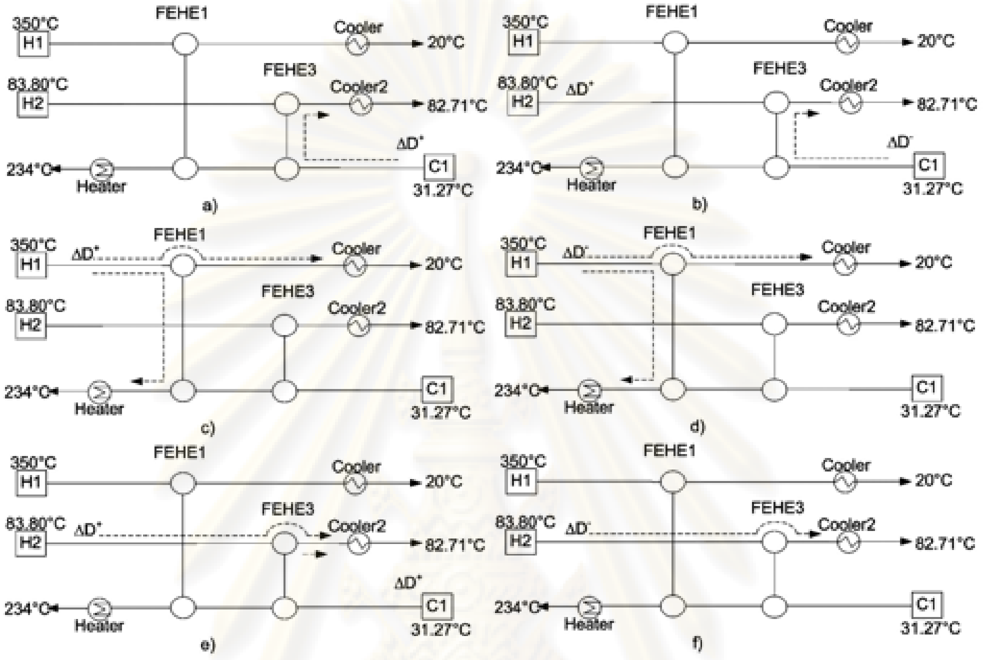


Figure 5.5 Heat pathways through alternative 3, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C1 to cooler2, (b) path 2is used to shift the negative disturbance load of the cold stream C1 to cooler2 ,(c) path 3 is used to shift the positive disturbance load of the hot stream H1 to heater or cooler, (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to heater or cooler, (e) path 5 is used to shift the positive disturbance load of the hot stream H3 to cooler2 (f) path 6 is used to shift the negative disturbance load of the hot stream H3 to cooler2.

The design of the heat pathways for alternative 3 is shown in figure 5.5.The controller of FEHE1 between H1 and C1 is like alternative 1. Consideration in other streams, when cold inlet (C1) temperature decreases (figure 5.5 a)) should be activated by controlling the cold outlet temperature of FEHE3 (VBP3). This will have the effect of shifting the positive disturbance load to cooler2. Thus, cooler2 duty will be decreased. When the inlet cold temperature increases (figure 5.5 b)) should be activated by controlling the cold outlet temperature of FEHE3 to shift its negative disturbance load to cooler. Thus, cooler2 duty will be increase. Consideration the case when disturbance in hot inlet (H2) temperature occurs (figure 5.5 e) and f)) should be activated by controlling the cold outlet temperature of FEHE3 (VBP3).

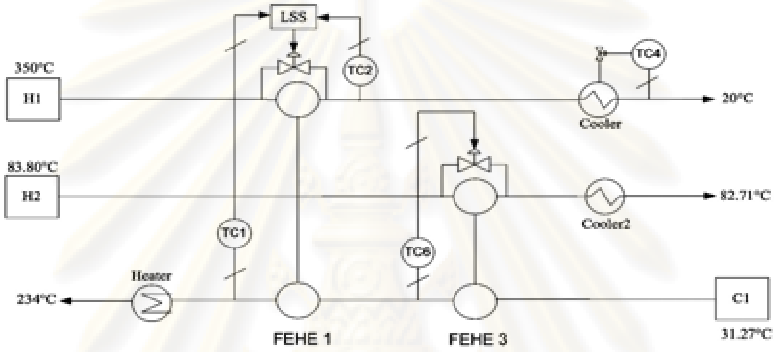


Figure 5.6 Control configurations of alternative 3

Figure 5.7 to 5.22 show the control structure 1, 2, 3 and 4 which simulatd by HYSYS for alternative 1, 2 and 3 in acetone process.

