การออกแบบโครงสร้างการควบคุมสำหรับกระบวนการ
ฟีนอลไฮโดรจีเนชันเป็นไซโคลเฮกซาโนน

นายกำชัย สุขก้องวารี

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต
สาขาวิชาวิศวกรรมเคมี ภาควิชาวิศวกรรมเคมี
คณะวิศวกรรมศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
ปีการศึกษา 2552

CONTROL STRUCTURE DESIGN FOR PHENOL HYDREOGENATION TO CYCLOHEXANONE PROCESS

Mr. Kumchai Sukkongwaree

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 2009

Thesis Title	CONTROL STRUCTURE DESIGN FOR PHENOL HYDROGENATION TO CYCLOHEXANONE PROCESS
By	Mr. Kumchai Sukkongwaree
Field of Study	Chemical Engineering
Thesis 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

M. Phisalaphong .... Chairman

(Associate Professor Muenduen Phisalaphong, Ph.D.)

Montree Wongsri .... Thesis Advisor

(Assistant Professor Montree Wongsri, D.Sc.)

Soorathep Kheawhom .... Examiner

(Assistant Professor Soorathep Kheawhom, Ph.D.)

.... External Examiner

(Veerayut Lersbamrungsuk, D.Eng.)

กำชัย สุขก้องวารี : การออกแบบโครงสร้างการควบคุมสำหรับกระบวนการฟีนอลไฮโดรจีเนชันเป็นไซโคลเฮกซาโนน. (CONTROL STRUCTURE DESIGN FOR PHENOL HYDROGENATION TO CYCLOHEXANONE PROCESS) อ. ที่ปรึกษาวิทยานิพนธ์หลัก : ผู้ช่วยศาสตราจารย์ ดร. มนตรี วงศ์ศรี, 169 หน้า.

การนำสารตั้งต้นและพลังงานกลับมาใช้ใหม่ สามารถลดต้นทุนการผลิตในโรงงานอุตสาหกรรม แต่สิ่งที่เป็นผลตามมาคือโครงสร้างของกระบวนการที่จะมีความซับซ้อนมากยิ่งขึ้น ดังนั้นการควบคุมกระบวนการโดยรวมให้มีสมรรถนะที่ดีจึงจัดเป็นสิ่งที่จำเป็น และมีความสำคัญในการดำเนินกระบวนการผลิตให้เป็นไปตามวัตถุประสงค์ ทั้งในด้านของความปลอดภัยและคุณภาพของผลิตภัณฑ์ นอกจากนี้ยังจะนำมาซึ่งการใช้สารตั้งต้นและพลังงานอย่างคุ้มค่าอีกด้วย งานวิจัยนี้ได้นำกระบวนการฟีนอลไฮโดรจีเนชันเป็นไซโคลเฮกซาโนนซึ่งประกอบไปด้วยสายป้อนกลับหลายสาย และมีการแลกเปลี่ยนพลังงานระหว่างกันภายในกระบวนการ มาศึกษาการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ตามขั้นตอนของลูเบน (1998) และขั้นตอนของวงศ์ศรี (2009) โดยในงานวิจัยนี้ใช้โปรแกรมไฮซีสเพื่อจำลองกระบวนการฟีนอลไฮโดรจีเนชันเป็นไซโคลเฮกซาโนน ทั้งที่สภาวะคงตัวและที่สภาวะพลวัต เมื่อทำการออกแบบโครงสร้างการควบคุมตามขั้นตอนของลูเบน (1998) และขั้นตอนของวงศ์ศรี (2009) ผลปรากฏว่าได้โครงสร้างการควบคุมเดียวกันซึ่งประกอบไปด้วยโครงสร้างการควบคุมทั้งหมด 4 โครงสร้าง จากนั้นทำการประเมินสมรรถนะและเปรียบเทียบผลของโครงสร้างการควบคุมทั้งหมดที่ได้ออกแบบด้วยการรบกวนระบบทั้งทางด้านมวลสารและด้านความร้อน ผลที่ได้พบว่าโครงสร้างการควบคุมที่ได้ออกแบบทั้งหมดมีสมรรถนะที่ดี สามารถกำจัดตัวแปรรบกวนที่เข้าสู่ระบบ และรักษาคุณภาพของผลิตภัณฑ์ได้ สรุปได้ว่าการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ตามขั้นตอนของวงศ์ศรี (2009) สามารถออกแบบโครงสร้างการควบคุมที่มีสมรรถนะที่ดีได้

ภาควิชา.......วิศวกรรมเคมี................. ลายมือชื่อนิสิต....กำชัย สุขก้องวารี..................
สาขาวิชา.......วิศวกรรมเคมี................. ลายมือชื่อ อ.ที่ปรึกษาวิทยานิพนธ์หลัก........
ปีการศึกษา....2552..................................

5170549221 : MAJOR CHEMICAL ENGINEERING
KEYWORDS : PHENOL HYDROGENATION TO CYCLOHEXANONE PROCESS / CONTROL STRUCTURE DESIGN / HYSYS

KUMCHAI SUKKONGWAREE : CONTROL STRUCTURE DESIGN FOR PHENOL HYDROGENATION TO CYCLOHEXANONE PROCESS. THESIS ADVISOR : ASSISTANT PROFESSOR MONTREE WONGSRI, D.Sc., 169 pp.

For industries, material and energy recycle are beneficial in economic aspect. However, they make processes more complex. So the good control structure is necessary and is the important thing in order to maintain process operation, safety and product quality. In this research, control structures for phenol hydrogenation to cyclohexanone process consisting of many recycle streams and energy integration is designed. Procedure of Luyben (1998) and procedure of Wongsri (2009) are applied in design. This study use software HYSYS to simulate phenol hydrogenation to cyclohexanone process at steady state and dynamic. Designed control structures using procedure of Luyben (1998) and designed control structures using procedure of Wongsri (2009) can also design the same control structures. The four control structures are designed by using these two procedures. Then all designed control structures are evaluated the dynamics performance and are compared with each others. The result shows that all designed control structures can eliminate disturbances, can maintain product quality and can achieve process constraints. In sum, the plantwide control procedure of Wongsri (2009) can design the good performance control system.

Department : Chemical Engineering
Field of Study : Chemical Engineering
Academic Year : 2009

Student's Signature Kumchai Sukkongwaree
Advisor's Signature

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 Muenduen Phisalaphong, Assistant Professor Soorathep Kheawhom and Dr. Veerayut Lersbamrungsuk 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 page

LIST OF TABLES

LIST OF FIGURES

page

.

CHAPTER I

INTRODUCTION

1.1 Importance and Reasons for Research

Today petrochemical industry is challenged by many circumstantial variations. The performance requirements for process plants have become increasingly difficult to satisfy. Stronger competition, tougher environmental and safety regulations, and rapidly changing economic conditions have been key factors in tightening product quality specifications. Some plants have become more difficult to operate because of the trend toward complex and highly integrated processes. For such plants, it is difficult to prevent disturbances from propagating from one unit to other interconnected units. By the way, plants should always operate under the design condition, use energy effectively, low waste production and meet the required specification of the products. Furthermore, the process will not operate smoothly in the real situation. 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.

A chemical plant may have thousands of measurements, hundreds to thousands of manipulated variables and hundreds of disturbance variables. Control structure design deals with the decisions of the control system, including what to control and how to pair the variables to form control loops. Control structure design for complete chemical plants consisting of many interconnected unit operations is also known as plantwide control (PWC). A typical industrial process comprises a complex flowsheet that includes many units, recycle streams, and energy integration. These factors combined with the chemical component inventories lead to more interactions, and hence, the need for a perspective beyond the individual units. The recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. They also interconnect separate unit operations and create a path for disturbance propagation. Therefore, strategies for plantwide control are required to operate an entire plant safely and achieve its design objectives. Essentially, the plantwide control problem is how to develop the control loops needed to operate an entire process and achieves its design objectives. The problem is extremely complex and is very much opened. There are a combinatorial number of possible choices and alternative strategies to control and manage the disturbance load entering the process.