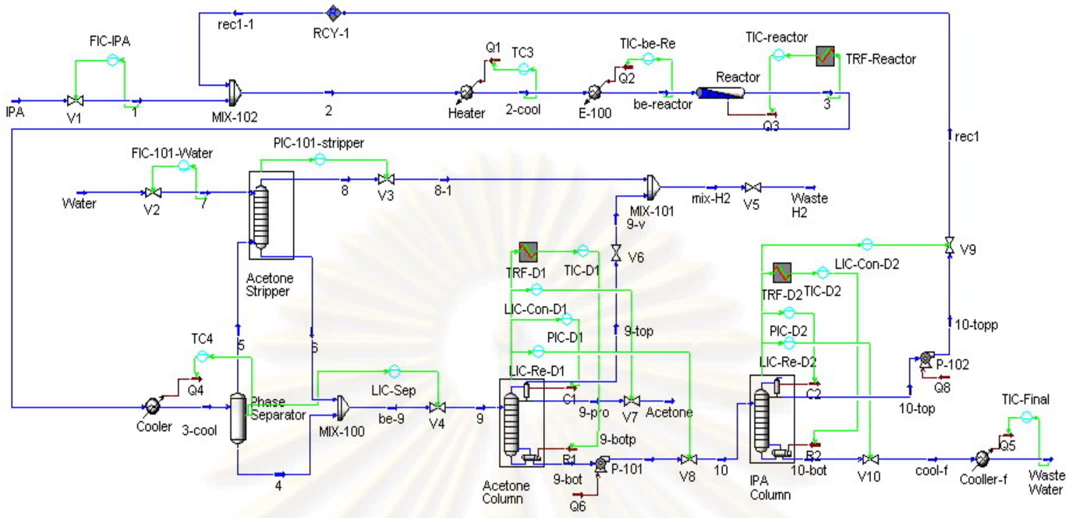


Figure 5.7 Application of reference control structure 1 (CS1) Base case

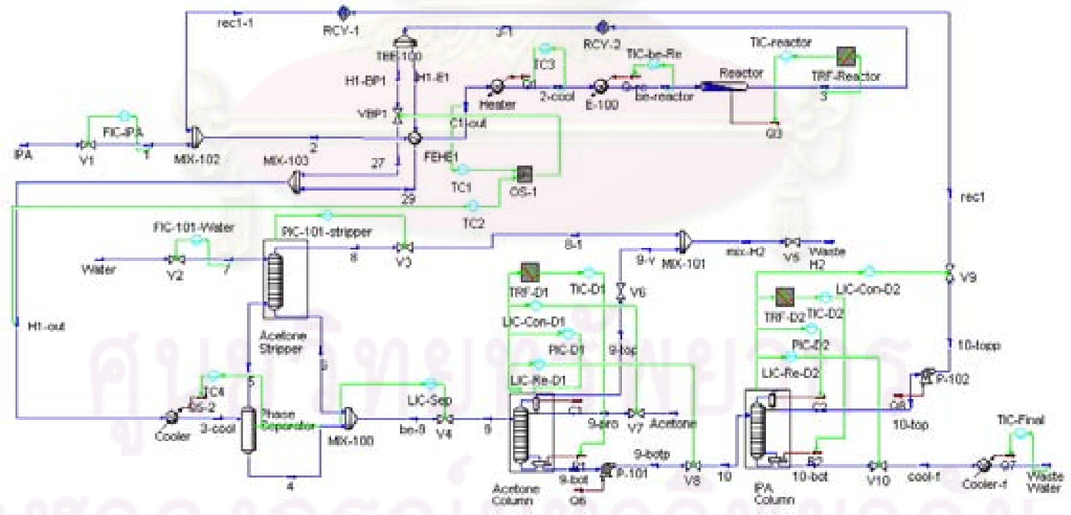


Figure 5.8 Application of reference control structure 1 (CS1) Alt. 1

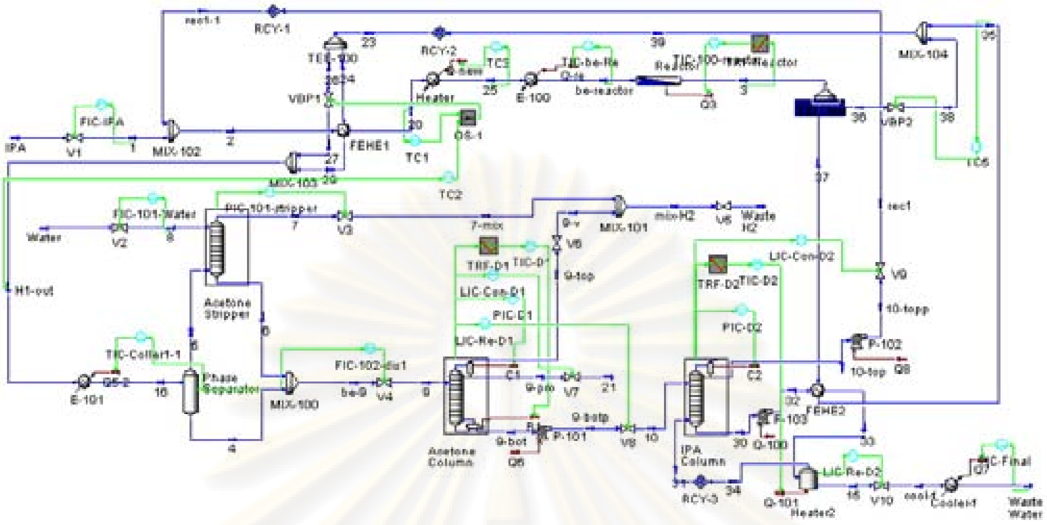


Figure 5.9 Application of reference control structure 1 (CS1) Alt. 2

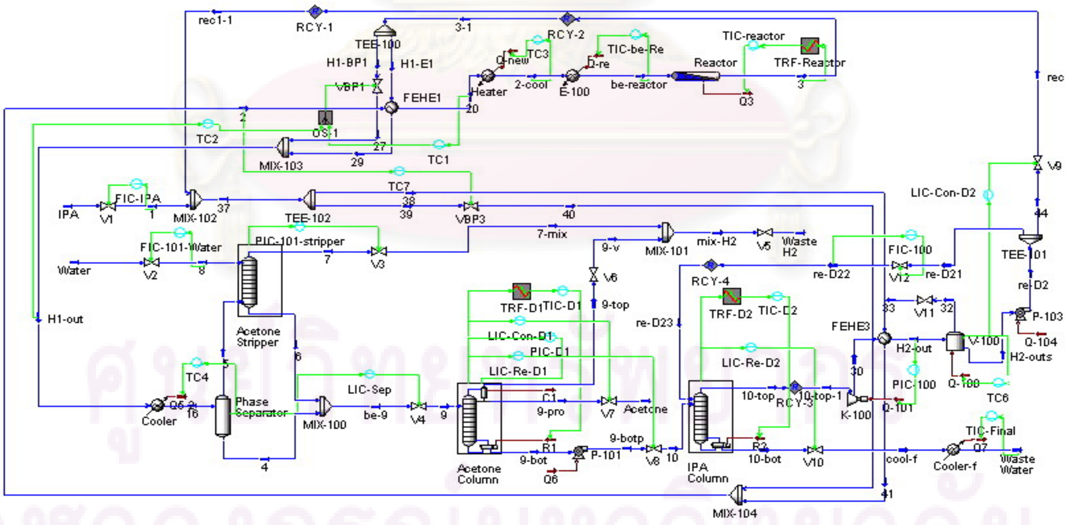


Figure 5.10 Application of reference control structure 1 (CS1) Alt. 3

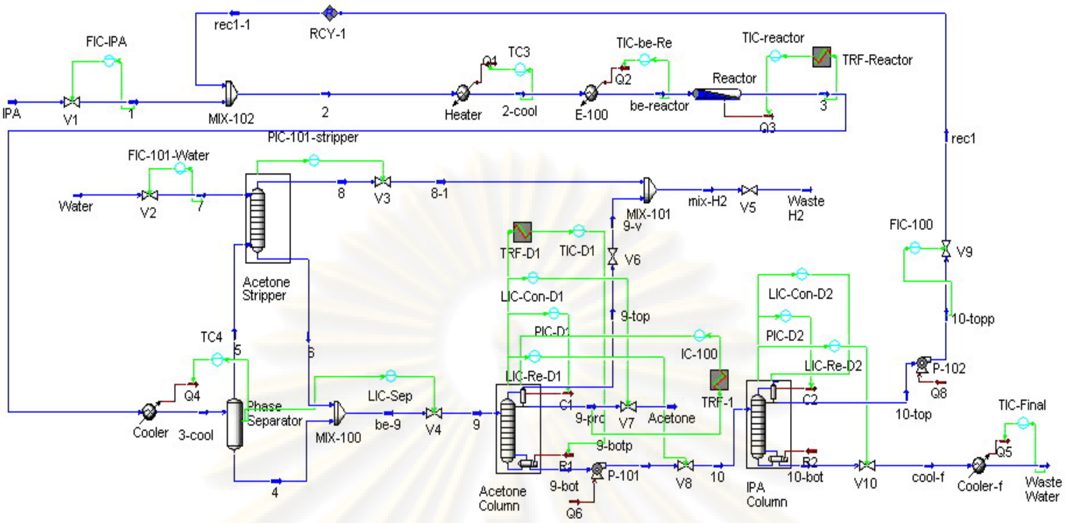


Figure 5.11 Application of reference control structure 2 (CS2) Base case

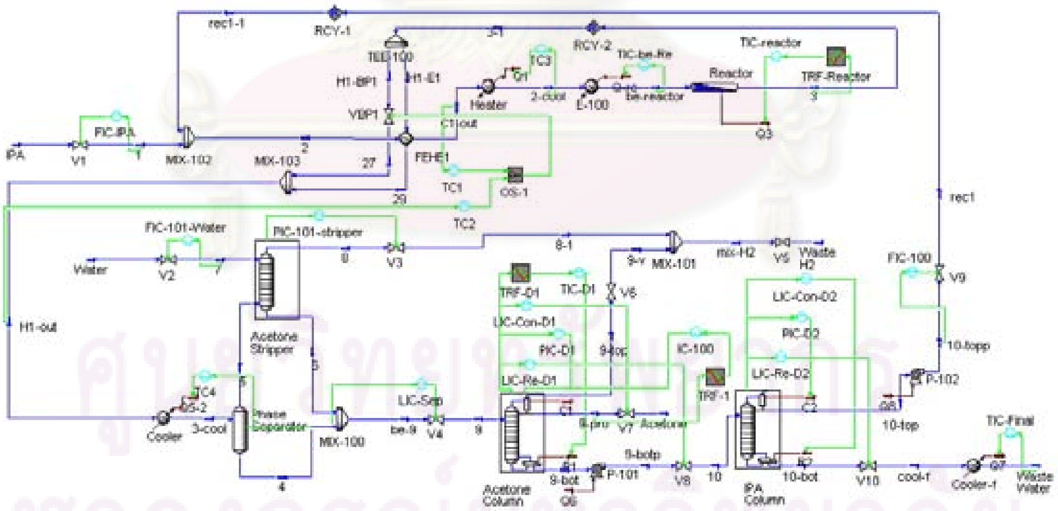


Figure 5.12 Application of reference control structure 2 (CS2) Alt.1

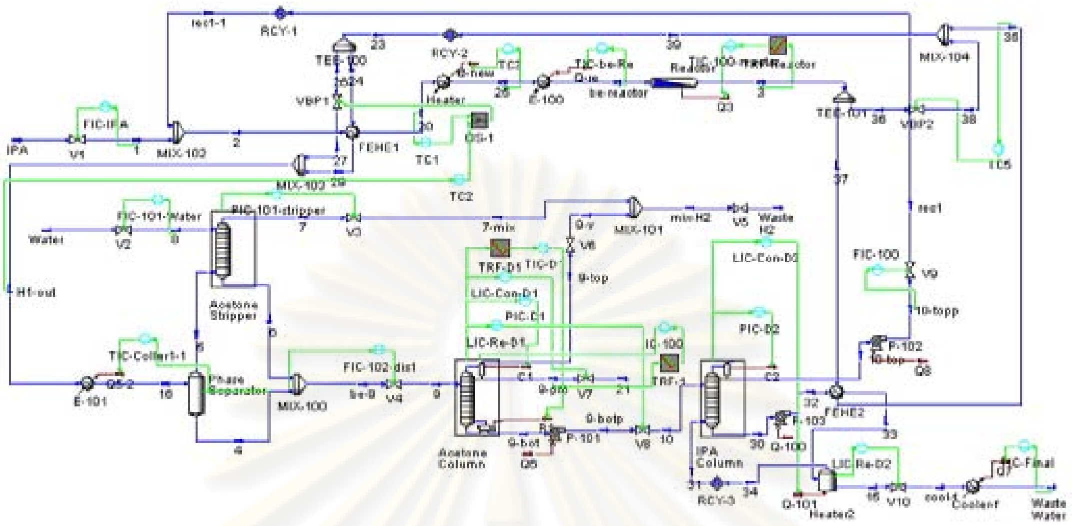


Figure 5.13 Application of reference control structure 2 (CS2) Alt.2

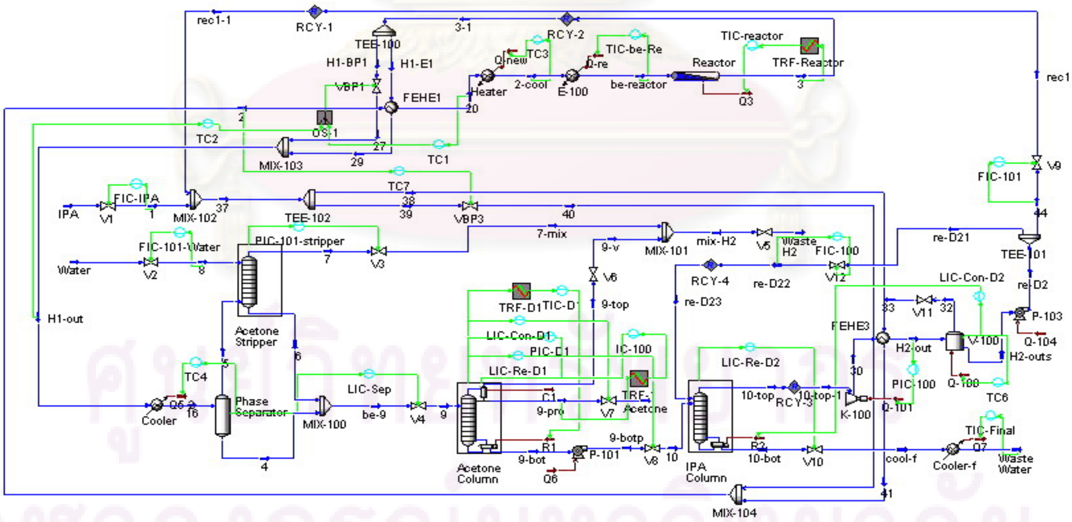


Figure 5.14 Application of reference control structure 2 (CS2) Alt.3

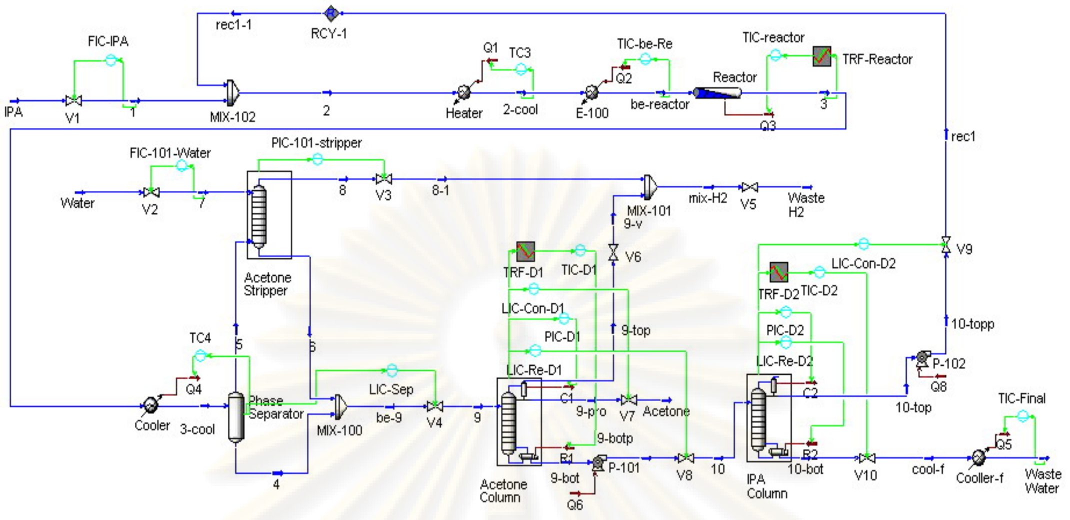


Figure 5.15 Application of reference control structure 3 (CS3) Base case

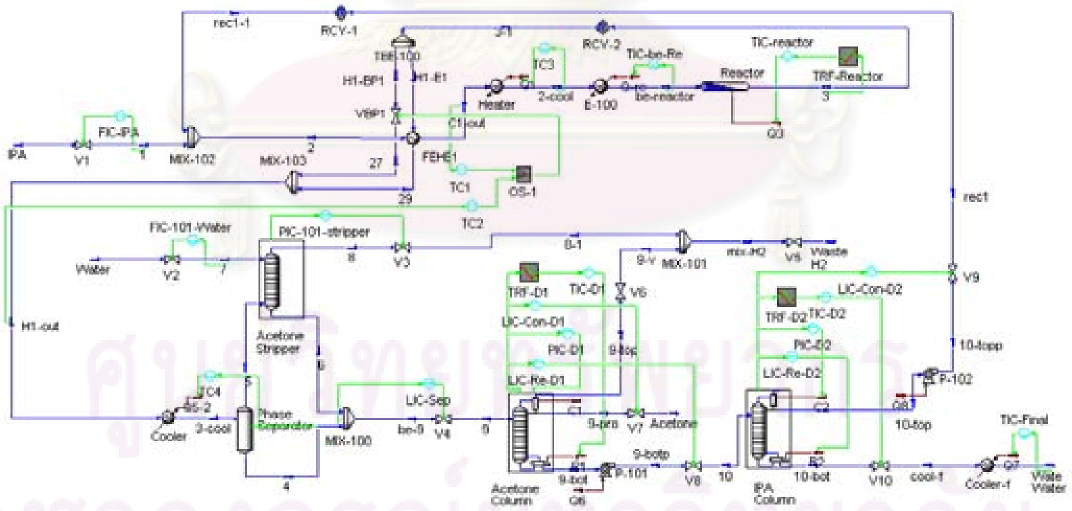


Figure 5.16 Application of reference control structure 3 (CS3) Alt.1

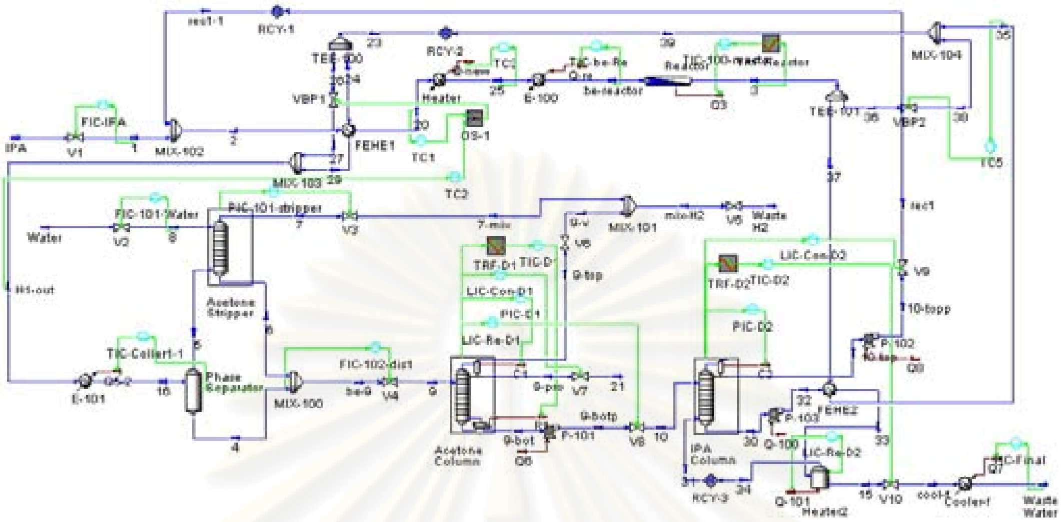


Figure 5.17 Application of reference control structure 3 (CS3) Alt.2

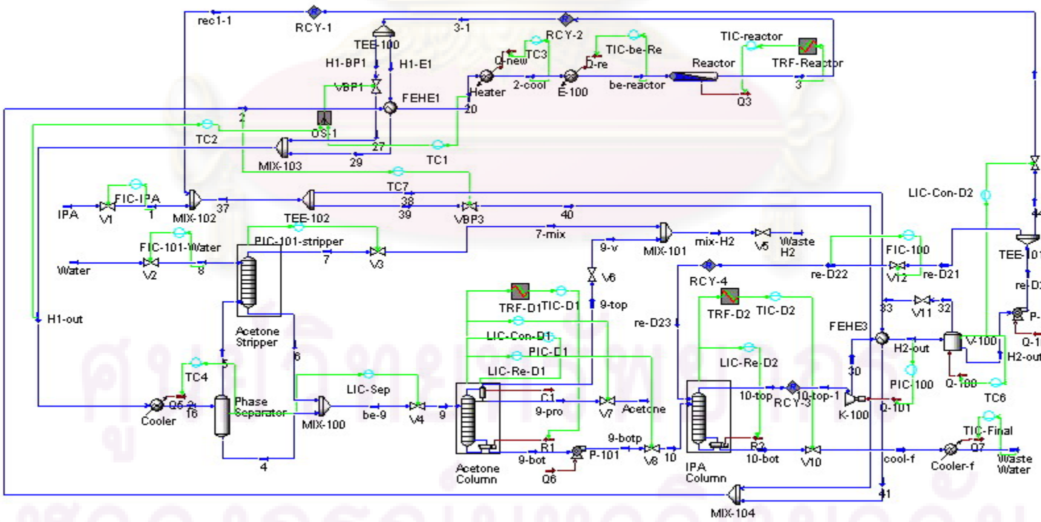


Figure 5.18 Application of reference control structure 3 (CS3) Alt.3

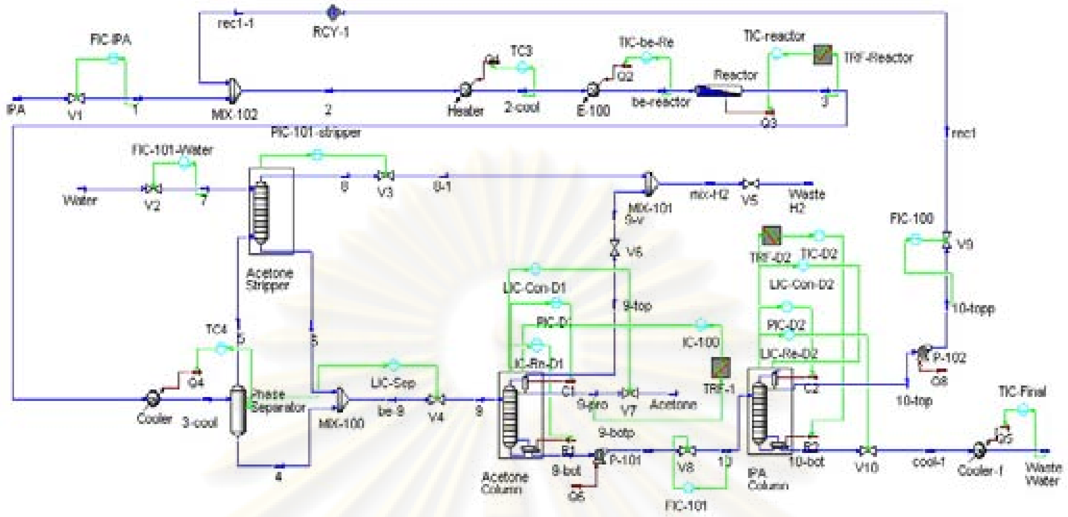


Figure 5.19 Application of reference control structure 4 (CS4) Base case

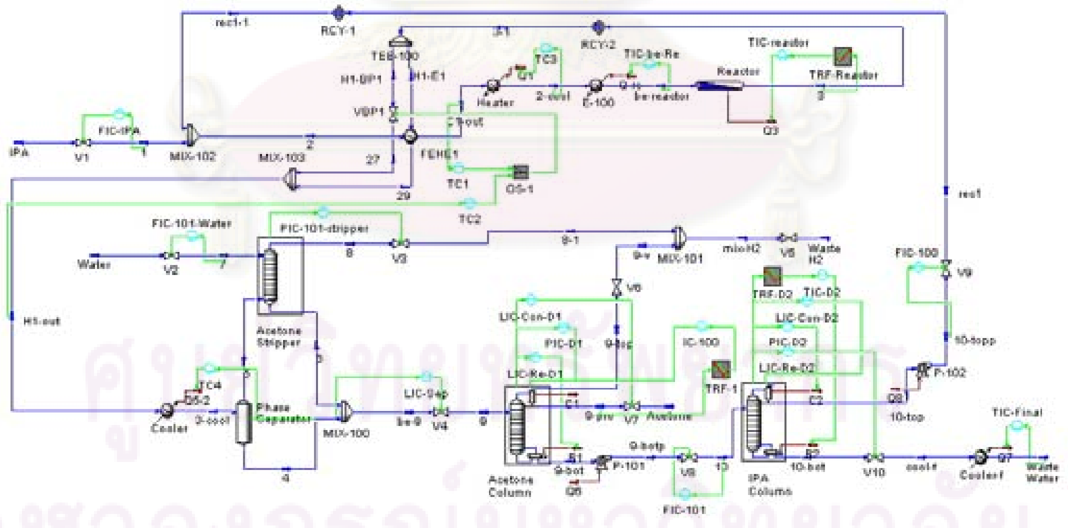


Figure 5.20 Application of reference control structure 4 (CS4) Alt.1

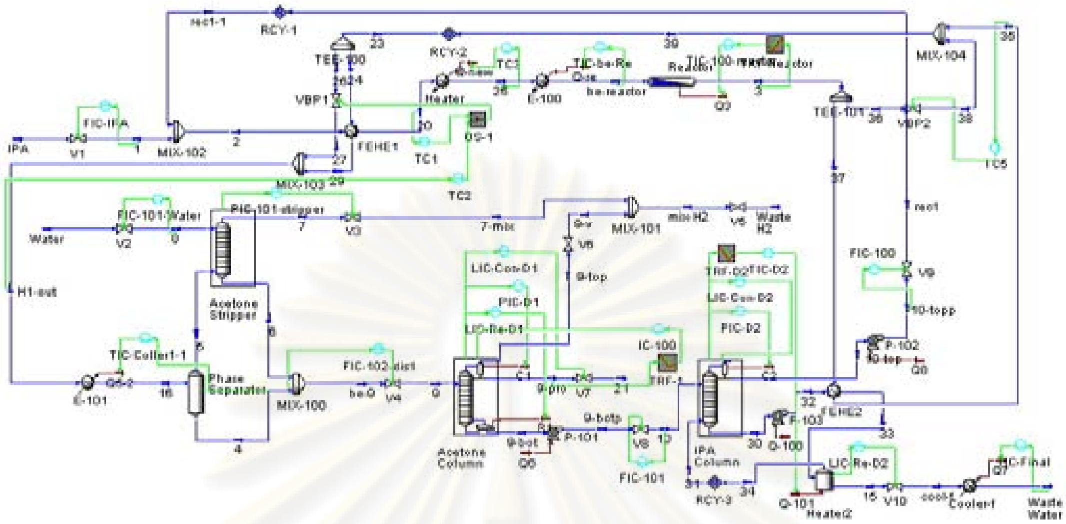


Figure 5.21 Application of reference control structure 4 (CS4) Alt.2

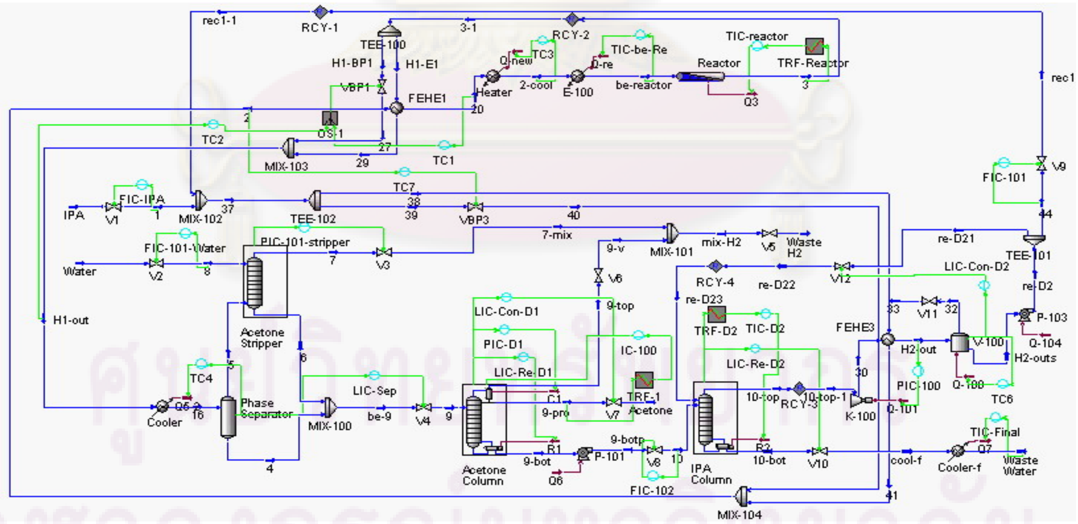


Figure 5.22 Application of reference control structure 4 (CS4) Alt.3

5.4 Dynamic simulation result

In order to illustrate the dynamic behaviors of our control structures, two types of disturbance: thermal and material disturbances are used to test response of the system. Temperature controllers are PIDs which are tuned using relay feedback. Temperature measurement lags of 0.5 minute are included in the temperature loops. A 3-minute deadtime is assumed in the product composition measurement (distillate from the acetone column). Flow and pressure controller are PIs and their parameters are heuristics values. Proportional-only level controllers are used and their parameters are heuristics values. All control valves are half-open at nominal operating condition.

5.4.1 Change in the thermal disturbance of hot stream (reactor outlet stream)CS 1 to CS 4 for base case

Figure 5.23 to 5.26 show the dynamic responses of the acetone plant in the heat load disturbance of the hot stream (the reactor outlet temperature stream). This disturbance made as follows: The reactor outlet temperature is increased from 350^0C to 355^0C at time equals 10 minutes, and the decreased from 355^0C to 345^0C at time equals 200 minutes and then return to its set point at time equals 400 minutes.

In all control structures give the same trend result to reject thermal disturbance which can reject disturbance and return to their setpoint. Effect from increasing temperature (positive disturbance), the IPA fresh feed flowrate (see figure above) and water flowrate are decreased (figure 5.23 to 5.26 h)). The acetone product flowrate is decreased too (figure 5.23 to 5.26 c)) because of endothermic reaction. This disturbance is direct effect to effluent cooler so it adjusts by increasing duty (figure 5.23 to 5.26 d)). When decrease 5^0C step decrease in outlet reactor exit temperature (negative disturbance), the dynamic responses of control system are contrary from increasing the outlet reactor exit temperature.

Consideration acetone product flowrate, it changes little flowrate when disturbance occurs (figure 5.23 to 5.26 g)) , so the reactor outlet temperature has reverse variation effect to the reaction rate. In IPA column, acetone product composition change little so IPA reboiler duty is quite smooth. All control structures mange disturbance by effluent cooler duty (figure 5.23 to 5.26 a)). Dynamic response of acetone purity in CS2 and CS4 are greater than CS1 and CS3 because CS 2 and CS 3 control purity by reflux flowrate.

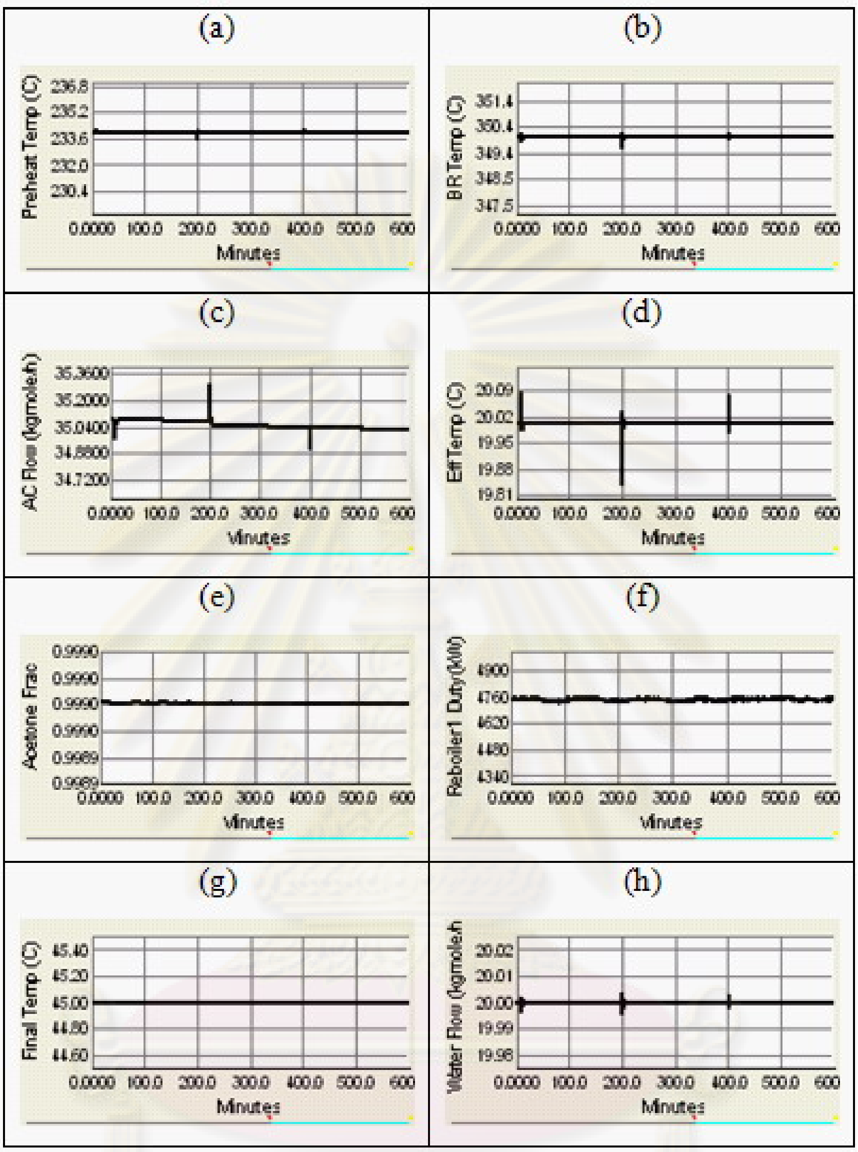


Figure 5.23 Dynamic responses of CS1 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

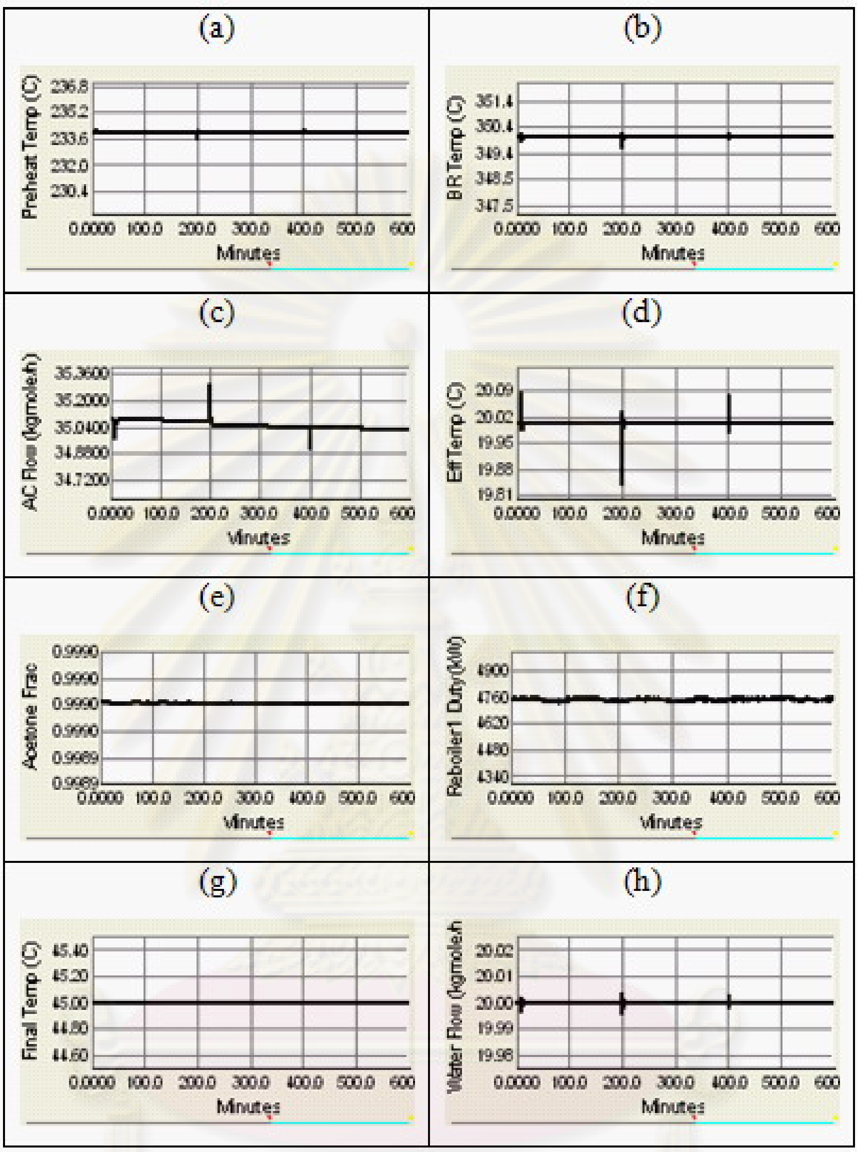


Figure 5.24 Dynamic responses of CS2 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

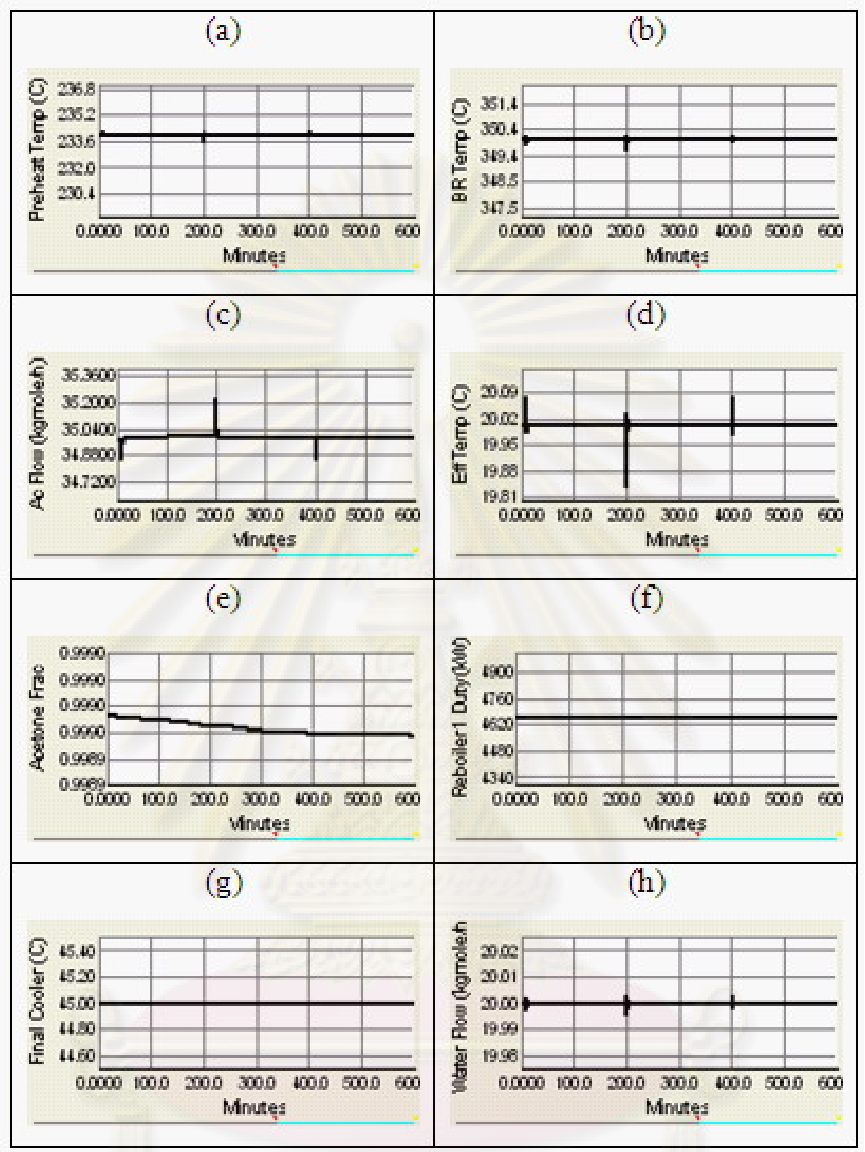


Figure 5.25 Dynamic responses of CS3 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

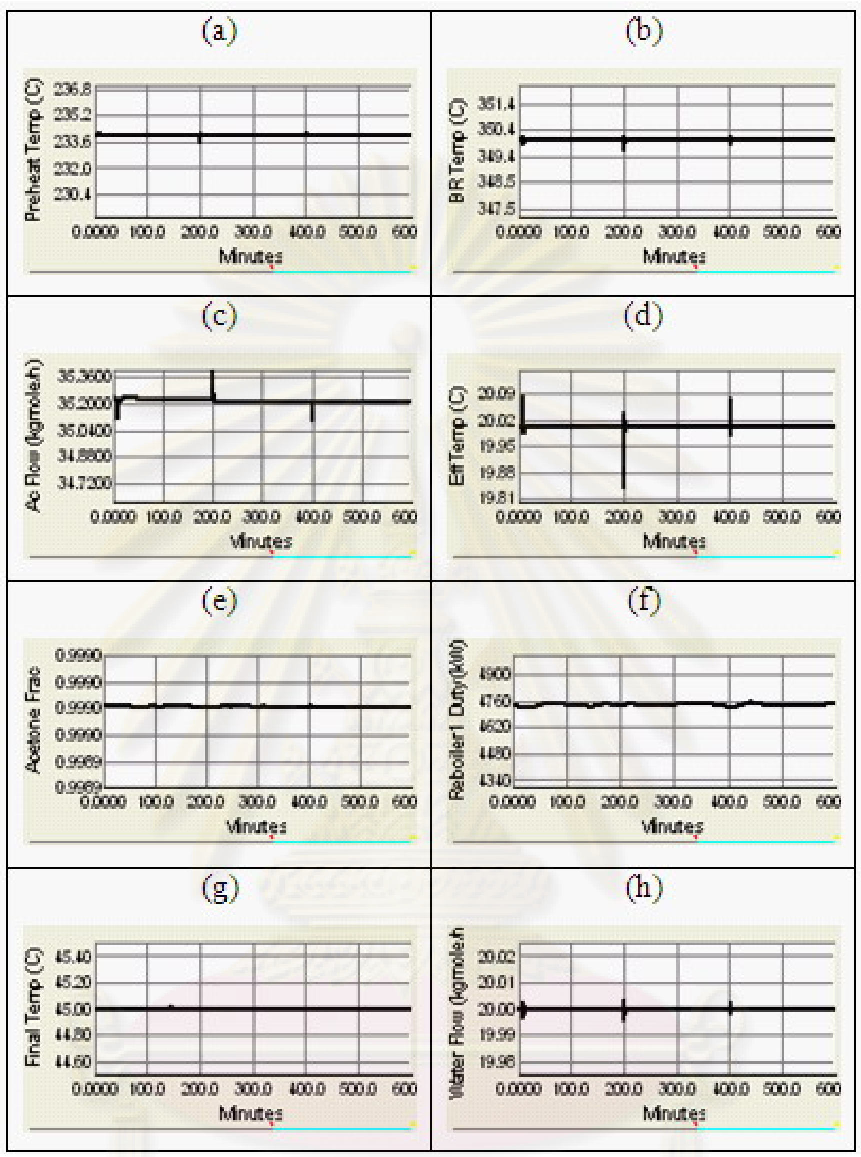


Figure 5.26 Dynamic responses of CS4 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

5.4.2 Change in the thermal disturbance of hot stream (reactor outlet stream)CS 1 to CS 4 for Alt. 1, Alt. 2 and Alt. 3

Figure 5.27 to 5.38 show the dynamic responses of the acetone plant in the heat load disturbance of the hot stream (the reactor outlet temperature stream). This disturbance made as follows: The reactor outlet temperature is increased from 350^0C to 355^0C at time equals 10 minutes, and the decreased from 355^0C to 345^0C at time equals 200 minutes and then return to its set point at time equals 400 minutes.

The dynamic response of alternative 1, 2 and 3 are similar base case. CS 2 and CS 4 are greatter than CS 1 and CS 3. All alternatives have been manages disturbance heat load propagation of hot stream difference from base case. All control structures in alternative 1 and 3 give the same result to shift the heat load disturbance to FEHE1. It control by adjusting bypass valve (VBP 1) and remain disturbance can transfer to heater or effluent cooler (figure a) and b)). In Alternative 2, When disturbance occurs, the heat load disturbance transfers to FEHE 2 so hot outlet temperature should be controlling by bypass valve (VBP 2). Thus, the remain disturbance which transfer to effluent cooler is smaller than alt. 1 and 3 (figure a) and b)). Acetone product flowrate isn't smooth when we compare with base case because of the effect from mangeability disturbance by valve.

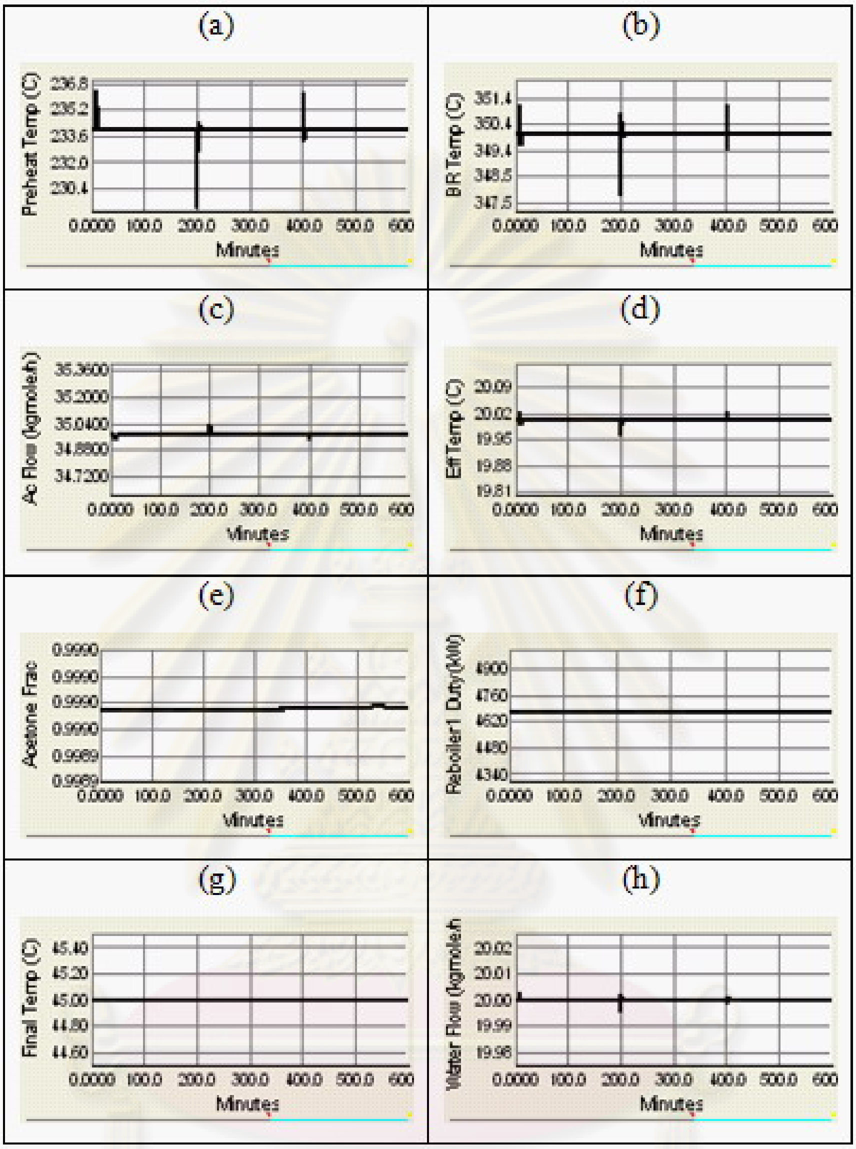


Figure 5.27 Dynamic responses of CS1 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

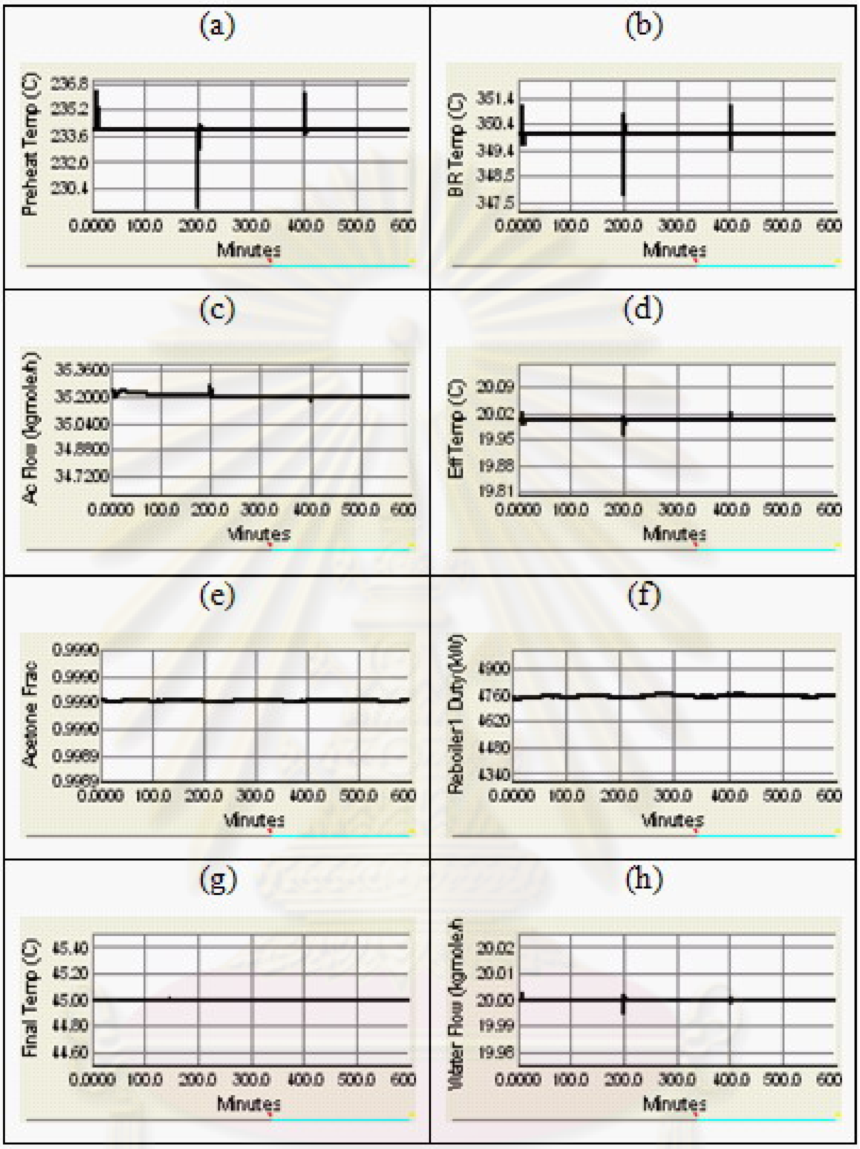


Figure 5.28 Dynamic responses of CS2 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

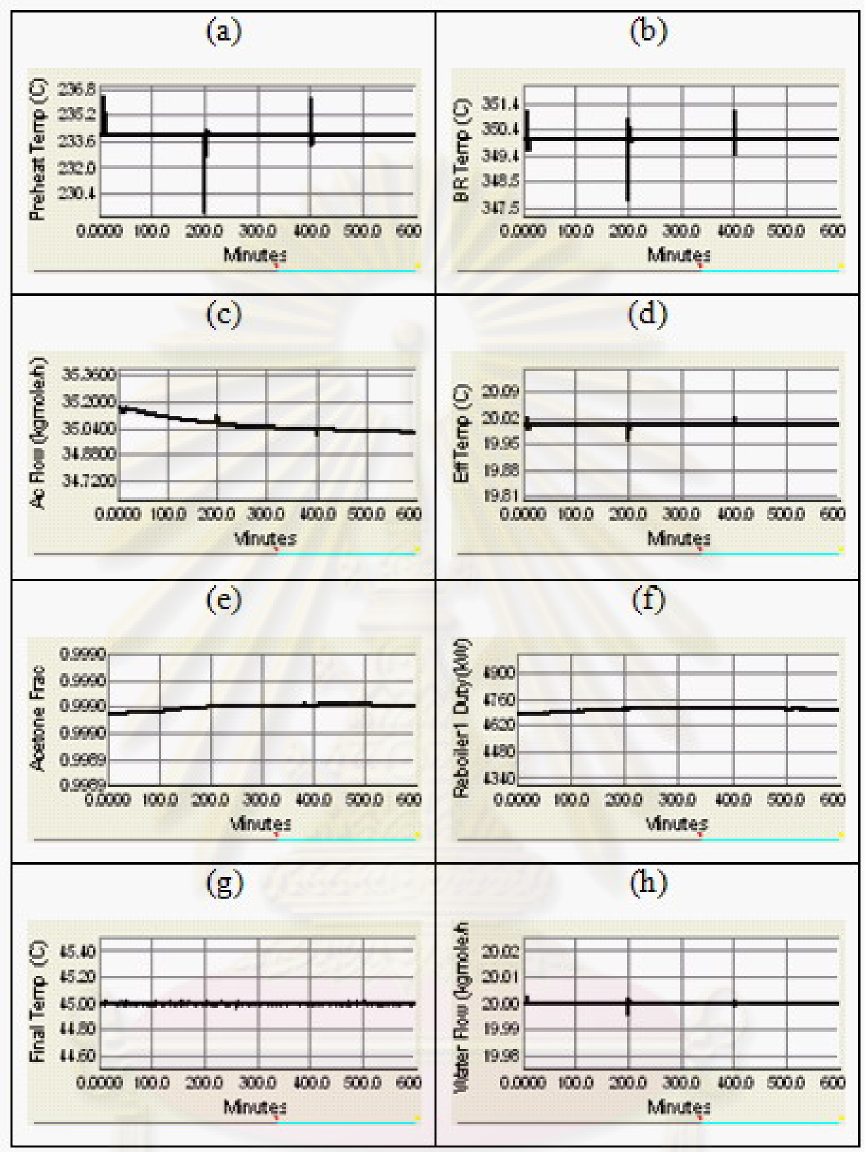


Figure 5.29 Dynamic responses of CS3 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

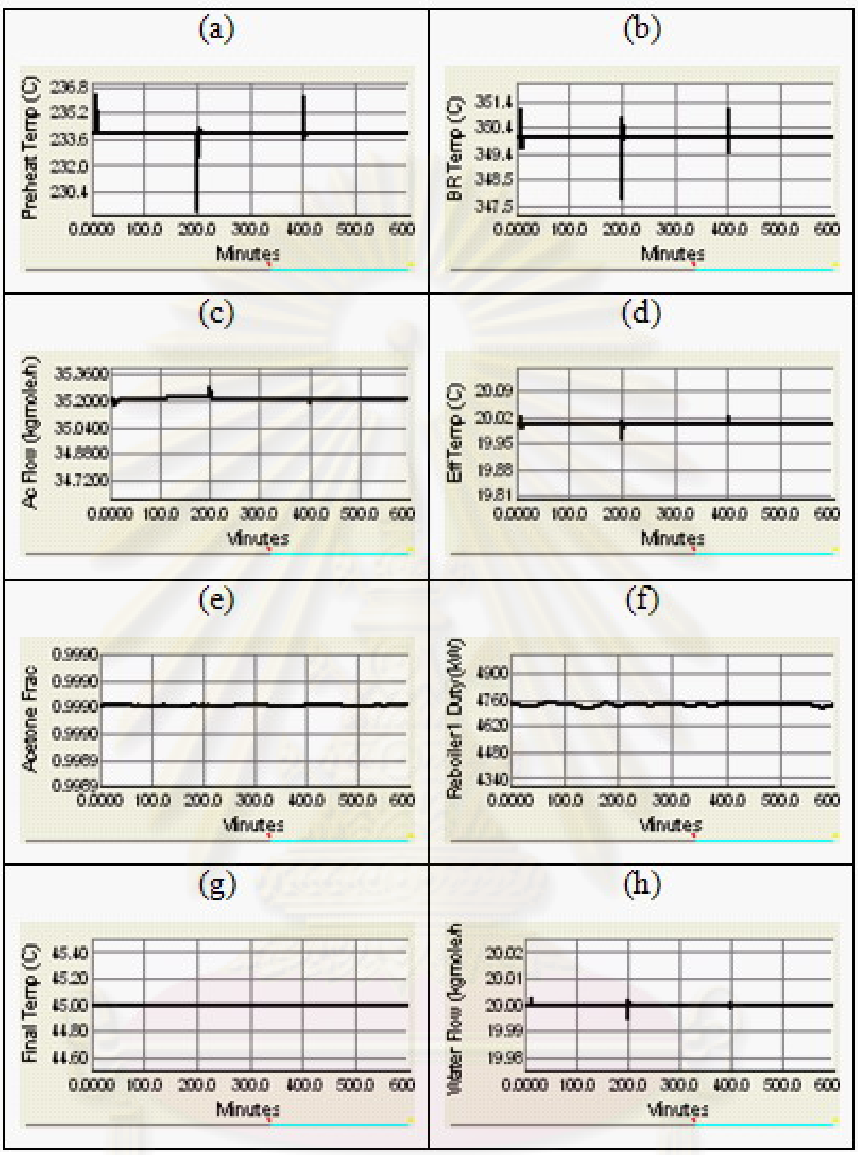


Figure 5.30 Dynamic responses of CS4 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

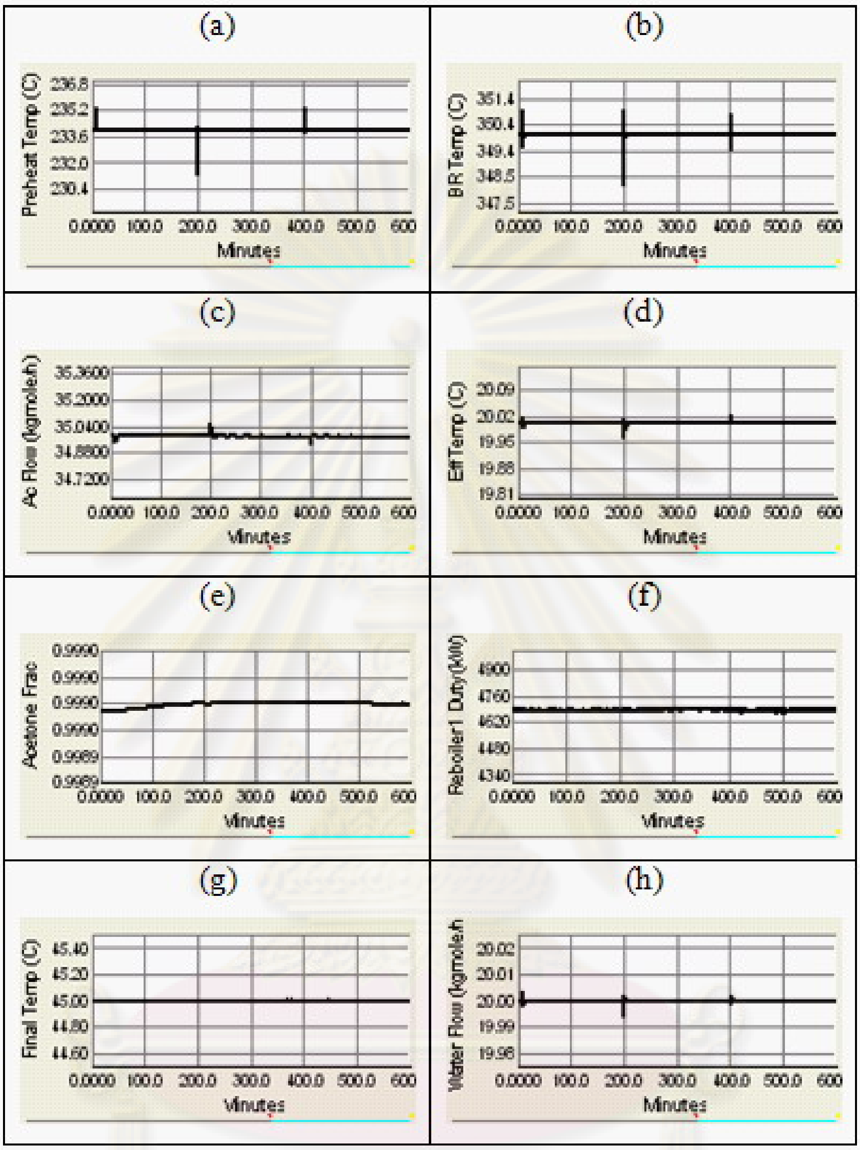


Figure 5.31 Dynamic responses of CS1 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

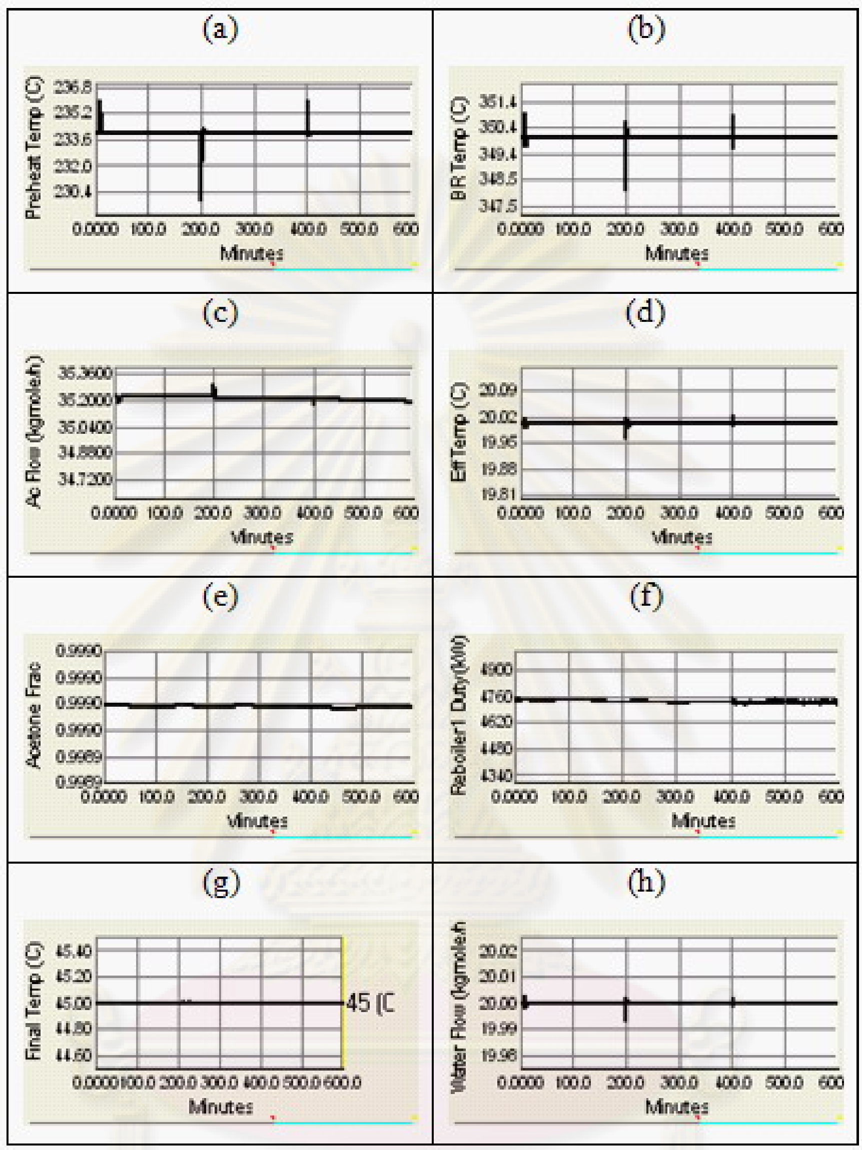


Figure 5.32 Dynamic responses of CS2 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

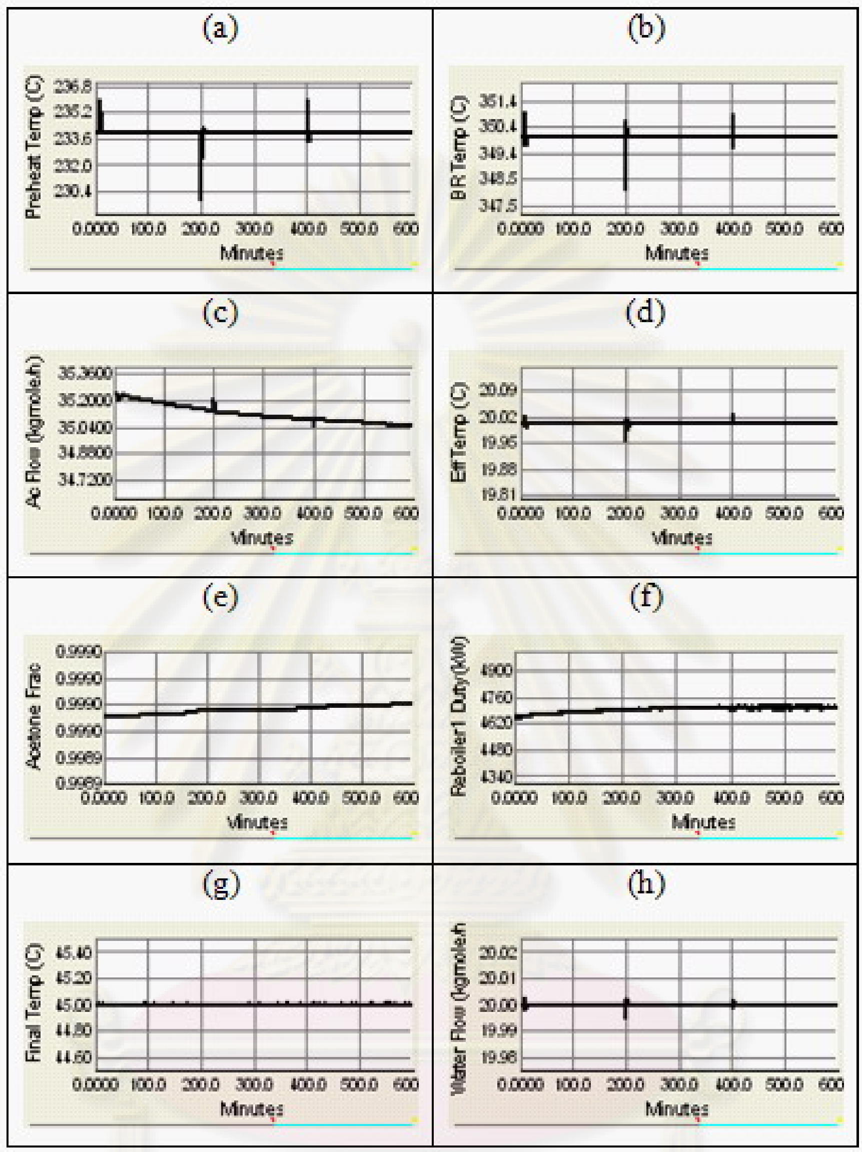


Figure 5.33 Dynamic responses of CS3 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

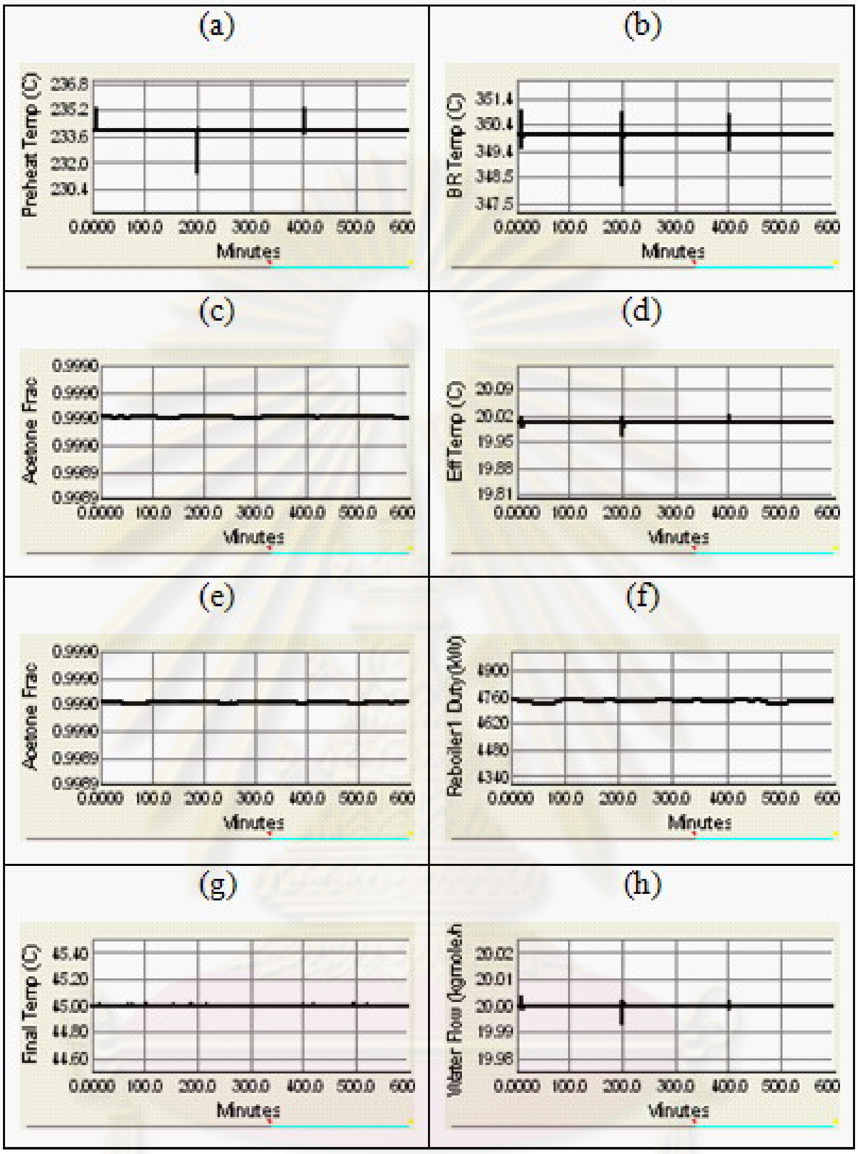


Figure 5.34 Dynamic responses of CS4 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