The goal of this research is to design heat exchanger networks and control structures of the phenol hydrogenation to cycloheaxanone process in order to better understand plantwide control problems and evaluate the plantwide control methodologies. The heat exchanger networks will be designed using disturbance load propagation method (Wongsri, 1990) and the plantwide control structure will be designed using Luyben heuristic design method (1999) and new plantwide control procedure (Wongsri, 2009). The performance of the heat exchanger network design and their control structures are evaluated via simulation using HYSYS.

1.2 Research Objectives

1. To design heat exchanger networks (HEN) of the phenol hydrogenation to cyclohexanone process using disturbance load propagation method (Wongsri, 1990).
2. To design control structure for a HEN-integrated phenol hydrogenation to cyclohexanone process using Luyben heuristic design method (1999).
3. To design control structure for a HEN-integrated phenol hydrogenation to cyclohexanone process using new plantwide control procedure (Wongsri, 2009).
4. To assess performance of the designed control structures for a HEN-integrated phenol hydrogenation to cyclohexanone process.

1.3 Scopes of research

1. Simulation of the phenol hydrogenation to cyclohexanone process is performed by using a commercial process simulator – HYSYS.

2. Description and data of the phenol hydrogenation to cyclohexanone process is obtained from Alexandre C. Dimian, and Costin Sorin Bildea (2008).
3. Plantwide control structures for a HEN-integrated phenol hydrogenation to cyclohexanone process are designed using Luyben's heuristics method and new plantwide control procedure (Wongsri, 2009).
4. The four control structures for the phenol hydrogenation to cyclohexanone process are designed.

1.4 Contributions of research

1. Better understand the control structure problems and evaluate the plantwide control methodologies.
2. The heat-intergrated process (HIPs) structures for phenol hydrogenation to cyclohexanone process.
3. The plantwide control structures for phenol hydrogenation to cyclohexanone process.

1.5 Research procedures

1. Study disturbance load propagation method and plantwide process control theory.
2. Study phenol hydrogenation to cyclohexanone process and concerned information.
3. Simulate the steady state of the phenol hydrogenation to cyclohexanone process.
4. Design of disturbance load propagation for heat exchanger networks of phenol hydrogenation to cyclohexanone process.
5. Design control structures of the phenol hydrogenation to cyclohexanone process.

6. Simulate the dynamic of the phenol hydrogenation to cyclohexanone process with heat exchanger network and control structure design.

7. Evaluate the dynamic performance of the designed control structures.

8. Analyze the design and simulation results.

9. Conclude 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 importance and reasons for research, research objectives, scopes of research, contributions of research and research procedures.

Chapter II reviews the work carried out on heat exchanger networks 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 phenol hydrogenation to cyclohexanone process.

Chapter V describes the design of plantwide control structures and dynamic simulation results.

Chapter VI presents the conclusion of this research and makes the recommendations for future work.

This is follow by:

References

Appendix A: Process stream data and equipment data

Appendix B: Parameter tuning of control structures

Appendix C: Fixture point theorem data

CHAPTER II

LITERATURE REVIEW

Our purpose of this chapter is to present a review of the previous works on the heat exchanger network (HEN) and plantwide control design.

2.1 Heat Exchanger Networks (HENs)

Energy conservation is important in process design. The fundamental result for the use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost.

Linhoff, B. and Hindmarsh, E. (1983) presented a novel method for the design of HEN. The method is the first to combine sufficient 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, B., Dunford, H., and Smith, R., (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.

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.

Linnhoff and Kotjabasakis (1984) developed a design procedure for operable HENs by inspection and using the concept of downstream paths, i.e. the paths that connect the disturbed variables downstream to the controlled variables. They generated HEN design alternatives by the pinch method for the nominal operating condition. Then, the alternative designs are inspected for the effects of disturbances on the controlled variables and they are removed by breaking the troublesome downstream paths. Path breaking can be done by relocating and/or removing exchangers. If this procedure is not feasible, control action is inserted into the structure.