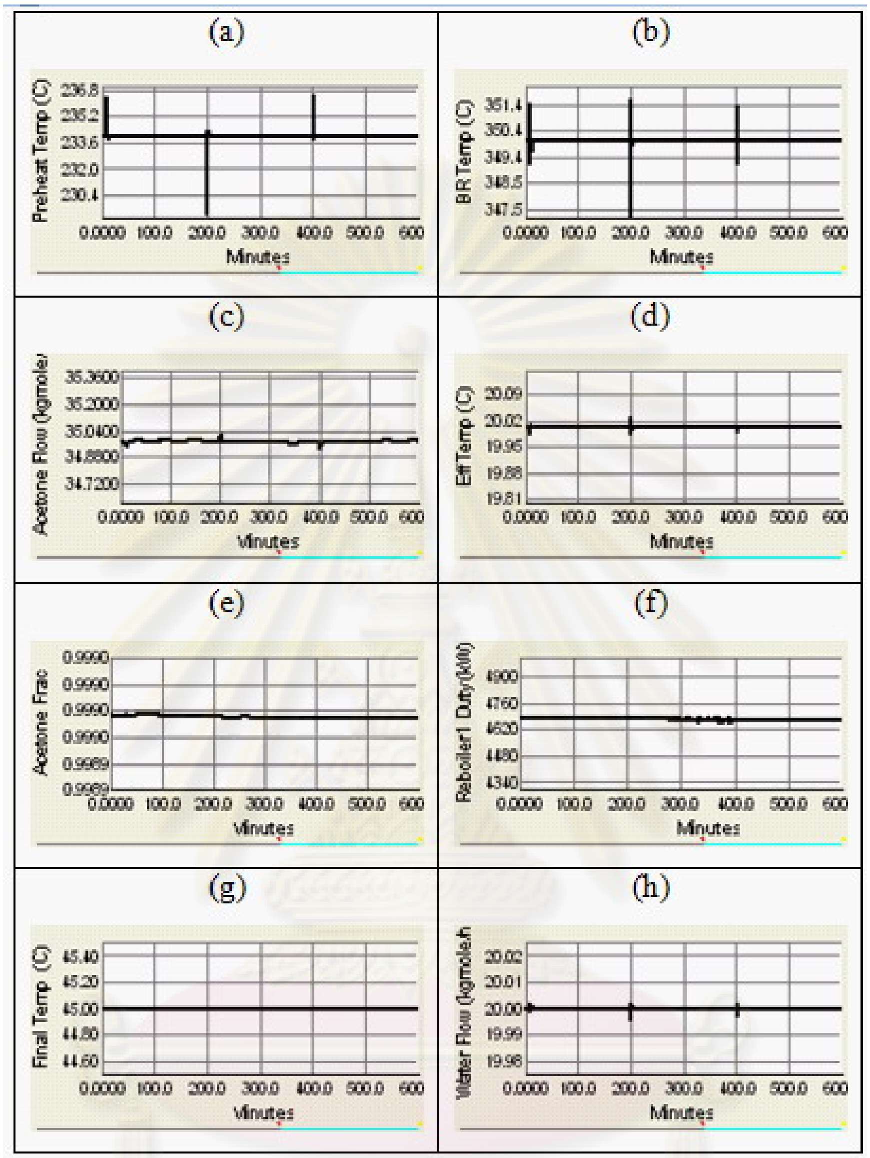


Figure 5.35 Dynamic responses of CS1 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

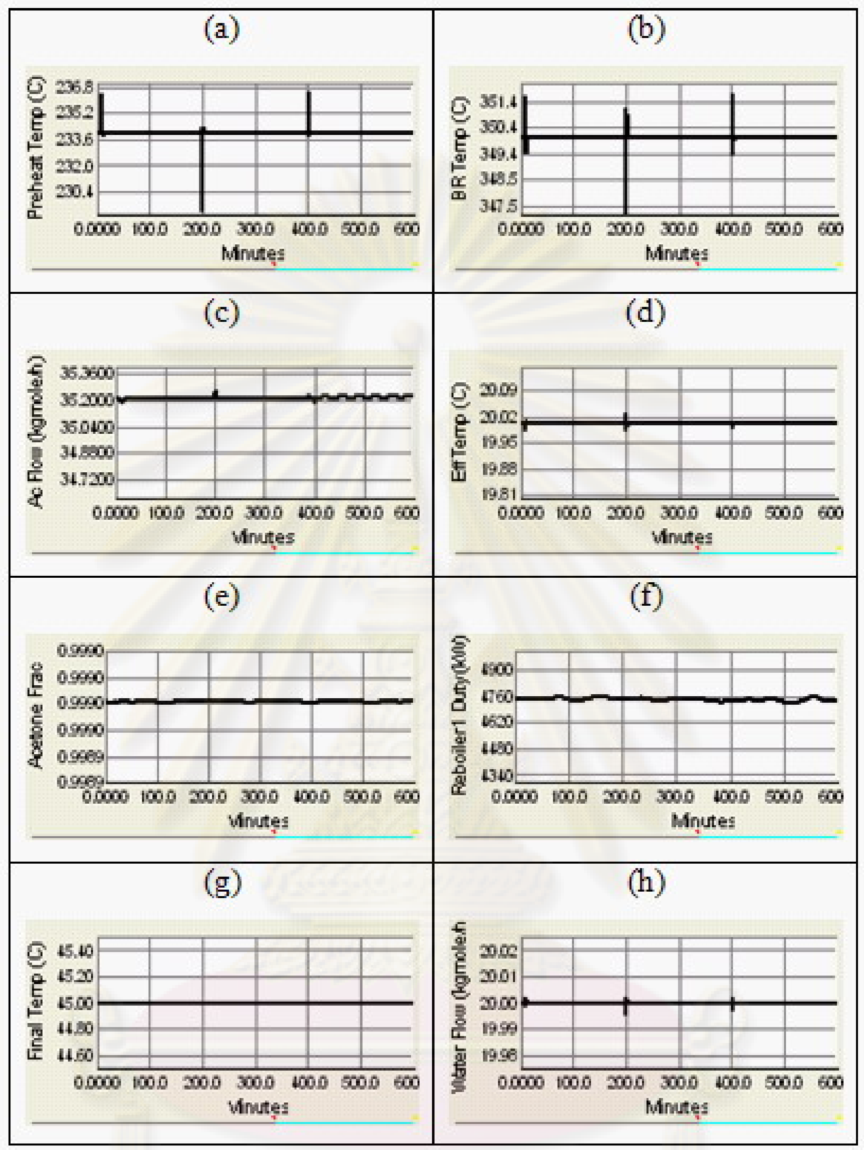


Figure 5.36 Dynamic responses of CS2 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

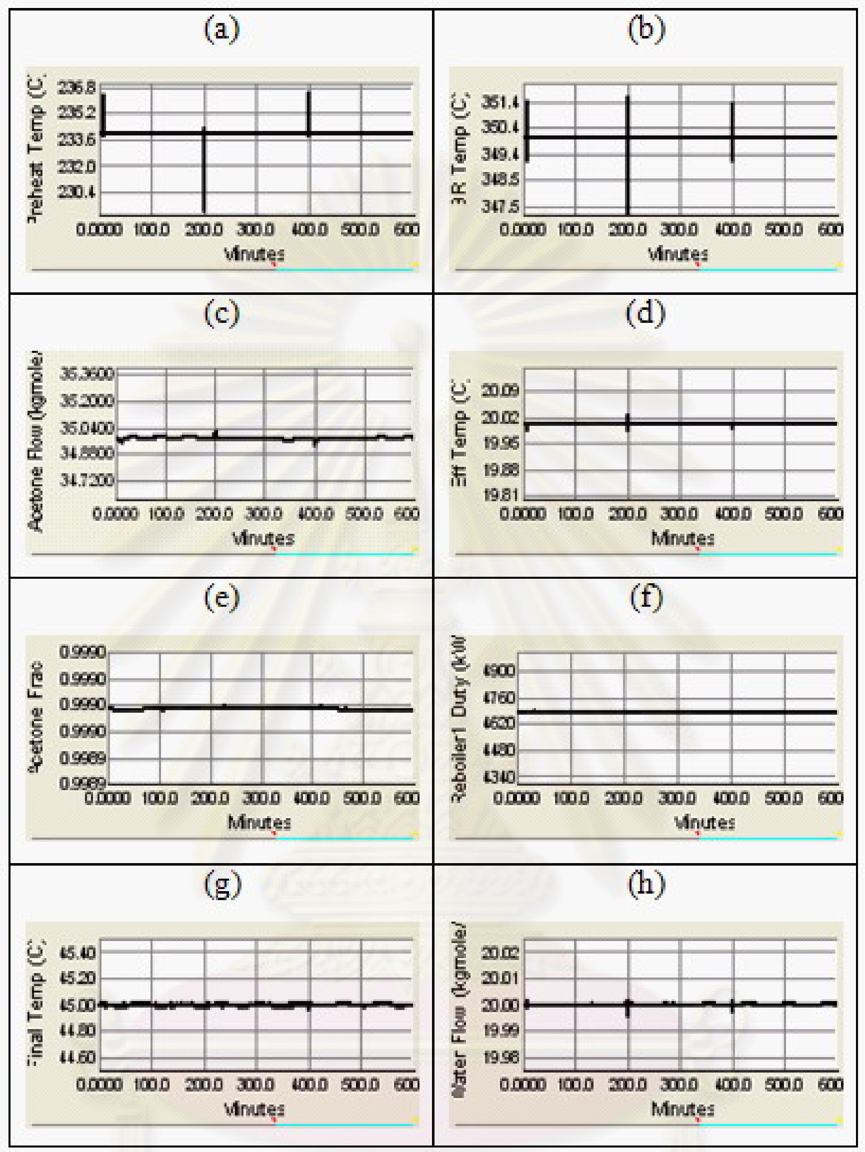


Figure 5.37 Dynamic responses of CS3 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

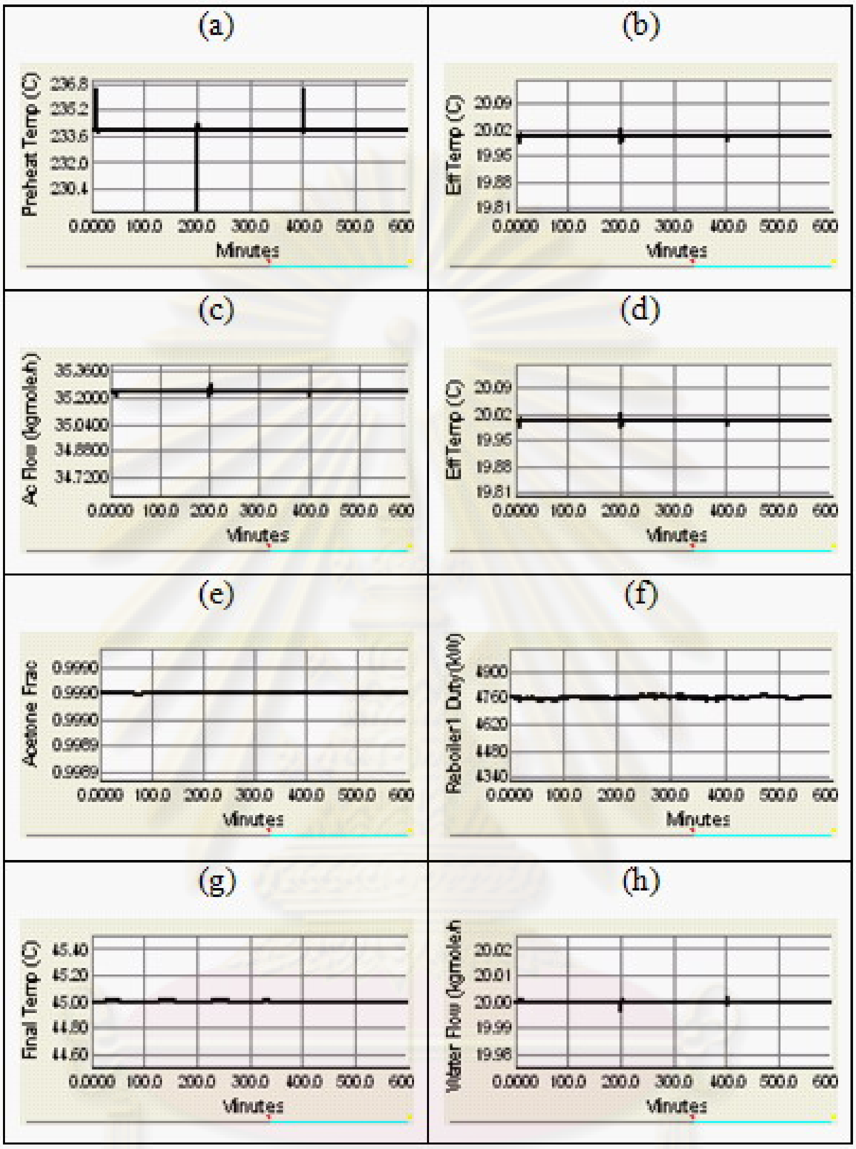
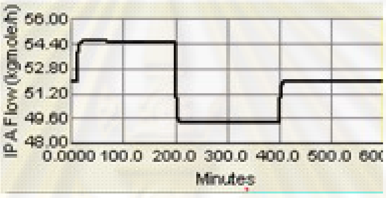


Figure 5.38 Dynamic responses of CS4 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

5.4.3 Change in the material disturbance of cold stream (IPA fresh feed stream) CS 1 to CS 4 for base case

Figure 5.39 to 5.42 show the dynamic responses of the acetone plant in the material disturbance. This disturbance made as follows (see figure below) : The IPA fresh feed is increased from 51.96 kgmole/h to 54.56 kgmole/h at time equals 10 minutes, and the decreased from 54.56 kgmole/h to 49.36 kgmole/h at time equals 200 minutes and then return to its set point at time equals 400 minutes.



All graphs have the same dynamic simulation results which can return to their set point. Consideration all graphs in figure 5.39 to 5.42 c), if fresh feed flowrate increase, acetone product flowrate is increased. When fresh feed flowrate decrease, acetone product flowrate is decreased. Thus, IPA fresh feed is direct effect to acetone product flowrate. Preheat temperature decreased because the temperature which mixed between recycle and fresh feed stream is decreased. This disturbance manage by heater. CS3 gave the worst dynamic response because of the effect from controlling tray temperature in IPA column by bottom valve.

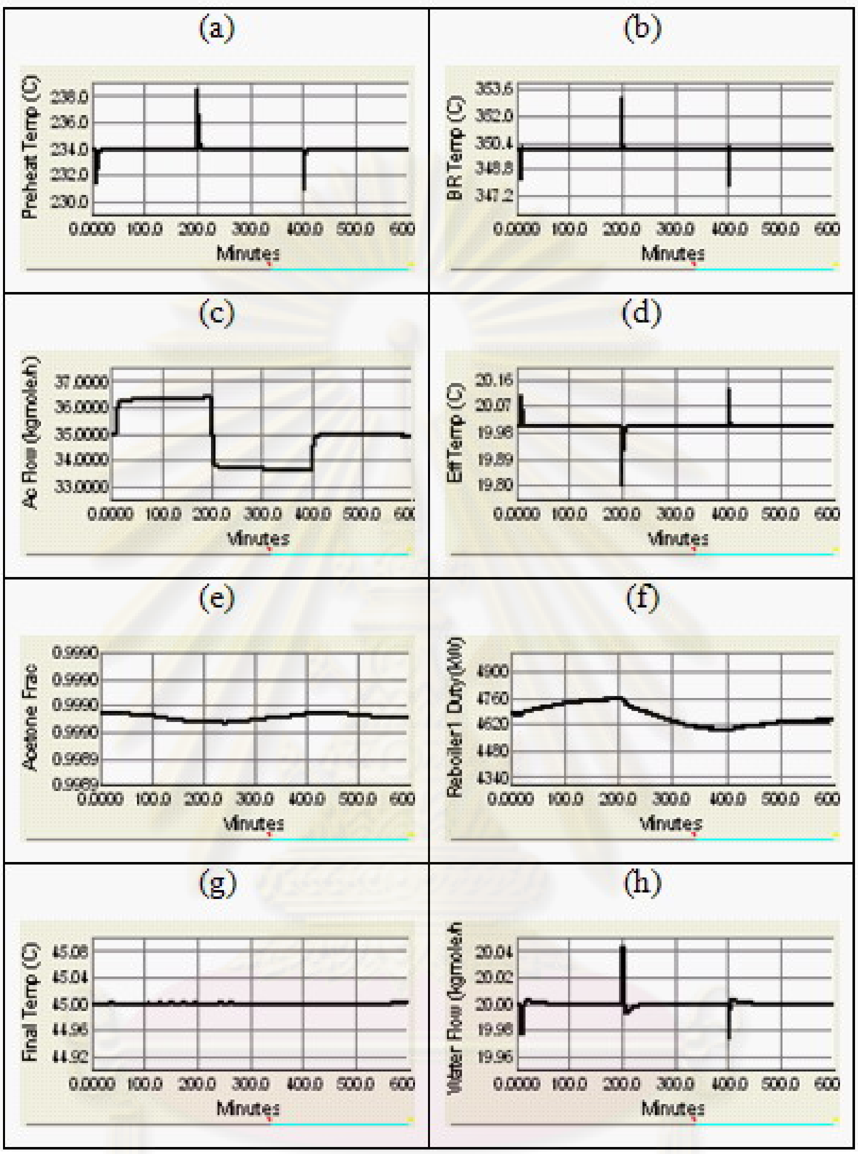


Figure 5.39 Dynamic responses of CS1 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

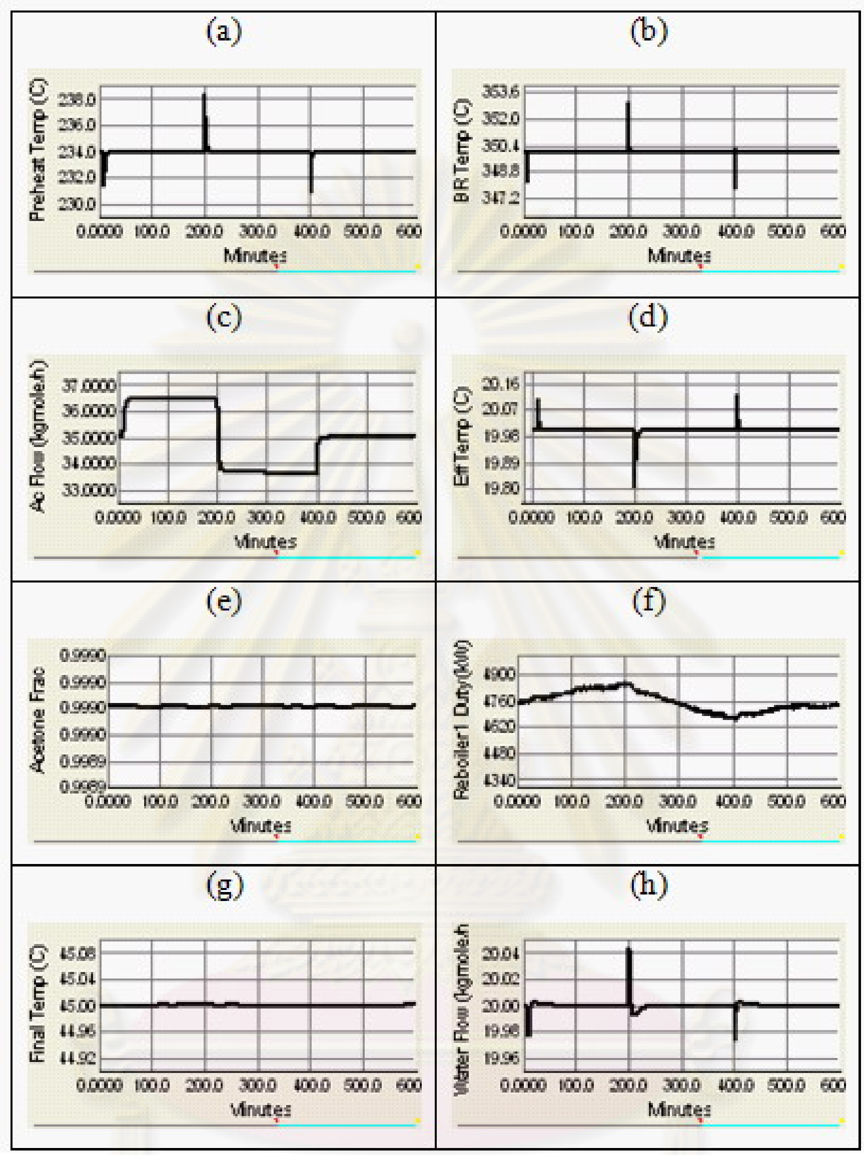


Figure 5.40 Dynamic responses of CS2 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

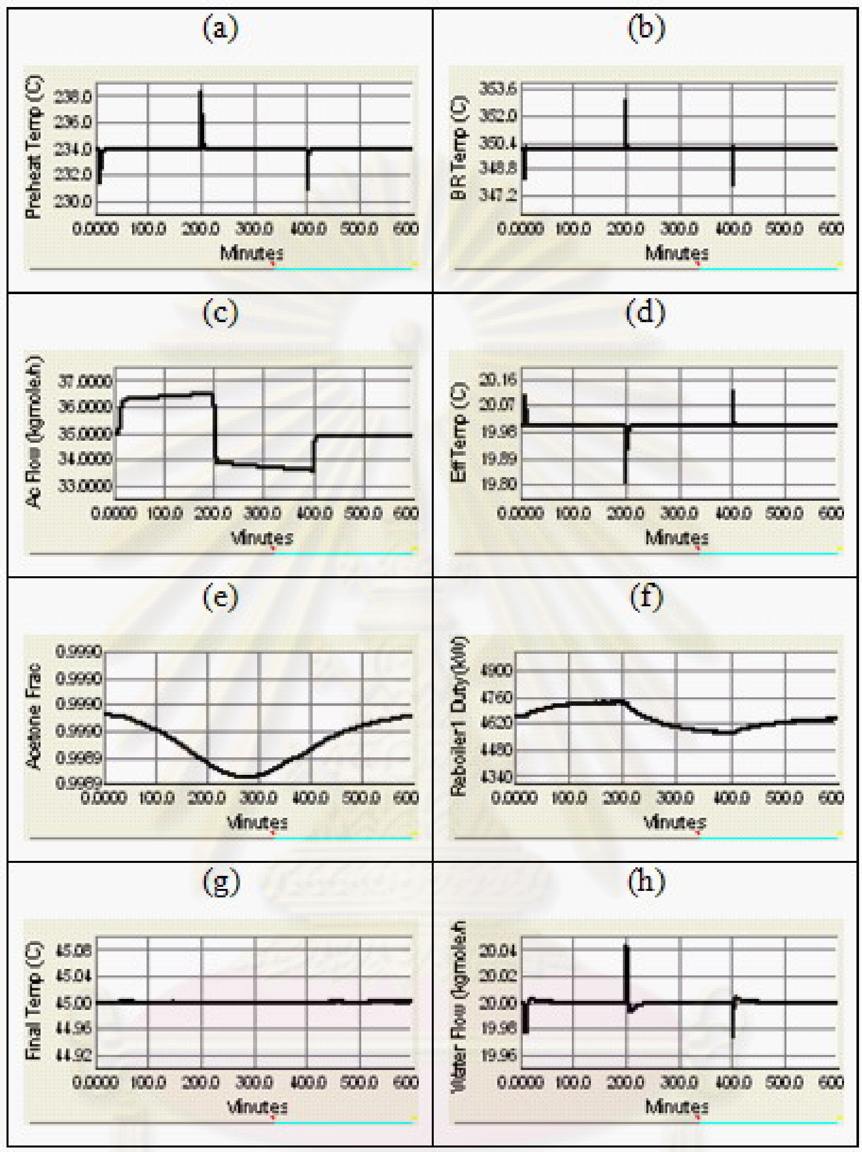


Figure 5.41 Dynamic responses of CS1 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

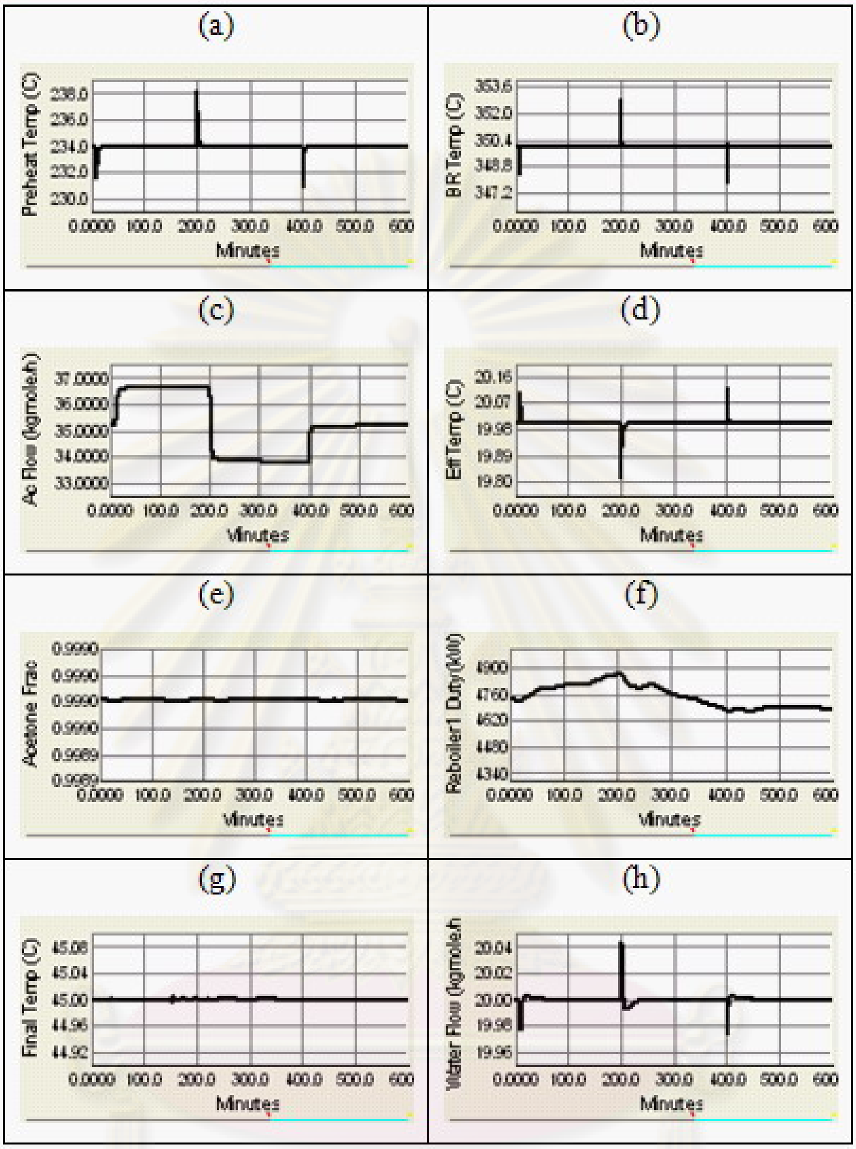


Figure 5.42 Dynamic responses of CS4 Base case where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

5.4.4 Change in the material disturbance of cold stream (IPA fresh feed stream) CS 1 to CS 4 for Alt. 1, Alt. 2 and Alt. 3

Figure 5.43 to 5.54 show the dynamic responses of the acetone plant in the material disturbance. This disturbance made as follows: The IPA fresh feed is increased from 51.96 kgmole/h to 54.56 kgmole/h at time equals 10 minutes, and the decreased from 54.56 kgmole/h to 49.36 kgmole/h at time equals 200 minutes and then return to its set point at time equals 400 minutes.

The dynamic response of alternative 1, 2 and 3 are similar base case. CS 2 and CS 4 are greatter than CS 1 and CS 3. All alternatives have been manages disturbance heat load propagation of hot stream difference from base case. All control structures in alternative 1 and 3 give the same result to shift the heat load disturbance to FEHE1. It control by adjusting bypass valve (VBP 1) and remain disturbance can transfer to heater or effluent cooler (figure a) and b)). In Alternative 2, When disturbance occurs, the heat load disturbance transfers to FEHE 2 so hot outlet temperature should be controlling by bypass valve (VBP 2). Thus, the remain disturbance which transfer to effluent cooler is smaller than alt. 1 and 3 (figure a) and b)). CS 3 is the worst control structure. It control IPA column temperature by bottom vale so recycle flowrate doesn't smooth. Thus, this factor has the direct effect to the process by recycle flowrate.

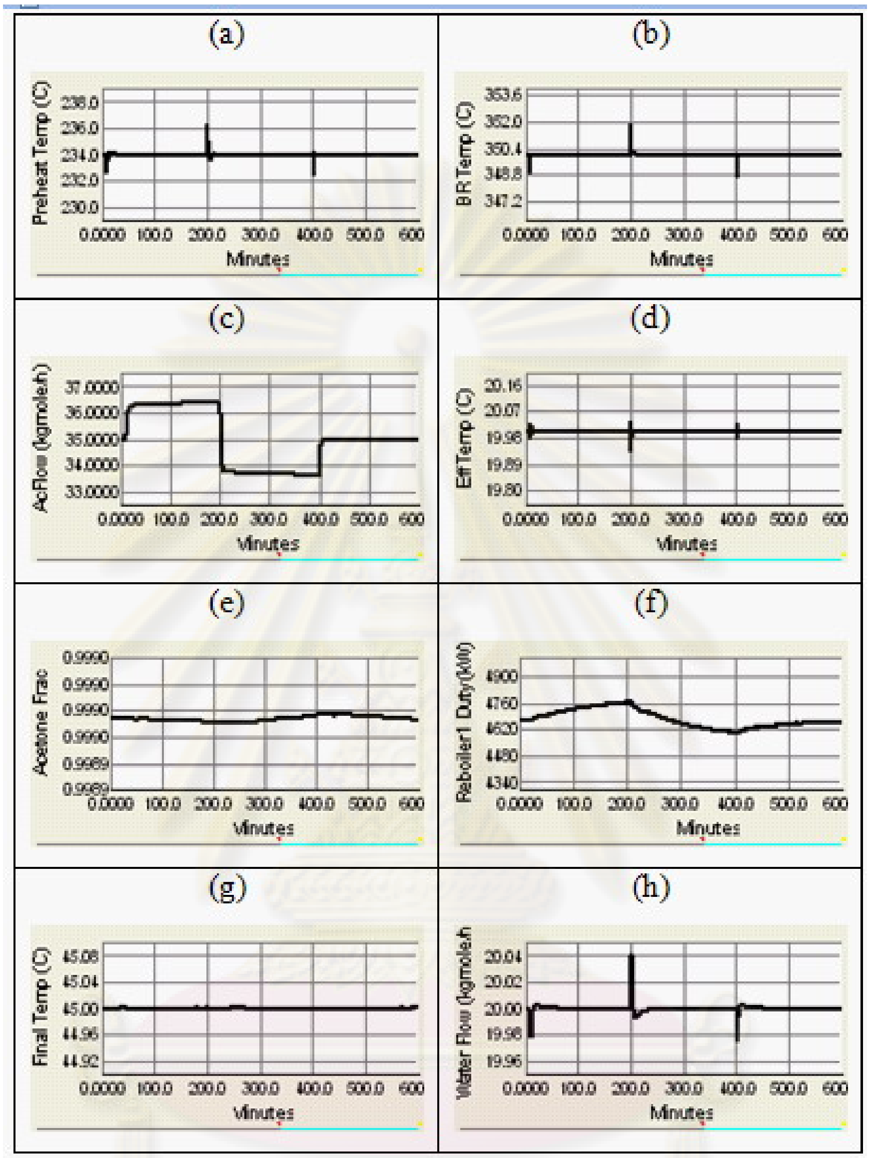


Figure 5.43 Dynamic responses of CS1 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

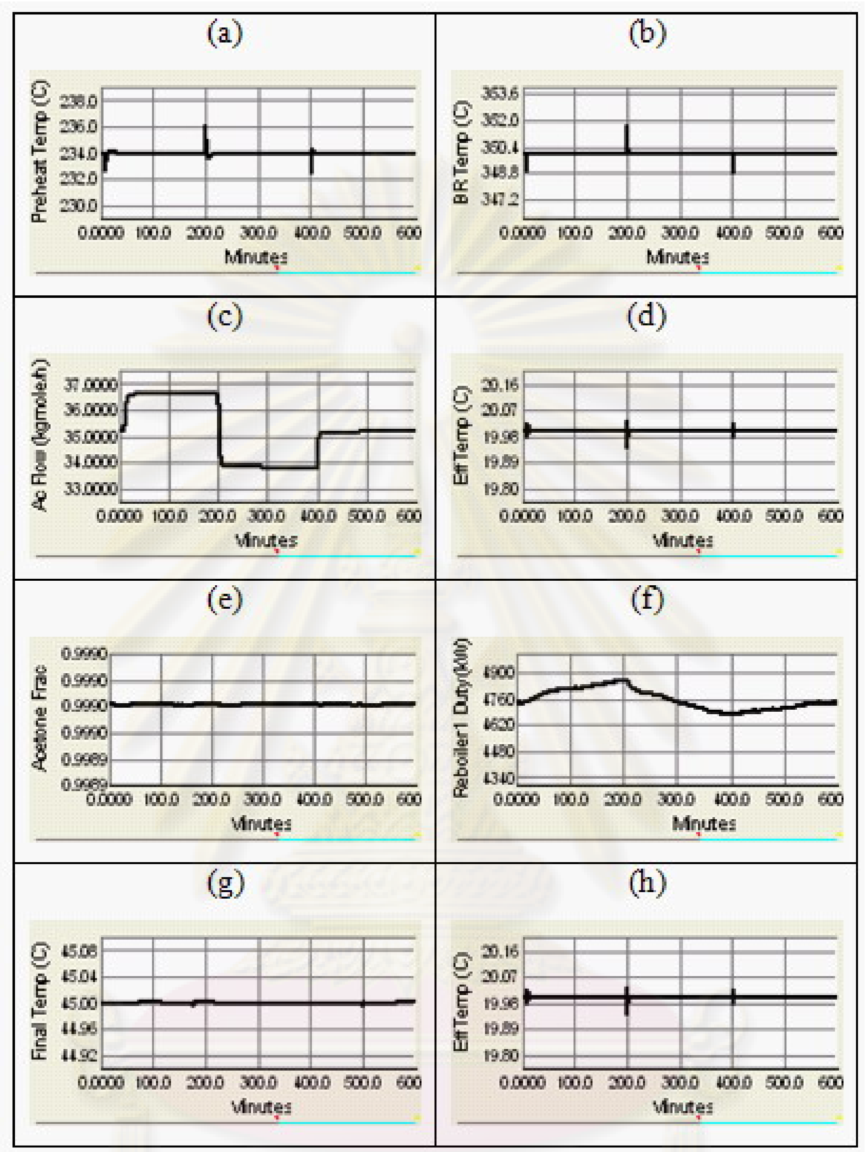


Figure 5.44 Dynamic responses of CS2 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

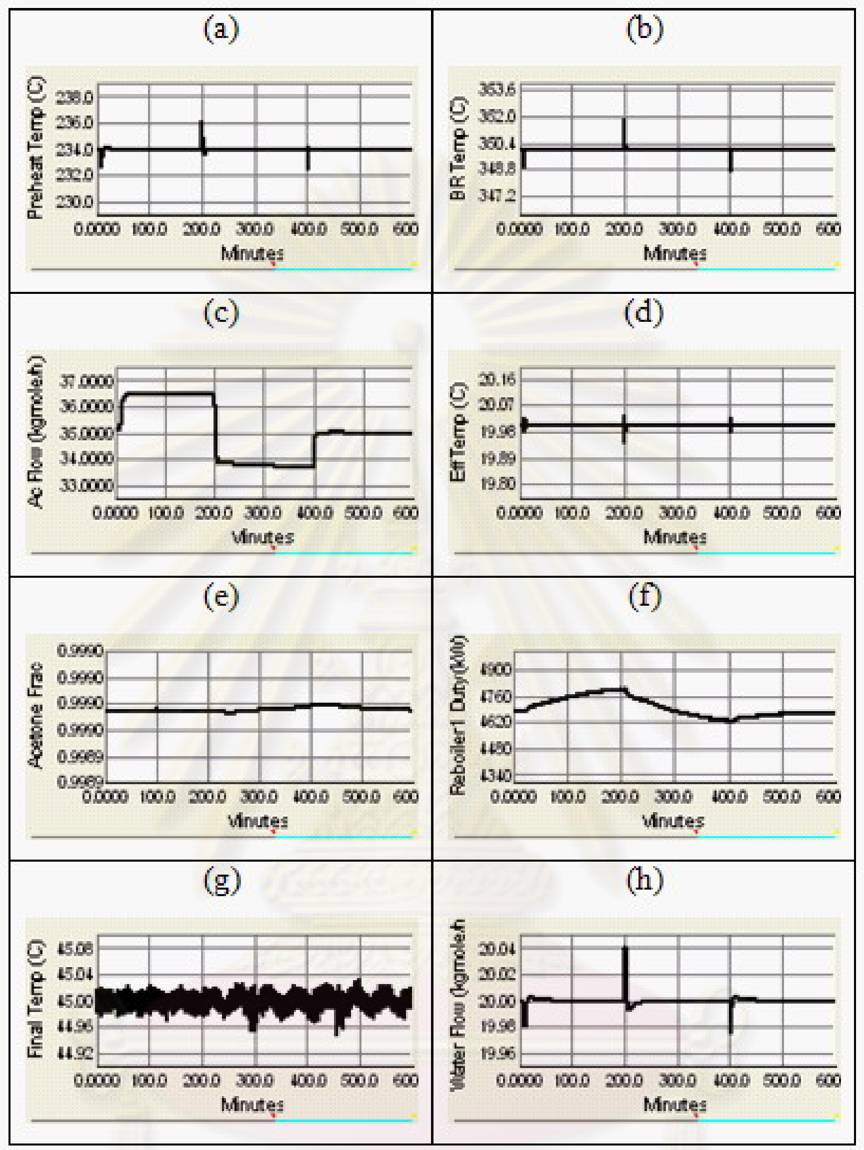


Figure 5.45 Dynamic responses of CS3 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

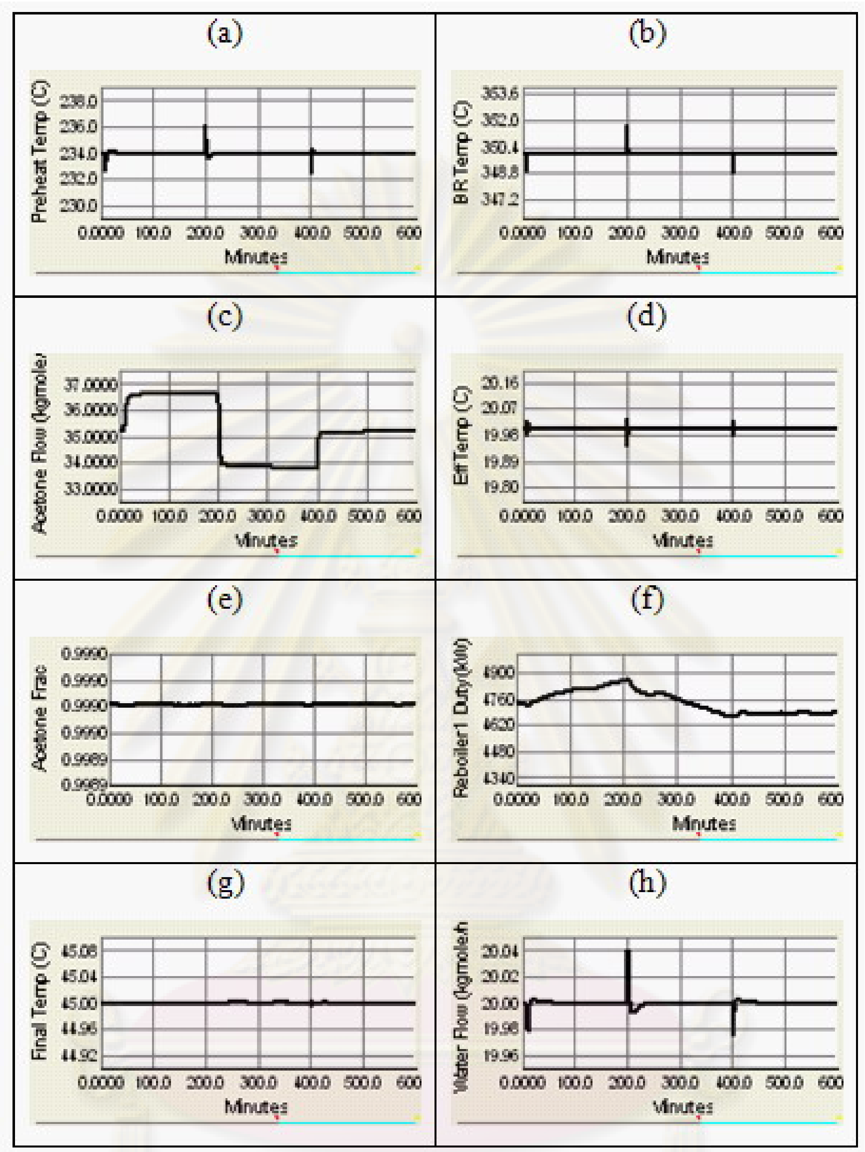


Figure 5.46 Dynamic responses of CS4 Alt. 1 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

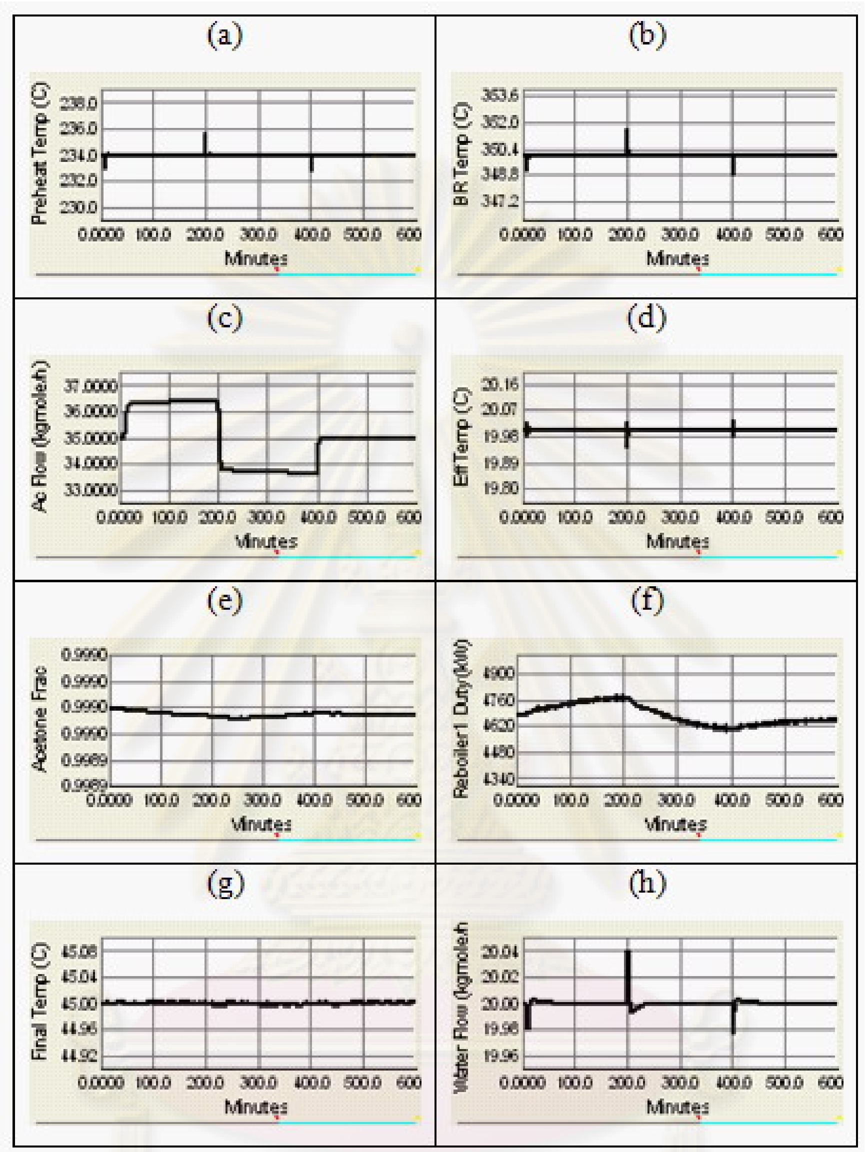


Figure 5.47 Dynamic responses of CS1 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

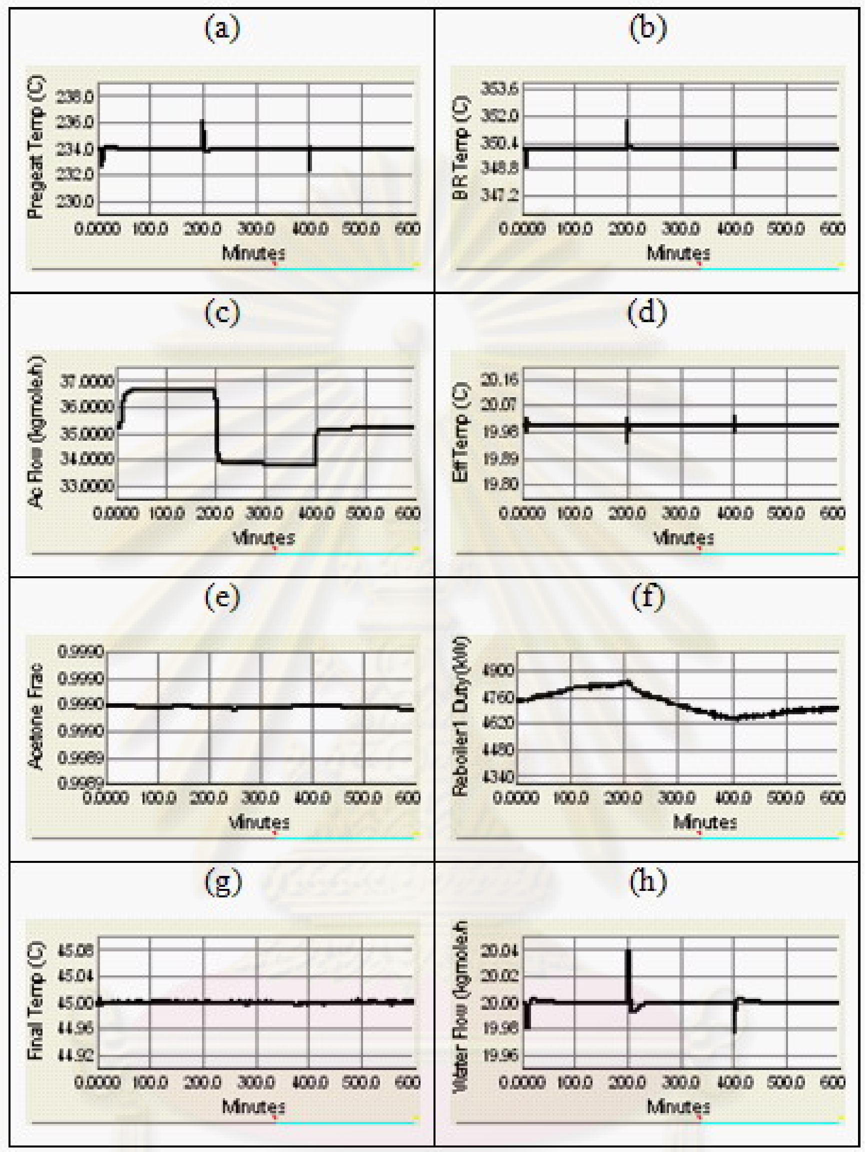


Figure 5.48 Dynamic responses of CS2 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