Saboo and Morari (1984) proposed the corner point theorem which states that for temperature variation only, if a network allows MER without violating $\triangle T_{min}$ at MER corner points, then the network is structurally resilient or flexible. This is the case where the constraint is convex, so examining the vertices of the polyhedron is sufficient. This procedure again can only apply to restricted classes of HEN problem.

Their design procedure is similar to Marselle et al. (1982), but using two extreme cases to develop the network structure. The strategy for both procedures is finding similar optional network structures for the extreme cases and the base case design in order that they may be easily merged and not have too many units. Two extreme cases are:

1. When all streams enter at their maximum inlet temperatures and the heat capacity flowrates of hot streams are maximal and those of cold streams minimal. This is the case of maximum cooling.

2. When all streams enter at their minimum inlet temperatures and the heat capacity flowrates of hot streams are minimal and those of cold streams maximal. This is an opposite case the above one and in this case maximum heating is required.

The 'base' design is then generated by using an optimization technique and the final design is obtained by combining these designs. A test for resiliency (calculating, RI) is required. If the design is not feasible a modification is done by attempting to reduce $\triangle T_{min}$ and if not successful, a new heat exchanger will added or some heat exchangers are located. If the modified network is still not resilient, synthesize network structures at all corner points where the current design is not feasible. The new structures should be as similar to the current design as possible. The new design is obtained by superimposing the current structure and the new structures. The unneeded heat exchangers are inspected and removed.

Floudas and Grossmann (1987) presented a synthesis procedure for resilient HENs. Their multiperiod operation transshipment model is used to find a match structure for selected design points. The design obtained for feasibility at the match level. If it is not feasible, the critical point is added as an additional operating point and the problem is reformulated and solved. If the match network is feasible then the multiperiod superstructure is derived and formulated as an NLP problem to find a minimum unit solution.

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.

Colberg (1989) suggested that flexibility should deal with planed, desirable changed that often have a discrete set of values. Whereas resilience deals with unplanned, undesirable changes which are naturally continuous values. Thus a flexibility problem is a 'multiple period' type pf problem. A resilience problem should be a problem with a continuous range of operating conditions in the neighborhood of nominal operating points.

Wongsri, M., (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. The ability of a HEN to tolerate unwanted changes is called resiliency. It should be noted that the ability of a HEN to tolerate wanted changes is called flexibility. 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, e.g. the input temperatures of hot streams are at the lowest and those of cold streams are at the highest.

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.

Wongsri and Sae-Leaw (2006) proposed the guide line to design workable of highly heat integrated process with minimum auxiliary reboiler. It starts with specifying the disturbances and their magnitudes, and then designing the resilient heat exchanger network is designed at the worst case condition as the minimum heat supply and maximum heat demand condition. There considered only one worst case to find the number of minimum auxiliary heating unit and the heat path way for disturbance load at worst case condition is no considering dynamic maximum energy recovery (DMER).

Wongsri and Sapsawaipol (2007) presented procedure for design control structure of heat exchanger network using heuristic approach to solve heat exchanger network problems in target temperature variation case that is able to maintain target temperatures at specified values and not violate maximum energy recovery.

2.2 Design and Control of Heat-Integrated Plants

Handogo, R. and Luyben, W. L., (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-integration systems 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 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.

Luyben, M.L. and Luyben, W.L., (1995) examines the plantwide design and control of a complex process. The plant contains two reaction 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 flow rates of the recycle streams. The total annual cost of the nonlinear optimization design is about 20 % 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, W.E., and Wilson, J.A., (1997) considered the range ability of flows in the bypass line of heat exchanger through interesting heat exchanger problems. Difficulty is immediately encountered when considering heat exchanger between two process streams; changing the flow rate of one will certainly affect the exit temperature of the other. Unfortunately, interfering with a process stream flow rate immediately upsets the plant mass balance, which is undesirable. The difficulty is overcome by using a bypass that does not affect the total flow rate but changes the proportion actually passing through the heat exchanger and hence the heat transfer. Good engineering practice would maintain a minimum flow rate of 5-10 percent through the bypass. This bypass is expected to be able to handle disturbances.