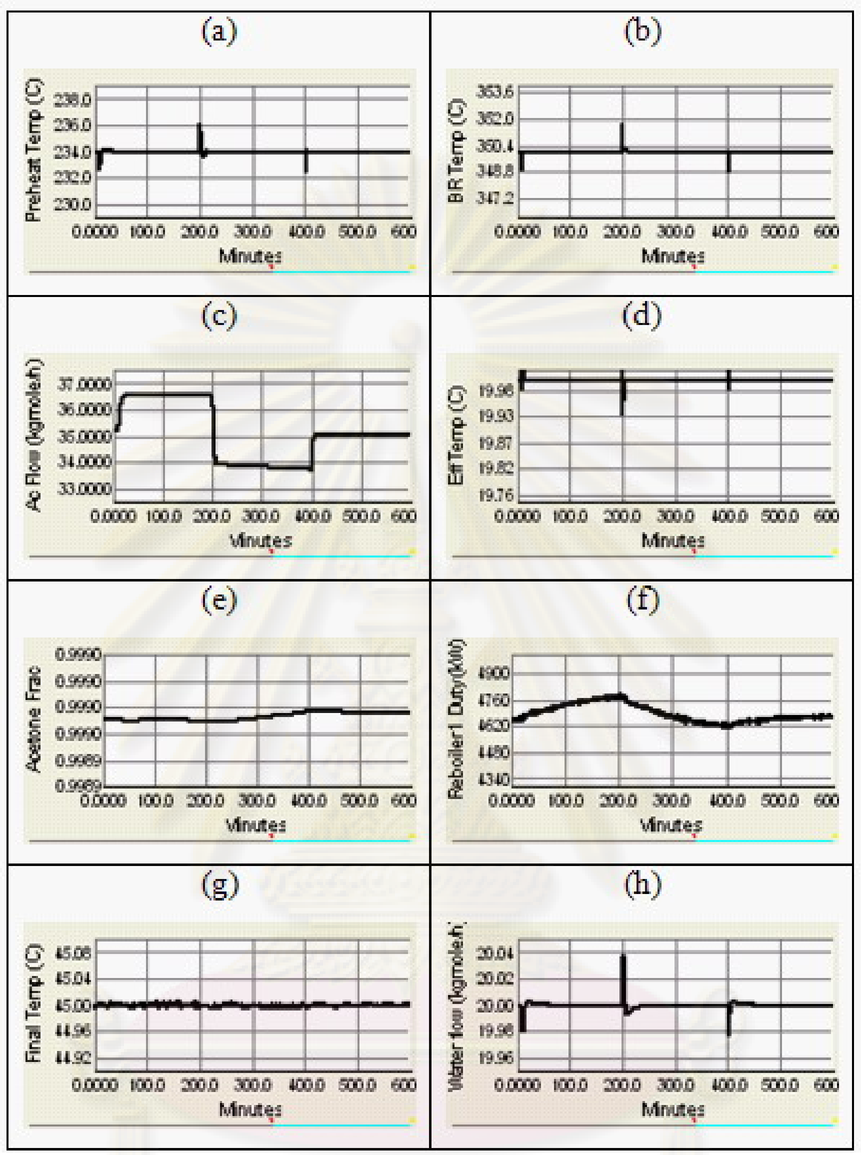


Figure 5.49 Dynamic responses of CS3 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

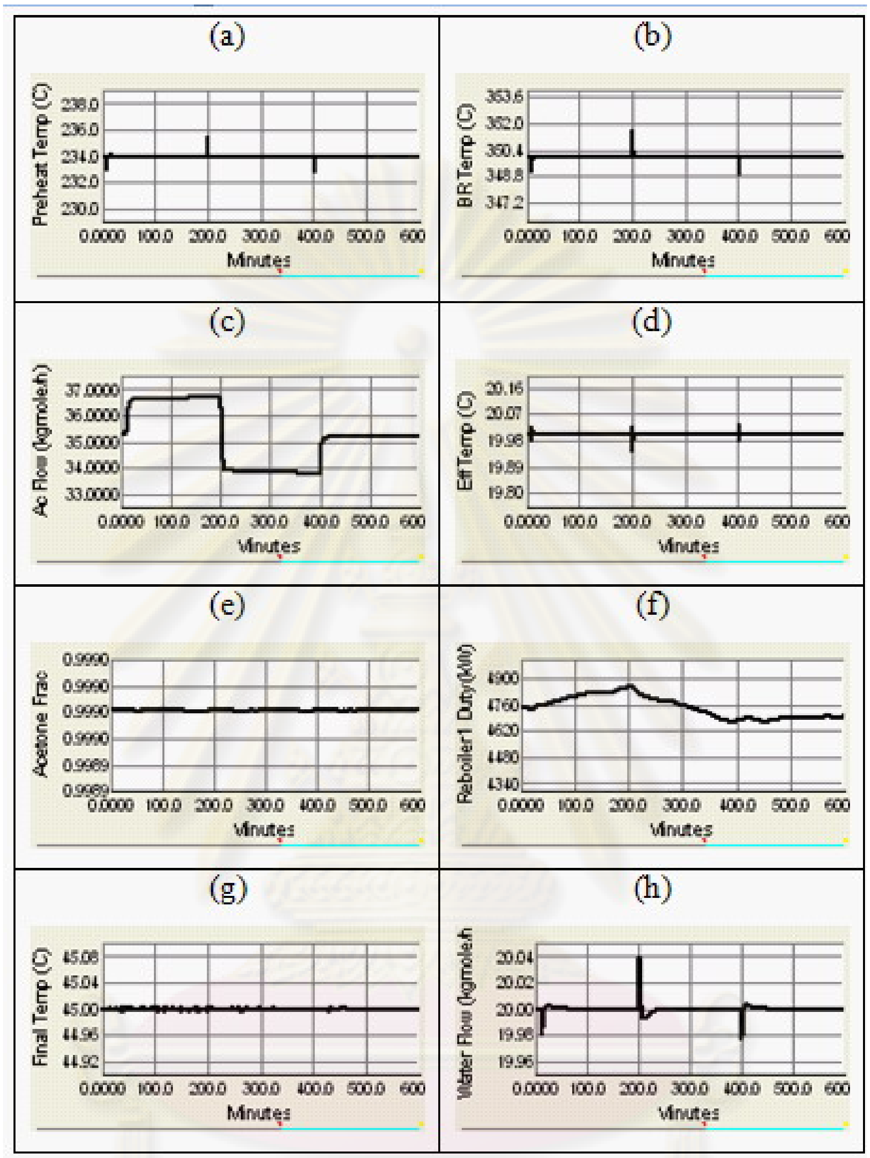


Figure 5.50 Dynamic responses of CS4 Alt. 2 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

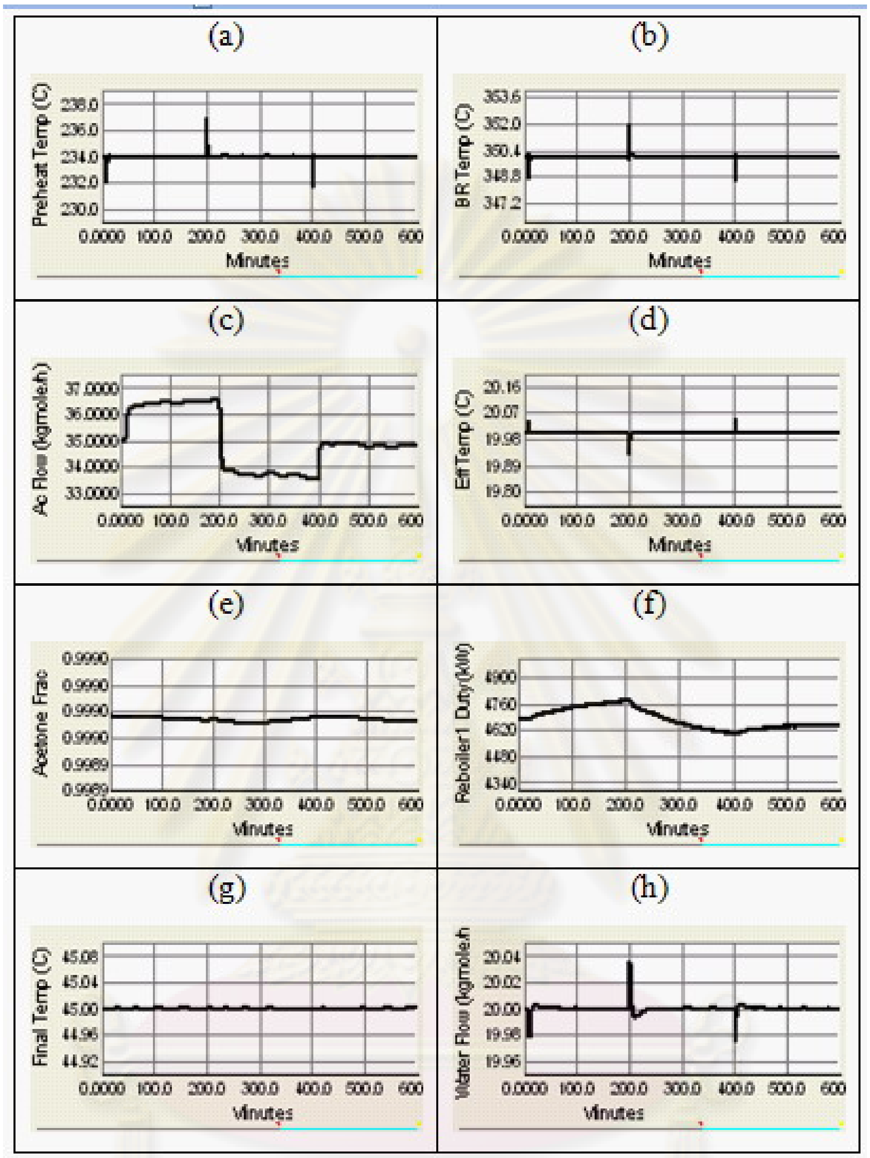


Figure 5.51 Dynamic responses of CS1 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

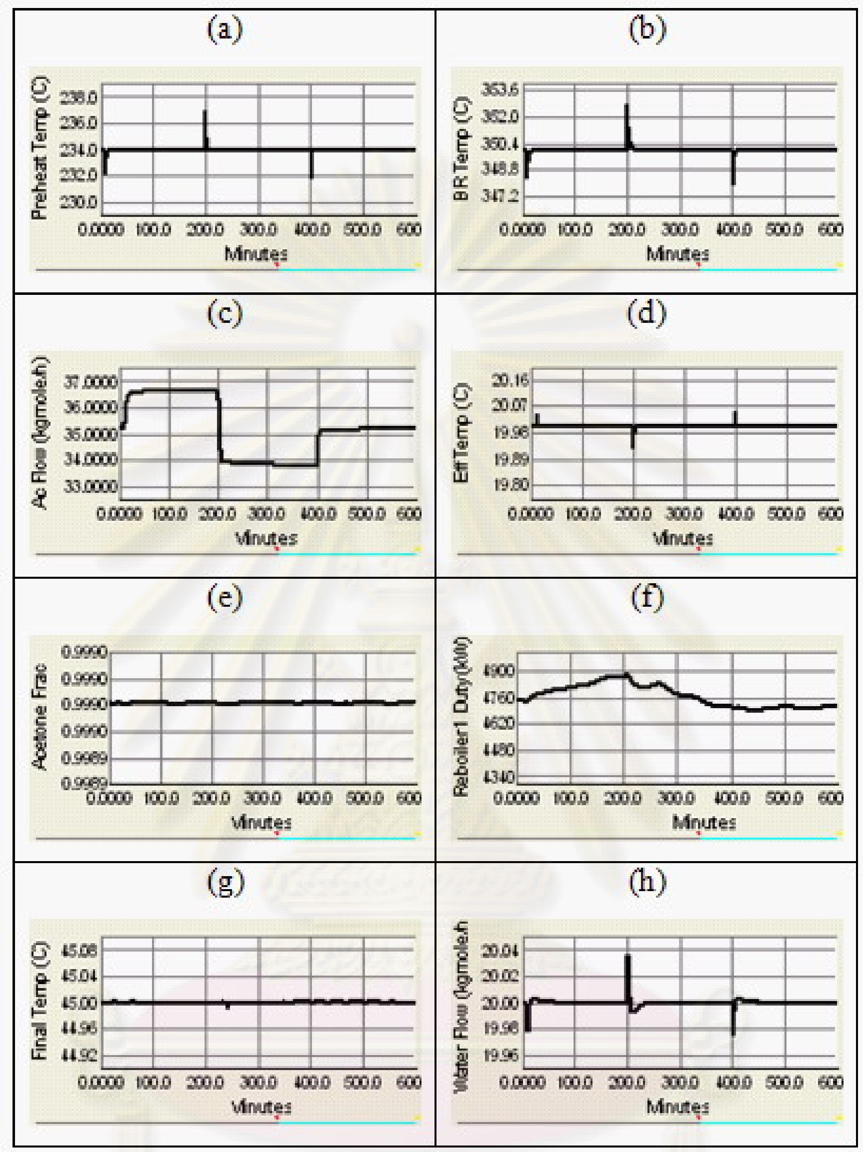


Figure 5.52 Dynamic responses of CS1 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

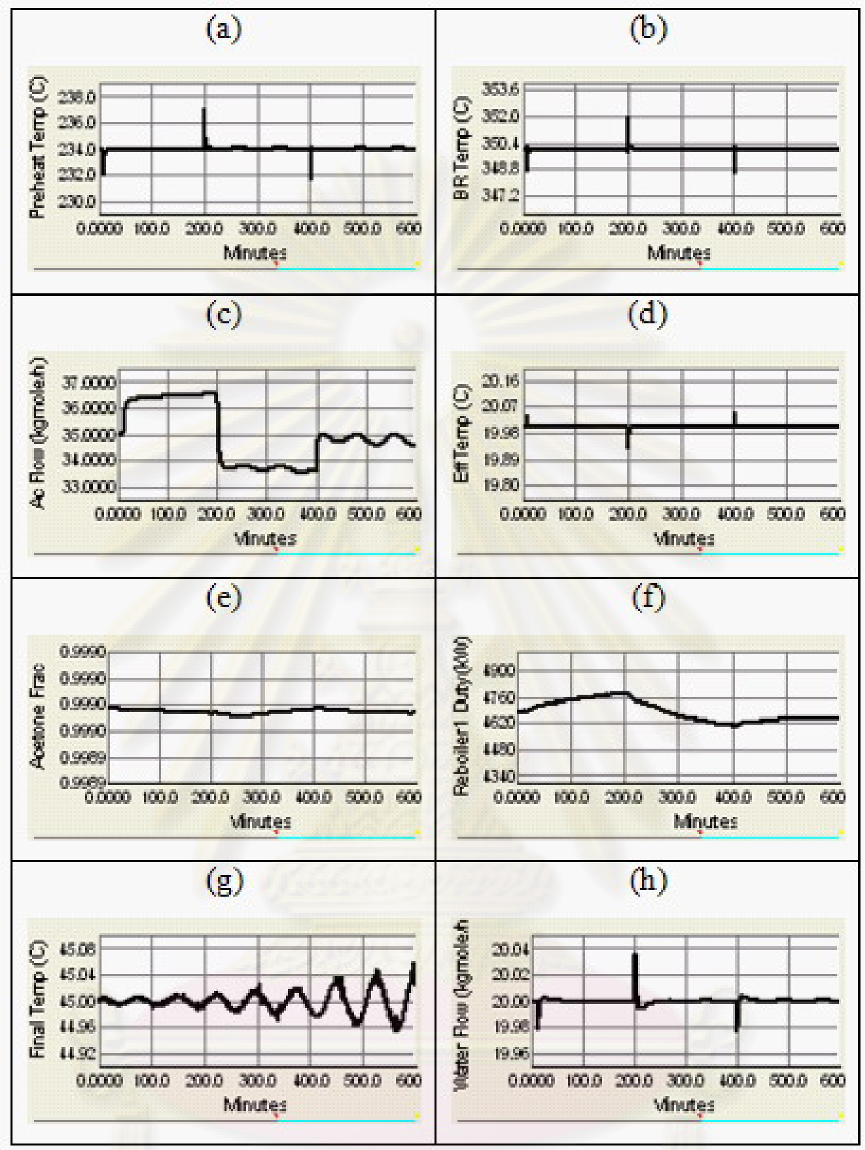


Figure 5.53 Dynamic responses of CS3 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

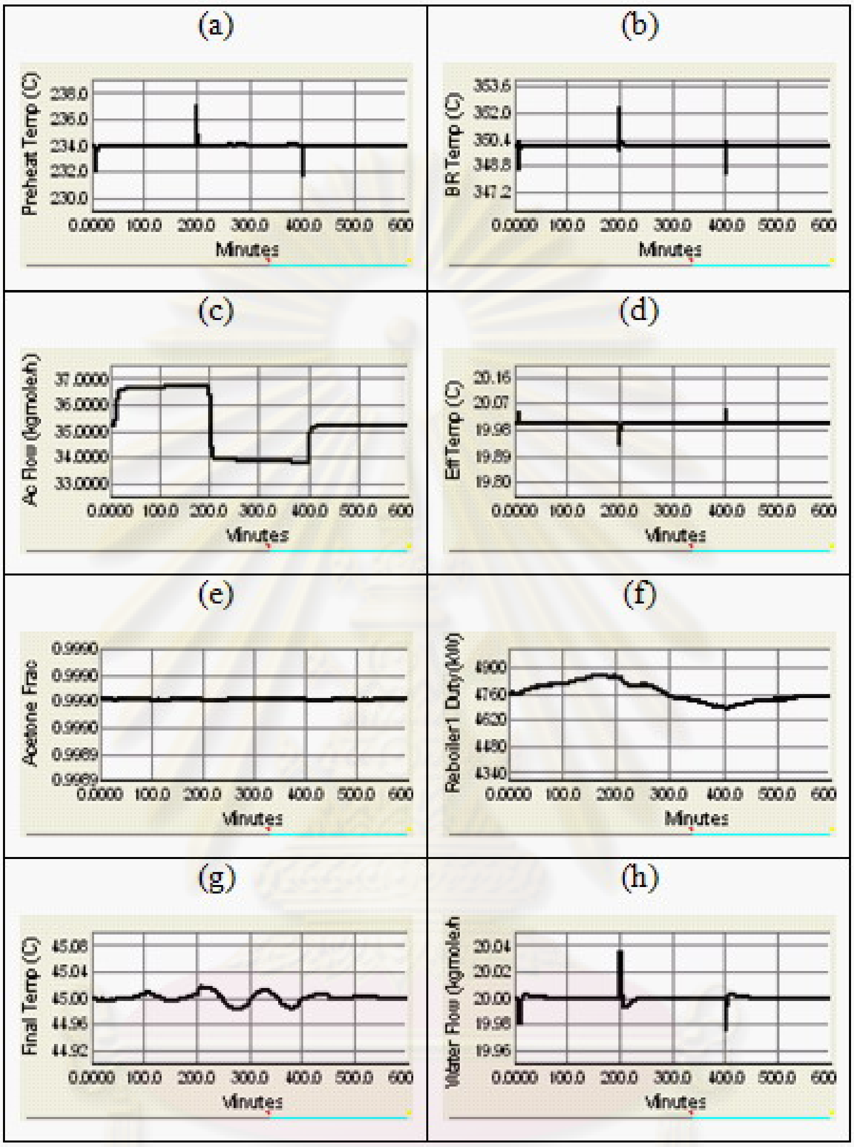


Figure 5.54 Dynamic responses of CS4 Alt. 3 where: (a) preheat temperature, (b) before entering reactor temperature, (c) acetone product flowrate, (d) effluent cooler temperature, (e) acetone product composition, (f) acetone column reboiler duty, (g) final cooler temperature, (h) water fresh feed flowrate

5.5 Evaluation of the Dynamic Performance

The dynamic performance index is focused on time related characteristics of the controller's response to setpoint changes or deterministic disturbances. There exist several candidate performance measures such as settling time and integral absolute error (IAE). Integral absolute error is well known and widely used. For the formulation of a dynamic performance as written below:

$$\mathrm{IAE} = \int |\epsilon(t)| \ \mathrm{dt}$$

Note that ϵ(t) = y_{sp}(t) - y(t) is the deviation (error) of the response from the desired setpoint.

In this work, IAE method is used to evaluate the dynamic performance of the designed control systems. Table 5.1 to table 5.4 show the IAE value result for the change in thermal disturbance of reactor outlet temperature in Base Case, Alternative 1, 2 and 3. Table 5.5 to table 5.8 show the IAE value result for the change in material disturbance of IPA fresh feed stream in Base Case, Alternative 1, 2 and 3.

In thermal disturbance, CS 2 is the best controller. When we compare CS 2 and CS 4, CS 2 gives smaller IAE value than CS 4 because CS 2 controls temperature in IPA column.

In material disturbance, CS 4 can manage flow disturbance better than other control structures because it controls flowrate two point at before entering IPA column and recycle stream. In this case, we can find IAE value of CS 2 close to CS4. Thus, CS 2 is the best control structure for handle disturbances due to it gives better control performances.

Table 5.1 The IAE Result of the acetone process in base case to a change in the thermal disturbance of reactor outlet temperature

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	0.111	0.130	0.106	0.117
T-BR	0.181	0.262	0.143	0.212
T-Re	0.752	0.517	0.369	1.558
T-cool	1.916	1.634	1.664	1.554
T-final	0.005	0.198	0.057	0.044
Ac-purity	0.640	0.239	3.780	0.139
Sum	3.605	2.979	6.119	3.625
Average	0.601	0.496	1.020	0.604

Table 5.2 The IAE Result of the acetone process in Alt.1 to a change in the thermal disturbance of reactor outlet temperature

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	2.074	1.953	2.030	1.84
T-BR	1.339	1.457	1.496	1.274
T-Re	.0.830	0.728	0.869	1.730
T-cool	0.891	0.627	0.669	0.837
T-final	0.006	0.175	4.140	0.054
Ac-purity	0.976	0.053	2.295	0.125
Sum	6.116	4.992	6.119	3.625
Average	0.601	0.496	1.020	0.604

Table 5.3 The IAE Result of the acetone process in Alt.2 to a change in the thermal disturbance of reactor outlet temperature

	Integral Absolute Error (IAE)			
Controller	CS1	CS2	CS3	CS4
T-pre	0.601	0.510	2.067	0.548
T-BR	0.876	0.725	1.339	0.983
T-Re	1.136	1.264	0.997	0.995
T-cool	1.247	0.746	1.144	1.022
T-final	0.324	0.730	1.519	1.148
Ac-purity	0.936	0.139	2.270	0.111
Sum	5.122	4.114	9.338	4.807
Average	0.854	0.686	1.556	0.801

Table 5.4 The IAE Result of the acetone process in Alt.3 to a change in the thermal disturbance of reactor outlet temperature

	Integral Absolute Error (IAE)			
Controller	CS1	CS2	CS3	CS4
T-pre	0.818	0.839	1.270	0.983
T-BR	1.220	2.072	1.135	1.285
T-Re	0.353	0.416	3.303	0.181
T-cool	0.284	0.295	0.970	0.499
T-final	0.020	0.278	5.717	1.585
Ac-purity	1.983	0.043	2.243	0.028
Sum	4.679	3.943	14.638	4.561
Average	0.780	0.657	2.440	0.760

Table 5.5 The IAE Result of the acetone process in Base Case to a change in material disturbance of feed Stream

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	1.792	1.817	1.825	1.817
T-BR	0.791	0.852	0.788	0.794
T-Re	0.996	1.014	0.994	1.060
T-cool	2.303	2.182	2.211	2.167
T-final	0.151	0.314	0.164	0.103
Ac-purity	1.907	0.138	5.715	0.118
Sum	7.941	6.319	11.697	6.060
Average	1.323	1.053	1.949	1.010

Table 5.6 The IAE Result of the acetone process in Alt. 1 to a change in material disturbance of feed Stream

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	0.723	0.813	0.771	0.842
T-BR	0.721	0.854	0.821	0.729
T-Re	0.984	1.054	0.993	1.050
T-cool	0.510	0.416	0.403	0.485
T-final	0.180	0.233	3.113	0.093
Ac-purity	1.044	0.029	1.124	0.104
Sum	4.164	3.401	7.226	3.304
Average	0.694	0.567	1.204	0.551

Table 5.7 The IAE Result of the acetone process in Alt. 2 to a change in material disturbance of feed Stream

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	0.216	0.224	0.933	0.225
T-BR	0.787	0.751	0.790	0.852
T-Re	0.994	1.046	0.961	1.041
T-cool	0.443	0.461	0.633	0.433
T-final	0.489	0.440	0.705	0.337
Ac-purity	1.295	0.082	1.579	0.018
Sum	4.225	3.005	5.601	2.906
Average	0.704	0.501	0.933	0.484

Table 5.8 The IAE Result of the acetone process in Alt. 3 to a change in material disturbance of feed Stream

Controller	Integral Absolute Error (IAE)			
	CS1	CS2	CS3	CS4
T-pre	0.856	0.818	1.328	0.998
T-BR	0.929	3.538	1.148	0.853
T-Re	1.004	1.040	1.193	0.573
T-cool	0.650	0.666	1.181	0.852
T-final	1.708	0.180	5.357	2.430
Ac-purity	1.494	0.016	1.303	0.031
Sum	6.642	6.258	11.510	5.737
Average	1.107	1.043	1.918	0.956

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

In this thesis, we considered two objectives. First, we design heat integrated process of acetone process by using resilient HEN synthesis method (Wongsri, 1990) for reduction of energy consumption when compare with Base case. The process is simulted by HYSYS. The result shows that alternative 1 can save energy 76.07%, 81.49% for alternative 2 and 62.81% for alternative 3 compare with Base Case.

Second, we considered the plantwide control structure of acetone process. All control structures are designed by using the disturbance load propagation method (Wongsri, M., 1990) and heat pathway heuristics,(HPH) (Wongsri, M. and Hermawan Y.D., 2005), respectively. Control structure 1(CS1) and control structure 2 (CS2) is designed by nine step approach of Luyben and co-workers, control structure 3 (CS3) and control structure 4 (CS4) are designed by fixture point method (Wongsri, 2008) to maintain good control performance.

Two kinds of disturbances: thermal and material disturbances are used in evaluation of the plantwide control structures. The performances of the heat integrated plants (HIPs) and the control structures evaluated dynamically by commercial software HYSYS. The IAE method is used to evaluate the dynamic performance of the designed control systems.

The IAE of control structures CS2 close to the IAE of CS4 but because the control structures are similar. However, CS2 is the most effective control structure to handle disturbance load in this work when compare with other constructures. It can maintain acetone product purity at set point.

The heat-integrated plants of acetone plant is selected to illustrate the concepts, the design procedures and the analysis is illustrated using time domain simulation-based approach through HYSYS rigorous dynamic simulator. Although heat-integration process is difficult to control, but proper control structure can reduce complication for complex heat integration process control and achieve to design objectives. However, the energy usage is important to consider because the good control structure with heat integration process is less energy consumption, namely decreasing operation cost.

6.2 Recommendations

1. Study and design the control structure complex heat-integrated plants of acetone process point of view.
2. Study the controllability characteristics of energy-integrated of acetone process.
3. Study and design the control structure of complex heat-exchanger networks and heat-integrated plants of the other process in plantwide control point of view.

REFERENCES

Alongkorn Ploypaisansang. Resilient Heat Exchanger Network Design of Hydrodealkylation Process. Master's Thesis, Department of Chemical Engineering, Engineering, Faculty of Engineering, Chulalongkorn University, 2003.

Calandranis, J., and Stephanopoulos, G. A Structure Approach to the Design of Control System in Heat Exchanger Networks. Comput. Chem. Eng. 12 (1988): 651-669.

Douglas, J.M. Conceptual Design of Chemical Process. New York: McGraw-Hill, (1988).

Handogo, R., and Luyben W.L. Design and Control of a Heat-Integrated Reactor /Column Process. Ind. Eng. Chem. Res. 26 (1987): 531-538.

Jones, W.E., and Wilson, J.A. An Introduction to Process Flexibility: Heat Exchanger. Chem. Eng. Ed. 31 (1997): 172-177.

Fisher, W.R., Doherty, M.F., and Douglas, J.M. The interface between design and control. 1, 2 and 3; 1: Process controllability, 2: Process operability 3: Selecting a set of controlled variables. Ind. Eng. Chem. Res. 27 (1988): 597-615.

Linhoff, B., Dunford, H., and Smith, R. Heat integration of distillation columns into overall processes. Chem. Eng. Sci. 38 (1983): 1175-1188.

Linhoff, B., and Hindmarsh E. The pinch design method for heat exchanger networks. Chem. Eng. Sci. 38 (1983): 745-763.

Luyben, M.L., and Luyben W.L. Design and control of a complex process involving two reaction steps three distillation columns and two recycle streams. Ind. Eng. Chem. Res. 34, 11 (1995): 3885-3898.

Marselle, D. F., Morari, M. and Rudd, D. F. Design of Resilient Processing Plants

II: Design and Control of Energy and Management Systems. Chem. Eng. Sci. 37 (1982): 259.

Montree Wongsri. Resilient of Heat Exchanger Network Design. Doctoral dissertation, Sever Institute of Technology, Science, Washington University, 1990.

Saboo, A. K., and Morari, M. Design of resilient processing plants-IV: some new result on heat exchanger network synthesis. Chem. Eng. Sci., 39, 3 (1984): 579-692.

Wongsri, M., and Hermawan, Y. D. Heat Pathway Management for Complex Energy Integrated Plant: Dynamic Simulation of HDA Plant. J. Chin. Inst. Chem. Engrs. 36 (2005): 1-27.

APPENDICES

APPENDIX A

PROCESS STREAM DATA FOR SIMULATION AND EQUIPMENT DATA SPECIFICATION

Table A.1 Column specifications of acetone process base Case

Name	IPA	2	3	5	6	8	Water
Temperature (^0C)	25	31.03	350.00	20.00	26.57	33.51	25.00
Pressure (bar)	2.60	2.30	1.90	1.63	1.63	1.50	2.00
Molar flow (kgmole/h)	51.96	57.84	92.65	39.74	20.97	38.77	20.00
Component Molar flow (kgmole/h)							
Hydrogen	0.00	0.00	34.81	34.80	0.00	34.80	0.00
Acetone	0.00	0.16	34.97	0.12	1.72	2.65	0.00
Isopropyl alchol	34.82	38.68	3.87	4.37	0.11	0.00	0.00
Water	17.14	19.00	19.00	0.45	19.13	1.32	20.00

Name	be-9	mix H_2	Acetone	9-bot	rec1	10-bot
Temperature (^0C)	21.47	33.45	4.59	94.22	82.78	106.77
Pressure (bar)	1.63	1.01	1.01	1.53	2.30	1.28
Molar flow (kgmole/h)	73.86	38.78	32.18	41.68	5.88	35.80
Component Molar flow (kgmole/h)						
Hydrogen	0.00	34.80	0.00	0.00	0.00	0.00
Acetone	32.32	2.65	32.16	0.16	0.16	0.00
Isopropyl alchol	3.86	0.01	0.00	3.86	3.86	0.00
Water	37.68	1.32	0.02	37.66	1.86	35.80

Table A.2 Equipment data and Specifications of heat-integrated plant of acetone process

Equipments	Specifications	Heat-integrated process of acetone process			
		Base case	Alternative 1	Alternative 2	Alternative 3
Reactor	Diameter (m)	1.85	1.85	1.85	1.85
	Length (m)	7.831	7.831	7.831	7.831
	Number of tube	1	1	1	1
Heater	Tube volume (m3)	0.1	0.1	0.1	0.1
Eff cooler	Tube volume (m3)	0.1	0.1	0.1	0.1
Final cooler	Tube volume (m3)	0.1	0.1	0.1	0.1
FEHE 1	Shell volume (m^3)	-	2.272	2.272	2.272
	Tube volume (m^3)	-	0.193	0.193	0.193
	UA (W/C)	-	2.366×10^4	1.994×10^4	2.366×10^4
FEHE 2	Shell volume (m3)	-	-	2.272	-
	Length (m)	-	-	0.193	-
	UA (kJ/C-h)	-	-	2.78×10^2	-
FEHE 3	Shell volume (m3)	-	-	-	2.272
	Length (m)	-	-	-	0.193
	UA (kJ/C-h)	-	-	-	1.42×10^3

Table A.3 Column Specifications of Acetone process Base Case

Parameters columns	Acetone Column	IPA Column
Model	Refluxed absorber	Refluxed absorber
Tray	Sieve Tray	Sieve Tray
Number of tray	66	19
Feed tray	33	16
Pressure (bar)	1.2	1.2
Diameter of Vessel (m)	1.25	1.36
Tray space (m)	0.457	0.610
Weir length (m)	4.292	1.2
Weir height (m)	0.05	0.05
Specification 1	H_2 composition in overhead (v)= 0.900	Ac composition in overhead = 0.027
Specification 2	Ac composition in overhead (l) = 0.999	H_2O composition in bottom = 0.999
Specification 3	Ac flow in = 0.160 kgmole/h	-

APPENDIX B

PARAMETER TUNING OF CONTROL STRUCTURES

B.1 Turning Flow, Level, Pressure, Temperature Control

Flow Controllers

The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be tuned with a small integral or reset time constant τ_I. A value of τ_I= 0.3 minutes works in most flow controllers. The value of controller gain should be kept modest because flow measurement signals are sometime noisy due to the turbulent flow through the orifice plate. A value of controller gain of $K_C = 0.5$ is often used. Derivative action should not be used.

Level Controllers

Most level controllers should use proportional-only action with a gain of 1 to 2. This provides the maximum amount of flow smoothing. Proportional control means there will be steady-state offset (the level will not be returned to its setpoint value). However, maintaining a liquid level at a certain value is often not necessary when the liquid capacity is simply being used as surge volume. So the recommended tuning of a level controller is K_C= 2.

Pressure Controllers

Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Of course the gain used depends on the span of the pressure transmitter. Some simple step tests can be used to find the value of controller gain that yields satisfactory pressure control. Typical pressure controller tuning constants for columns and tanks are K_C= 2 and $\tau_I = 10$ minutes.

Temperature Controllers

Temperature dynamic responses are generally slow, so PID control is used. Typically, the controller gain, Kc, should be set between 2 and 10, the integral time, τ_I, should set between 2 and 10 minutes, and the derivative time τ_d, should be set between 0 and 5 minutes.

B.2 Relay-Feedback Testing

If we have a controller that needs tuning and after we have inserted reasonable lags and deadtimes, we need a quick and simple method for identifying the dynamic parameters that are important for designing a feedback controller. The relay-feedback test is a tool that serves this purpose well. The results of the test are the ultimate gain and the ultimate frequency. This information is usually sufficient to permit us to calculate some reasonable controller tuning constants.

IThe method consists of merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the high of the relay h. This height is typically 5 to 10% of the controller-output scale. The loop starts to oscillate around the setpoint, with the controller output switching every time the process variable (PV) signal crosses the setpoint.

Relay feedback testing can be done in HYSYS. It simply click the Tuning botton on the controller faceplate, select Autotuning and click the Start Autotuning botton. The loop will start to oscillate. After several cycles, the tuning is stopped and some ewcommended settings for a PID controller are suggested.

Table B.1 Parameter tuning of acetone process CS 1

Controller	controlled variable	manipulated variable	Control action	K_C	τ_I	τ_d
F-IPA	IPA flowrate	V1	Reverse	0.5	0.3	-
T-C3	Preheat temperature	Heater duty (Q1)	Reverse	0.086	0.216	0.048
T-reactor	Outlet temperature	Reactor duty (Q3)	Reverse	14.6	4.1	0.911
Cooler	Separator temperature	Cooler duty(Q4)	Direct	0.84	0.186	0.041
F-water	Water flowrate	V2	Reverse	0.5	0.3	-
P-stripper	Stripper Pressure	V3	Direct	2	10	-
T-D1	Ac column stage 64 temperature	Ac column reboiler duty	Reverse	14.8	14.7	0.1
P-D1	Ac column condenser pressure	Ac column condenser duty	Direct	2	10	-
Lcon-D1	Ac column condenser level	Distillate valve (V7)	Direct	2	-	-
Lreboil-D1	Ac column reboiler level	Botom valve (V8)	Direct	2	-	-
T-D2	IPA column stage 11 temperature	Ac column reboiler duty	Reverse	14.5	1.24	0.27
P-D2	IPA column condenser pressure	Ac column condenser duty	Direct	2	-	-
Lcon-D2	IPA column condenser level	Distillate valve (V9)	Direct	2	-	-
Lreboil-D2	IPA column reboiler level	Botom valve (V10)	Direct	2	-	-

Table B.2 Parameter tuning of acetone process CS 2

Controller	controlled variable	manipulated variable	Control action	K_C	τ_I	τ_d
F-IPA	IPA flowrate	V1	Reverse	0.5	0.3	-
T-C3	Preheat temperature	Heater duty (Q1)	Reverse	0.086	0.216	0.048
T-reactor	Outlet temperature	Reactor duty (Q3)	Reverse	14.6	4.1	0.911
Cooler	Separator temperature	Cooler duty(Q4)	Direct	0.84	0.186	0.041
F-water	Water flowrate	V2	Reverse	0.5	0.3	-
P-stripper	Stripper Pressure	V3	Direct	2	10	-
T-D1	Ac column stage 64 temperature	Ac column reboiler duty	Reverse	14.8	14.7	0.1
P-D1	Ac column condenser pressure	Ac column condenser duty	Direct	2	10	-
Lcon-D1	Ac column condenser level	Distillate valve (V7)	Direct	2	-	-
Lreboil-D1	Ac column reboiler level	Botom valve (V8)	Direct	2	-	-
CC-Ac	Ac compsition	Reflux valve	Reverse	1	10	-
P-D2	IPA column condenser pressure	Ac column condenser duty	Direct	2	-	-
Lcon-D2	IPA column condenser level	Ac column reboiler duty	Reverse	2	-	-
Lreboil-D2	IPA column reboiler level	Bottom valve (V10)	Direct	2	-	-
F-rec1	Recycle flowrate	V9	Reverse	0.5	0.3	-

Table B.3 Parameter tuning of acetone process CS 3

Controller	controlled variable	manipulated variable	Control action	K_C	τ_I	τ_d
F-IPA	IPA flowrate	V1	Reverse	0.5	0.3	-
T-C3	Preheat temperature	Heater duty (Q1)	Reverse	0.086	0.216	0.048
T-reactor	Outlet temperature	Reactor duty (Q3)	Reverse	14.6	4.1	0.911
Cooler	Separator temperature	Cooler duty(Q4)	Direct	0.84	0.186	0.041
F-water	Water flowrate	V2	Reverse	0.5	0.3	-
P-stripper	Stripper Pressure	V3	Direct	2	10	-
T-D1	Ac column stage 64 temperature	Ac column reboiler duty	Reverse	14.8	14.7	0.1
P-D1	Ac column condenser pressure	Ac column condenser duty	Direct	2	10	-
Lcon-D1	Ac column condenser level	Distillate valve (V7)	Direct	2	-	-
Lreboil-D1	Ac column reboiler level	Botom valve (V8)	Direct	2	-	-
T-D2	IPA column stage 11 temperature	Bottom valve (V10)	Reverse	0.704	41.9	9.32
P-D2	IPA column condenser pressure	Ac column condenser duty	Direct	2	-	-
Lcon-D2	IPA column condenser level	Distillate valve (V9)	Direct	2	-	-
Lreboil-D2	IPA column reboiler level	Ac column reboiler duty	Direct	2	-	-

Table B.4 Parameter tuning of acetone process CS 4

Controller	controlled variable	manipulated variable	Control action	K_C	τ_I	τ_d
F-IPA	IPA flowrate	V1	Reverse	0.5	0.3	-
T-C3	Preheat temperature	Heater duty (Q1)	Reverse	0.086	0.216	0.048
T-reactor	Outlet temperature	Reactor duty (Q3)	Reverse	14.6	4.1	0.911
Cooler	Separator temperature	Cooler duty(Q4)	Direct	0.84	0.186	0.041
F-water	Water flowrate	V2	Reverse	0.5	0.3	-
P-stripper	Stripper Pressure	V3	Direct	2	10	-
P-D1	Ac column condenser pressure	Ac column condenser duty	Direct	2	10	-
Lcon-D1	Ac column condenser level	Distillate valve (V7)	Direct	2	-	-
Lreboil-D1	Ac column reboiler level	Ac column reboiler duty	Direct	2	-	-
CC-Ac	Ac compsition	Reflux valve	Reverse	1	10	-
F-botAC	Ac bottom flowrate	V8	Reverse	0.5	0.3	-
T-D2	IPA column stage 11 temperature	Ac column reboiler duty	Reverse	14.5	1.24	0.27
P-D2	IPA column condenser pressure	IPA column condenser duty	Direct	2	-	-
Lcon-D2	IPA column condenser level	Reflux valve	direct	2	-	-
Lreboil-D2	IPA column reboiler level	Bottom valve (V10)	Direct	2	-	-
F-rec1	Recycle flowrate	V9	Reverse	0.5	0.3	-

APPENDIX C

FIXTURE POINT THEOREM DATA

Table C.1 IAE result of temperature deviation

Stream	IPA	2-liquid	2-cool	3	3-cool	8
V1	0.0000	0.0831	1.6737	0.1620	0.7276	0.3830
V2	0.0000	0.0262	0.2016	0.0117	0.0727	0.2327
V3	0.0000	0.0421	2.1873	0.1133	0.9202	0.4392
V4	0.0000	0.0841	0.0596	0.0147	0.0153	0.0067
V5	0.0000	0.0244	0.0995	0.0056	0.0261	0.0183
V6	0.0000	0.0374	1.1010	0.0136	0.4566	0.1959
V7	0.0000	0.1766	0.1487	0.0082	0.0879	0.0444
V8	0.0000	0.0400	0.0954	0.0113	0.0236	0.0117
V9	0.0000	0.2027	0.1971	0.0059	0.0691	0.0396
V10	0.0000	0.0202	0.0906	0.0123	0.0260	0.0114
Q-new	0.0000	0.0202	42.0671	2.7200	0.6117	0.3560
reactor	0.0000	0.0341	6.6061	7.2498	0.7517	0.4380
TIC-cooler1-1	0.0000	0.1692	7.8025	0.6921	3.3964	1.5325
TIC-final	0.0000	0.0219	0.0851	0.0099	0.0216	0.0116
D1-con	0.0000	0.0642	0.0463	0.0122	0.0145	0.0113
D1-re	0.0000	0.1300	6.0437	0.5090	2.7750	1.2470
D2-con	0.0000	0.1059	0.1364	0.0024	0.0225	0.0147
D2-re	0.0000	0.2232	0.2502	0.0242	0.0458	0.0255
sum	0.0000	1.5053	68.8919	11.5783	10.0642	5.0194

Stream	9	10	becool	water	rec1	waste water
V1	0.6235	1.1016	0.1014	0.0000	0.4338	0.8870
V2	0.2153	1.8058	0.0372	0.0000	0.1776	0.3207
V3	0.8362	1.8904	0.0337	0.0000	0.1979	0.2696
V4	0.0459	1.1966	0.1303	0.0000	0.5372	1.1935
V5	0.0360	1.8856	0.0339	0.0000	0.1708	0.2945
V6	0.4018	2.1236	0.3382	0.0000	0.2049	0.3149
V7	0.0976	1.6983	0.0395	0.0000	0.8677	3.0987
V8	0.0206	1.3320	0.0738	0.0000	0.2519	0.6672
V9	0.0698	1.7301	0.1711	0.0000	0.4028	1.5384
V10	0.0239	1.3950	0.2446	0.0000	0.1310	4.4545
Q-new	0.5710	0.4559	0.0242	0.0000	0.0843	0.2309
reactor	0.7540	0.7529	0.1266	0.0000	0.1539	1.1467
TIC-cooler1-1	3.036	1.7023	0.0780	0.0000	0.1982	0.5714
TIC-final	0.0281	1.6620	0.0371	0.0000	0.1525	4.5048
D1-con	0.0191	1.3577	0.0660	0.0000	0.4436	0.5735
D1-re	2.6401	1.7182	0.1142	0.0000	0.3351	0.8611
D2-con	0.0337	1.6893	0.3055	0.0000	0.5672	2.7938
D2-re	0.0312	1.5459	0.6326	0.0000	1.0888	5.5557
sum	9.4840	27.0433	2.5878	0.0000	6.3992	29.2770

Table C.2 IAE Result of pressure deviation

Stream	IPA	2-liquid	2-cool	3	3-cool	8
V1	0.0000	0.0188	0.0182	0.0200	0.0214	0.0193
V2	0.0000	0.0002	0.0003	0.0004	0.0006	0.0043
V3	0.0000	0.0021	0.0031	0.0041	0.0063	0.0145
V4	0.0000	0.0003	0.0003	0.0003	0.0004	0.0004
V5	0.0000	0.0001	0.0002	0.0002	0.0002	0.0004
V6	0.0000	0.0011	0.0016	0.0021	0.0031	0.0061
V7	0.0000	0.0020	0.0018	0.0020	0.0021	0.0019
V8	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002
V9	0.0000	0.0017	0.0016	0.0018	0.0019	0.0017
V10	0.0000	0.0001	0.0002	0.0002	0.0001	0.0001
Q-new	0.0000	0.0024	0.0036	0.0063	0.0073	0.0065
reactor	0.0000	0.0062	0.0091	0.0087	0.0098	0.0091
TIC-cooler1-1	0.0000	0.0070	0.0102	0.0131	0.0198	0.0452
TIC-final	0.0000	0.0001	0.0002	0.0002	0.0001	0.0001
D1-con	0.0000	0.0002	0.0002	0.0002	0.0003	0.0003
D1-re	0.0000	0.0055	0.0080	0.0101	0.0151	0.0389
D2-con	0.0000	0.0005	0.0005	0.0005	0.0005	0.0005
D2-re	0.0000	0.0011	0.0010	0.0010	0.0011	0.001
sum	0.0000	0.0495	0.0601	0.0713	0.0904	0.1505

Stream	9	10	becool	water	rec1	waste water
V1	0.0105	0.0085	0.0214	0.0000	0.0000	0.0000
V2	0.0198	0.0030	0.0006	0.0000	0.0000	0.0000
V3	0.0182	0.0028	0.0063	0.0000	0.0000	0.0000
V4	0.011	0.0109	0.0004	0.0000	0.0000	0.0000
V5	0.0209	0.0028	0.0002	0.0000	0.0000	0.0000
V6	0.0201	0.0032	0.0031	0.0000	0.0000	0.0000
V7	0.0157	0.0283	0.0021	0.0000	0.0000	0.0000
V8	0.0164	0.0061	0.0002	0.0000	0.0000	0.0000
V9	0.0196	0.0143	0.0000	0.0000	0.0000	0.0000
V10	0.0176	0.0040	0.0001	0.0000	0.0000	0.0000
Q-new	0.0050	0.0020	0.0073	0.0000	0.0000	0.0000
reactor	0.0173	0.0102	0.0098	0.0000	0.0000	0.0000
TIC-cooler1-1	0.0179	0.0065	0.0198	0.0000	0.0000	0.0000
TIC-final	0.0194	0.0030	0.0001	0.0000	0.0000	0.0000
D1-con	0.0140	0.0054	0.0003	0.0000	0.0000	0.0000
D1-re	0.0190	0.0091	0.0151	0.0000	0.0000	0.0000
D2-con	0.0160	0.0257	0.0005	0.0000	0.0000	0.0000
D2-re	0.0153	0.0531	0.0011	0.0000	0.0000	0.0000
sum	0.2938	0.1989	0.0885	0.0000	0.0000	0.0000

Table C.3 IAE Result of flow deviation

Stream	IPA	2-liquid	2-cool	3	3-cool	8
V1	0.2005	0.1484	0.1486	0.2825	0.2826	0.2482
V2	0.0203	0.0195	0.0191	0.0269	0.0272	0.0245
V3	0.2018	0.2008	0.2006	0.2815	0.2820	0.2219
V4	0.0256	0.0026	0.0022	0.0144	0.0143	0.0191
V5	0.0105	0.0107	0.0095	0.0142	0.0150	0.0157
V6	0.104	0.1011	0.1003	0.1396	0.1403	0.0850
V7	0.1896	0.0181	0.0178	0.0236	0.024	0.0182
V8	0.0144	0.0112	0.0096	0.0148	0.0159	0.0135
V9	0.1626	0.0174	0.0170	0.0294	0.0297	0.0273
V10	0.0090	0.0115	0.0098	0.0149	0.0163	0.0129
Q-new	0.2299	0.2387	0.2374	0.2277	0.2278	0.2088
reactor	0.5834	0.6194	0.6145	0.2448	0.2439	0.4725
TIC-cooler1-1	0.6915	0.6964	0.6964	0.9104	0.9205	0.4416
TIC-final	0.0094	0.0103	0.0088	0.0138	0.0150	0.0143
D1-con	0.0162	0.0027	0.0026	0.0147	0.0151	0.0204
D1-re	0.5513	0.5238	0.5237	0.6908	0.6979	0.4509
D2-con	0.0477	0.0096	0.0084	0.0118	0.0124	0.0141
D2-re	0.1012	0.0116	0.0113	0.0164	0.0169	0.0152
sum	3.1690	2.6538	2.6375	2.9723	2.9968	2.3242

Stream	9	10	becool-ff-F	water	rec1	waste water
V1	2.0662	1.5198	0.4355	0.3865	0.0522	0.4373
V2	2.6431	2.4853	0.1540	1.2807	0.0074	0.1543
V3	1.5650	2.318	0.1394	0.2838	0.0052	0.1403
V4	2.4619	1.5316	0.5626	0.0073	0.0265	0.5638
V5	2.1857	2.5861	0.1401	0.0083	0.0067	0.1404
V6	1.7601	2.5807	0.1629	0.1174	0.0059	0.1639
V7	1.4757	1.7664	1.4779	0.0384	0.2071	1.4827
V8	1.7103	3.7686	0.3102	0.0038	0.0134	0.3107
V9	2.0910	2.3929	0.7262	0.0339	0.1723	0.7275
V10	1.8291	2.1286	2.6599	0.0021	0.0084	2.6666
Q-new	0.4819	0.7669	0.0996	0.1297	0.0087	0.0992
reactor	1.2806	1.5754	0.5186	0.1825	0.0357	0.5178
TIC-cooler1-1	1.6496	1.8827	0.3142	0.8358	0.0173	0.3168
TIC-final	2.0209	2.4025	0.1535	0.0025	0.0069	0.1566
D1-con	1.3274	2.0193	0.2761	0.0057	0.0145	0.2769
D1-re	0.9829	1.9919	0.5507	0.7062	0.0291	0.5572
D2-con	1.6897	2.0116	1.3216	0.0097	0.0533	1.3259
D2-re	1.5683	1.7861	2.6485	0.0190	0.1111	2.6524
sum	30.7895	37.5144	12.6514	4.0535	0.7816	12.6902

Table C.4 IAE Result of Temperature Deviation at Ac column

	Tray 1	Tray 2	Tray 3	Tray 4	Tray 5	Tray 6	Tray 7	Tray 8	Tray 9	Tray 10
V1	0.8832	0.8794	0.8753	0.8713	0.8676	0.8637	0.8595	0.8558	0.8520	0.8484
V2	0.9981	0.9939	0.9891	0.9845	0.9797	0.9751	0.9710	0.9665	0.9622	0.9577
V3	0.9826	0.9785	0.9739	0.9693	0.9647	0.9603	0.9561	0.9517	0.9475	0.9432
V4	0.8865	0.8826	0.8785	0.8744	0.8705	0.8666	0.8624	0.8586	0.8547	0.8511
V5	0.9968	0.9926	0.9879	0.9833	0.9785	0.9740	0.9699	0.9654	0.9611	0.9567
V6	0.9908	0.9867	0.9820	0.9775	0.9728	0.9683	0.9641	0.9597	0.9555	0.9511
V7	1.0480	1.0437	1.0391	1.0344	1.0299	1.0254	1.0209	1.0165	1.0121	1.0077
V8	0.9927	0.9887	0.9839	0.9794	0.9744	0.9699	0.9661	0.9616	0.9573	0.9528
V9	1.0048	1.0006	0.9959	0.9912	0.9863	0.9817	0.9776	0.9731	0.9688	0.9643
V10	0.9981	0.9940	0.9893	0.9847	0.9797	0.9751	0.9713	0.9668	0.9625	0.9579
Q-new	1.0273	1.0237	1.0188	1.0144	1.0088	1.0045	1.0018	0.9972	0.9933	0.9883
reactor	1.1430	1.1388	1.1332	1.1282	1.1216	1.1165	1.1136	1.1082	1.1036	1.0979
TIC-cooler1-1	1.0213	1.0169	1.0121	1.0074	1.0027	0.9980	0.9936	0.9890	0.9846	0.9801
TIC-final	0.9944	0.9903	0.9855	0.9810	0.9761	0.9716	0.9676	0.9631	0.9589	0.9544
D1-con	0.9137	0.9097	0.9054	0.9011	0.8970	0.8929	0.8888	0.8848	0.8808	0.8767
D1-re	1.0005	0.9962	0.9916	0.9870	0.9825	0.9780	0.9736	0.9693	0.9649	0.9606
D2-con	0.9932	0.9891	0.9844	0.9798	0.9749	0.9704	0.9664	0.9619	0.9576	0.9532
D2-re	1.0115	1.0073	1.0025	0.9978	0.9929	0.9883	0.9842	0.9796	0.9753	0.9707
sum	17.8867	17.8124	17.7283	17.6468	17.5606	17.4804	17.4085	17.3288	17.2526	17.1729

	Tray 11	Tray 12	Tray 13	Tray 14	Tray 15	Tray 16	Tray 17	Tray 18	Tray 19	Tray 20
V1	0.8446	0.8411	0.8373	0.8338	0.8303	0.8269	0.8235	0.8199	0.8169	0.8135
V2	0.9537	0.9494	0.9454	0.9413	0.9373	0.9333	0.9293	0.9256	0.9214	0.9177
V3	0.9392	0.9350	0.9310	0.9270	0.9231	0.9191	0.9153	0.9115	0.9076	0.9039
V4	0.8472	0.8436	0.8398	0.8363	0.8327	0.8293	0.8258	0.8222	0.8191	0.8157
V5	0.9527	0.9484	0.9445	0.9404	0.9364	0.9324	0.9284	0.9247	0.9206	0.9169
V6	0.9471	0.9428	0.9389	0.9348	0.9309	0.9269	0.9230	0.9192	0.9152	0.9116
V7	1.0035	0.9992	0.9950	0.9908	0.9866	0.9824	0.9783	0.9743	0.9702	0.9662
V8	0.9489	0.9445	0.9408	0.9366	0.9328	0.9287	0.9248	0.9212	0.9169	0.9134
V9	0.9603	0.9559	0.9520	0.9478	0.9438	0.9398	0.9358	0.9321	0.9279	0.9242
V10	0.9541	0.9497	0.9459	0.9418	0.9379	0.9338	0.9299	0.9263	0.9219	0.9183
Q-new	0.9853	0.9807	0.9777	0.9737	0.9701	0.9659	0.9621	0.9589	0.9537	0.9503
reactor	1.0944	1.0890	1.0856	1.0808	1.0768	1.0720	1.0677	1.0643	1.0583	1.0547
TIC-cooler1-1	0.9758	0.9715	0.9673	0.9631	0.9590	0.9549	0.9508	0.9468	0.9428	0.9390
TIC-final	0.9505	0.9461	0.9423	0.9382	0.9342	0.9302	0.9263	0.9226	0.9184	0.9148
D1-con	0.8729	0.8689	0.8652	0.8615	0.8578	0.8541	0.8505	0.8468	0.8435	0.8402
D1-re	0.9565	0.9523	0.9482	0.9441	0.9401	0.9361	0.9322	0.9284	0.9245	0.9207
D2-con	0.9492	0.9449	0.9410	0.9369	0.9330	0.9289	0.9250	0.9214	0.9172	0.9136
D2-re	0.9667	0.9623	0.9583	0.9542	0.9501	0.9460	0.9420	0.9383	0.9341	0.9303
sum	17.1024	17.0252	16.9563	16.8832	16.8128	16.7406	16.6708	16.6046	16.5301	16.4650

Table C.4(Cont)

	Tray 21	Tray 22	Tray 23	Tray 24	Tray 25	Tray 26	Tray 27	Tray 28	Tray 29	Tray 30
V1	0.8105	0.8072	0.8041	0.8007	0.7976	0.7945	0.7916	0.7881	0.7846	0.7817
V2	0.9138	0.9101	0.9067	0.9033	0.8998	0.8962	0.8923	0.8888	0.8847	0.8788
V3	0.9001	0.8965	0.8930	0.8897	0.8862	0.8827	0.8791	0.8756	0.8717	0.8666
V4	0.8126	0.8093	0.8061	0.8028	0.7996	0.7965	0.7936	0.7901	0.7866	0.7836
V5	0.9130	0.9094	0.9059	0.9026	0.8991	0.8954	0.8916	0.8881	0.8840	0.8780
V6	0.9077	0.9041	0.9006	0.8972	0.8937	0.8902	0.8865	0.8829	0.8789	0.8736
V7	0.9621	0.9581	0.9541	0.9501	0.9461	0.9419	0.9375	0.9328	0.9276	0.9214
V8	0.9093	0.9058	0.9024	0.8993	0.8959	0.8923	0.8884	0.8851	0.8810	0.8742
V9	0.9202	0.9165	0.9130	0.9097	0.9062	0.9025	0.8986	0.8951	0.8909	0.8847
V10	0.9143	0.9107	0.9073	0.9041	0.9006	0.8969	0.8930	0.8896	0.8855	0.8787
Q-new	0.9451	0.9412	0.9371	0.9335	0.9286	0.9224	0.9143	0.9063	0.8946	0.8735
reactor	1.0490	1.0448	1.0405	1.0370	1.0320	1.0260	1.0182	1.0115	1.0017	0.9825
TIC-cooler1-1	0.9351	0.9313	0.9276	0.9240	0.9203	0.9167	0.9131	0.9095	0.9058	0.9019
TIC-final	0.9108	0.9072	0.9038	0.9005	0.8971	0.8935	0.8896	0.8862	0.8821	0.8758
D1-con	0.8367	0.8332	0.8299	0.8267	0.8234	0.8202	0.8171	0.8135	0.8099	0.8029
D1-re	0.9170	0.9133	0.9097	0.9062	0.9027	0.8993	0.8958	0.8924	0.8890	0.8855
D2-con	0.9096	0.9060	0.9026	0.8993	0.8959	0.8923	0.8884	0.8850	0.8809	0.8746
D2-re	0.9263	0.9227	0.9192	0.9158	0.9122	0.9086	0.9047	0.9011	0.8969	0.8907
sum	16.3931	16.3275	16.2636	16.2025	16.1370	16.0681	15.9933	15.9215	15.8365	15.7088

	Tray 31	Tray 32	Tray 33	Tray 34	Tray 35	Tray 36	Tray 37	Tray 38	Tray 39	Tray 40
V1	0.7755	0.7692	0.7537	0.7521	0.7472	0.7444	0.7407	0.7375	0.7341	0.7310
V2	0.8743	0.8642	0.8469	0.8414	0.8396	0.8356	0.8328	0.8294	0.8264	0.8233
V3	0.8624	0.8544	0.8415	0.8356	0.8322	0.8276	0.8239	0.8200	0.8164	0.8130
V4	0.7775	0.7712	0.7586	0.7560	0.7509	0.7474	0.7432	0.7396	0.7360	0.7330
V5	0.8736	0.8633	0.8457	0.8401	0.8383	0.8343	0.8315	0.8281	0.8251	0.8220
V6	0.8691	0.8603	0.8458	0.8400	0.8367	0.8322	0.8287	0.8249	0.8214	0.8180
V7	0.9135	0.9012	0.8771	0.8736	0.8705	0.8673	0.8643	0.8612	0.8583	0.8554
V8	0.8709	0.8600	0.8436	0.8363	0.8356	0.8310	0.8285	0.8250	0.8220	0.8190
V9	0.8805	0.8700	0.8526	0.8466	0.8450	0.8409	0.8381	0.8347	0.8317	0.8285
V10	0.8753	0.8644	0.8481	0.8406	0.8399	0.8354	0.8328	0.8292	0.8263	0.8231
Q-new	0.8571	0.8169	0.7630	0.7491	0.7530	0.7463	0.7451	0.7411	0.7387	0.7357
reactor	0.9728	0.9398	0.9006	0.8837	0.8886	0.8807	0.8792	0.8742	0.8714	0.8680
TIC-cooler1-1	0.8985	0.8952	0.8966	0.8917	0.8877	0.8834	0.8794	0.8753	0.8713	0.8673
TIC-final	0.8719	0.8613	0.8443	0.8379	0.8367	0.8324	0.8298	0.8263	0.8233	0.8203
D1-con	0.8006	0.7923	0.7756	0.7733	0.7695	0.7662	0.7627	0.7600	0.7571	0.7538
D1-re	0.8826	0.8804	0.8841	0.8798	0.8760	0.8720	0.8681	0.8642	0.8604	0.8566
D2-con	0.8706	0.8602	0.8430	0.8368	0.8355	0.8313	0.8285	0.8252	0.8222	0.8190
D2-re	0.8864	0.8759	0.8582	0.8523	0.8507	0.8466	0.8438	0.8403	0.8373	0.8342
sum	15.6130	15.4003	15.0788	14.9665	14.9339	14.8550	14.8010	14.7362	14.6795	14.6213

Table C.4(Cont)

	Tray 41	Tray 42	Tray 43	Tray 44	Tray 45	Tray 46	Tray 47	Tray 48	Tray 49	Tray 50
V1	0.7279	0.7242	0.7221	0.7192	0.7142	0.7174	0.7126	0.7093	0.7072	0.7045
V2	0.8201	0.8179	0.8139	0.8109	0.8045	0.8068	0.8006	0.7987	0.7959	0.7942
V3	0.8095	0.8067	0.8030	0.7999	0.7937	0.7962	0.7902	0.7881	0.7854	0.7836
V4	0.7301	0.7266	0.7245	0.7217	0.7166	0.7198	0.7149	0.7117	0.7095	0.7068
V5	0.8189	0.8166	0.8126	0.8097	0.8032	0.8056	0.7993	0.7974	0.7946	0.7929
V6	0.8147	0.8120	0.8083	0.8053	0.7991	0.8016	0.7956	0.7934	0.7907	0.7889
V7	0.8526	0.8499	0.8471	0.8444	0.8391	0.8416	0.8365	0.8341	0.8315	0.8290
V8	0.8159	0.8142	0.8094	0.8065	0.7997	0.8016	0.7950	0.7937	0.7908	0.7897
V9	0.8254	0.8232	0.8190	0.8161	0.8094	0.8117	0.8054	0.8036	0.8007	0.7991
V10	0.8200	0.8183	0.8135	0.8105	0.8037	0.8057	0.7989	0.7977	0.7947	0.7936
Q-new	0.7328	0.7336	0.7264	0.7239	0.7163	0.7160	0.7091	0.7108	0.7081	0.7103
reactor	0.8643	0.8654	0.8567	0.8535	0.8441	0.8440	0.8353	0.8372	0.8335	0.8355
TIC-cooler1-1	0.8634	0.8597	0.8557	0.8520	0.8447	0.8481	0.8411	0.8380	0.8349	0.8322
TIC-final	0.8170	0.8151	0.8107	0.8078	0.8012	0.8034	0.7970	0.7953	0.7925	0.7911
D1-con	0.7511	0.7485	0.7453	0.7424	0.7369	0.7397	0.7340	0.7320	0.7291	0.7267
D1-re	0.8528	0.8492	0.8453	0.8417	0.8344	0.8379	0.8307	0.8275	0.8242	0.8213
D2-con	0.8159	0.8139	0.8096	0.8066	0.8001	0.8023	0.7959	0.7942	0.7915	0.7899
D2-re	0.8311	0.8288	0.8247	0.8217	0.8152	0.8175	0.8110	0.8092	0.8063	0.8046
sum	14.5636	14.5238	14.4479	14.3938	14.2762	14.3171	14.2030	14.1719	14.1212	14.0938

	Tray 51	Tray 52	Tray 53	Tray 54	Tray 55	Tray 56	Tray 57	Tray 58	Tray 59	Tray 60
V1	0.7035	0.7019	0.7026	0.7033	0.7099	0.7189	0.7371	0.7711	0.8406	0.9787
V2	0.7914	0.7904	0.7889	0.7904	0.7906	0.7971	0.8093	0.8333	0.8758	0.9637
V3	0.7812	0.7800	0.7790	0.7803	0.7819	0.7890	0.8025	0.8290	0.8781	0.9796
V4	0.7055	0.7040	0.7044	0.7051	0.7112	0.7200	0.7377	0.7711	0.8388	0.9734
V5	0.7901	0.7891	0.7875	0.7891	0.7893	0.7958	0.8081	0.8323	0.8751	0.9637
V6	0.7864	0.7853	0.7841	0.7853	0.7866	0.7934	0.8063	0.8316	0.8784	0.9753
V7	0.8262	0.8233	0.8198	0.8156	0.8097	0.8013	0.7879	0.7654	0.7252	0.6536
V8	0.7864	0.7858	0.7839	0.7863	0.7852	0.7925	0.8053	0.8307	0.8725	0.9594
V9	0.7961	0.7951	0.7934	0.7949	0.7947	0.8009	0.8125	0.8355	0.8755	0.9585
V10	0.7902	0.7897	0.7876	0.7901	0.7887	0.7958	0.8082	0.8329	0.8731	0.9569
Q-new	0.7063	0.7090	0.7072	0.7158	0.7126	0.7270	0.7475	0.7853	0.8327	0.9281
reactor	0.8292	0.8312	0.8269	0.8336	0.8236	0.8317	0.8411	0.8596	0.8673	0.8870
TIC-cooler1-1	0.8295	0.8276	0.8262	0.8262	0.8273	0.8321	0.8421	0.8624	0.9022	0.9855
TIC-final	0.7881	0.7873	0.7855	0.7875	0.7871	0.7940	0.8064	0.8312	0.8735	0.9613
D1-con	0.7251	0.7237	0.7230	0.7245	0.7281	0.7369	0.7509	0.7828	0.8415	0.9582
D1-re	0.8185	0.8163	0.8148	0.8147	0.8163	0.8218	0.8337	0.8578	0.9056	1.0060
D2-con	0.7870	0.7861	0.7845	0.7863	0.7861	0.7930	0.8056	0.8304	0.8733	0.9622
D2-re	0.8017	0.8007	0.7989	0.8002	0.7998	0.8057	0.8167	0.8387	0.8769	0.9563
sum	14.0423	14.0266	13.9981	14.0293	14.0288	14.1467	14.3592	14.7811	15.5059	17.0073

Table C.4(Cont)

	Tray 61	Tray 62	Tray 63	Tray 64	Tray 65	Tray 66
V1	1.2662	1.9228	3.2994	4.9372	4.5809	2.8779
V2	1.1621	1.6027	2.4714	3.2428	2.7581	1.9477
V3	1.2054	1.7098	2.6707	3.4334	2.8361	1.9986
V4	1.2536	1.8922	3.2381	4.8801	4.5929	2.8984
V5	1.1638	1.6082	2.4847	3.2638	2.7753	1.9528
V6	1.1915	1.6742	2.5932	3.3176	2.7437	1.9660
V7	0.5699	0.9431	1.9449	3.2291	3.0154	1.7660
V8	1.1605	1.6008	2.4872	3.3290	2.8807	1.9964
V9	1.1478	1.5663	2.3964	3.1457	2.6921	1.9108
V10	1.1516	1.5771	2.4344	3.2509	2.8191	1.9625
Q-new	1.1620	1.6425	2.6317	3.6489	3.2655	2.2913
reactor	0.9679	1.0965	1.3687	1.6306	1.5324	1.3529
TIC-cooler1-1	1.1713	1.5782	2.2538	2.6016	2.0737	1.6817
TIC-final	1.1618	1.6042	2.4870	3.3034	2.8367	1.9763
D1-con	1.2029	1.7582	2.9472	4.4731	4.3115	2.7894
D1-re	1.2296	1.7166	2.5059	2.8759	2.2298	1.6494
D2-con	1.1646	1.6118	2.5030	3.3234	2.8495	1.9842
D2-re	1.1375	1.5381	2.3312	3.0423	2.6043	1.8643
sum	20.4700	28.6435	45.0490	60.9288	53.3977	36.8667

Table C.5 IAE Result of Temperature Deviation at IPA column

	Tray 1	Tray 2	Tray 3	Tray 4	Tray 5	Tray 6	Tray 7	Tray 8	Tray 9	Tray 10
V1	0.1435	0.1182	0.1129	0.1123	0.1137	0.1174	0.1264	0.1503	0.2346	0.6525
V2	0.0644	0.0531	0.0516	0.0525	0.0557	0.0645	0.0931	0.2312	1.4404	4.6929
V3	0.0662	0.0530	0.0512	0.0531	0.0598	0.0830	0.2416	1.1377	2.5235	4.3947
V4	0.1817	0.1530	0.1473	0.1468	0.1485	0.1528	0.1629	0.1883	0.2639	0.6121
V5	0.0596	0.0488	0.0474	0.0482	0.0511	0.0589	0.0842	0.2027	1.2635	4.5276
V6	0.0706	0.0582	0.0565	0.0582	0.0644	0.0856	0.2215	1.1227	2.5659	4.3101
V7	0.3452	0.3266	0.3230	0.3222	0.3228	0.3249	0.3310	0.3482	0.4008	0.7260
V8	0.1124	0.0988	0.0966	0.0968	0.0990	0.1047	0.1209	0.1751	0.4609	3.0222
V9	0.2267	0.2175	0.2160	0.2160	0.2175	0.2221	0.2377	0.3033	0.8490	3.7926
V10	0.0704	0.0647	0.0649	0.0649	0.0658	0.0683	0.0785	0.1219	0.4021	3.2711
Q-new	0.0484	0.0408	0.0456	0.0445	0.0414	0.0441	0.0567	0.1054	0.3489	2.5932
reactor	0.1970	0.2048	0.2109	0.2093	0.2062	0.1978	0.1829	0.1449	0.1024	1.2396
TIC-cooler1-1	0.1268	0.1233	0.1674	0.4320	0.7336	1.0277	1.3160	1.6426	2.1266	3.1593
TIC-final	0.0595	0.0502	0.0493	0.0498	0.0518	0.0573	0.0745	0.1434	0.6514	4.1790
D1-con	0.1311	0.1030	0.0973	0.0972	0.0991	0.1035	0.1127	0.1350	0.2018	0.5165
D1-re	0.1813	0.4347	0.6792	0.9067	1.1338	1.3841	1.6534	1.9114	2.1668	2.3742
D2-con	0.3720	0.3761	0.3765	0.3750	0.3722	0.3670	0.3565	0.3928	0.7255	2.9356
D2-re	0.6009	0.6026	0.6014	0.5989	0.5952	0.5889	0.5735	0.5460	0.8960	2.8578
sum	3.0579	3.1273	3.3948	3.8843	4.4317	5.0524	6.0239	9.0031	17.6240	49.8571

	Tray 11	Tray 12	Tray 13	Tray 14	Tray 15	Tray 16	Tray 17	Tray 18	Tray 19
V1	3.8493	6.7175	3.5043	1.1193	0.7383	0.7047	0.2589	0.1130	0.1129
V2	5.7805	1.7917	1.0901	1.0397	1.0494	1.0645	0.2721	0.0650	0.0478
V3	4.5525	1.5095	0.9968	0.9607	0.9680	0.9790	0.2593	0.0668	0.0437
V4	3.2331	5.8715	4.0656	1.4946	0.8225	0.7436	0.3125	0.1597	0.1397
V5	5.9988	1.8644	1.1218	1.0686	1.0791	1.0954	0.2754	0.0615	0.0432
V6	4.3034	1.5218	1.0554	1.0245	1.0333	1.0456	0.2805	0.0733	0.0486
V7	3.2734	5.0927	2.6939	1.1462	0.9414	0.9230	0.4887	0.3465	0.3234
V8	6.8860	2.2670	1.2661	1.1882	1.1946	1.2091	0.3848	0.1187	0.0982
V9	5.8508	1.7284	1.0450	1.0039	1.0131	1.0267	0.3761	0.2377	0.2196
V10	7.6694	2.2382	1.1591	1.0748	1.0838	1.1011	0.2553	0.0727	0.0730
Q-new	10.1628	2.4056	0.8179	0.6729	0.6619	0.6625	0.1435	0.0452	0.0585
reactor	9.3515	2.7782	0.9771	0.8172	0.8152	0.8277	0.1161	0.1901	0.2313
TIC-cooler1-1	2.9186	1.1353	0.8971	0.8863	0.8910	0.8972	0.2693	0.1305	0.1194
TIC-final	6.8460	2.0339	1.1361	1.0686	1.0782	1.0947	0.2664	0.0606	0.0493
D1-con	2.8836	5.2564	4.3387	2.3306	1.1679	0.9144	0.3248	0.1116	0.0747
D1-re	1.9030	0.8841	0.7262	0.7156	0.7181	0.7218	0.2588	0.1333	0.1133
D2-con	5.2279	1.4914	1.0791	1.0611	1.0737	1.0894	0.5311	0.3942	0.4029
D2-re	4.2433	1.3453	0.8058	0.7678	0.7720	0.7800	0.5419	0.6335	0.6493
sum	94.9340	47.9328	28.7761	19.4405	17.1016	16.8804	5.6156	3.0139	2.8488

Table C.6 IAE result of level deviation at acetone column and IPA column

Stream	D1-con-L	D1-re-L	D1-con-P	D2-con-L	D2-re-L
V1	0.0959	14.9758	0.0109	0.0859	0.2956
V2	0.0251	6.3547	0.0051	0.0081	0.5791
V3	0.1682	9.0452	0.0177	0.0358	1.7667
V4	0.2703	7.3123	0.0186	0.0236	1.4334
V5	0.1391	14.5489	0.0168	0.0275	4.3193
V6	0.1588	11.8151	0.0180	0.0244	2.7688
V7	0.3153	14.4230	0.0160	0.3824	2.2310
V8	0.2105	12.3025	0.0204	0.0302	0.6414
V9	0.1985	12.5536	0.0202	0.3683	1.9455
V10	0.1785	13.3662	0.0199	0.0303	0.7676
Q-new	0.3094	10.0156	0.0197	0.1202	2.6251
reactor	0.8187	17.4723	0.0145	0.0700	0.2861
TIC-cooler1-1	0.1545	8.9610	0.0158	0.2457	5.6611
TIC-final	0.1510	11.2527	0.0164	1.3035	4.2449
D1-con	0.1983	13.6495	0.0188	0.0336	0.4176
D1-re	0.2109	14.4413	0.0208	0.0296	0.4191
D2-con	0.2090	14.1877	0.0215	0.0318	0.6652
D2-re	0.1014	15.9248	0.0113	0.0691	0.7099
sum	3.9132	222.6023	0.3024	2.9198	31.7775

VITA

Miss Sirikorn Juengtanakornkul was born in Bangkok, Thailand on January 17, 1985. She received the Bachelor Degree in Chemical Engineering from Kasetsart University in 2006. After that he entered the Graduate School of Chulalongkorn University to pursue the Master of Engineering in Chemical Engineering and completed in 2009.