Luyben, M.L., Tyreus, B.D. and Luyben, W.L., (1997) presented a general heuristic design procedure. Their procedure generated an effective plantwide control structure for an entire complex process flowsheet and not simply individual 17 units. The nine step of the proposed procedure center around the fundamental principles of plantwide control: energy management, production rate, product quality, operational, environmental and safety constraints, liquid-level and gas-pressure inventories, makeup of reactants, component balances and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, Eastman process and HDA process. The procedure produced a workable plantwide control strategy for a given process design. The control system was tested on a dynamic model built with TMODS, Dupont's in-house simulator.

After that, Luyben, W.L. (2000) studied the process had the exothermic, irreversible, gas-phase reaction $A + B \longrightarrow C$ occurring in an adiabatic tubular reactor. A gas recycle returns unconverted reactants from the separation section. Four alternative plantwide control structures for achieving reactor exit temperature control had been compared. Manipulation of reactor inlet temperature appeared to be the least attractive scheme. Manipulation of recycle flow rate gave the best control but may be undesirable in some system because of compressor limitations. The on-demand structure provided effective control in the face of feed composition disturbances.

Wongsri and Kietawarin (2002) presented a comparison among 3 control structure designs for reduced effect from disturbances that caused production rate change of HDA process. The first control scheme measured toluene flow rate in the process and adjusted the fresh toluene feed rate accordingly. The second was modified from the first scheme by added a cooling unit to control the outlet temperature from the reactor. In the third scheme, a ratio was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process. These three control structures was compared with reference on plantwide process control book, Luyben (1999), the result was performance of these structure higher than reference.

Wongsri and Thaicharoen (2004) presented the new control structures for the hydrodealkylation of toluene (HDA) process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben's structure (CS1). The dynamic simulation of this process with various disturbances was made to evaluate performance of each control structures: increasing and decreasing the reactor inlet temperature, increasing and decreasing total toluene flow rate, increasing and decreasing benzene production rate. The result shown that hydrodealkylation of toluene process with heat integration can reduce energy cost, which this process can be operated well by using plantwide methodology to design the control structure.

Wongsri and Hermawan Y.D. (2004) 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. 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.

Wongsri and Gayapan (2008) studied nine alternatives (8 new alternative designs and base case) of heat exchanger networks and three control structure designs of the natural gas expander plant are proposed. The resilient heat exchanger networks are designed using the disturbance load propagation method (Wongsri, M., 1990) and the control structures of HENs using the heat pathway heuristics (Wongsri, M. and Hermawan Y.D., 2005). The plantwide control structures are designed by using Luyben heuristic design method (1999) for the CS1 control structure and Fixture point theorem (Wongsri, 2008) for the CS2 and CS3 control structure. The result shows the CS3 control structure can reject disturbances better than other control structures.

CHAPTER III

THEORY

This chapter is aimed to summarize heuristic approach from the previous researches and this approach in heat pathway view point which was developed by Wongsri and Hermawan (2004). Furthermore, we propose the plantwide control involving the system and strategies required to control entire plant consisting of many interconnected unit operations.

3.1 Basic Knowledge for Pinch Technology

3.1.1 Pinch Technology

Pinch technology has been developed for more than two decades and now provides a systematic methodology for analysis chemical processes and surrounding utility systems. The concept was first developed by two independent research groups (Flower and Linnhoff, 1978; Umeda et al., 1979), based on an applied thermodynamics point of view.

3.1.2 Basic Pinch Analysis Concept

The pinch analysis concept is originated to design the heat recovery in network for a specified design task. Starting with do calculate heat and material balance of the process obtained after the core process, i.e. reaction and separation system, has been designed. By using thermal data from the process, we can set the target for energy saving prior to the design of the heat exchanger networks. The necessary thermal data is source, target temperature and heat capacity flow rate for each stream as shown in Table 3.1.

Table 3.1 Thermal data for process streams (Linnhoff and Hindmarsh, 1983)

Stream No.	Stream type	Start Temperature (Ts), °C	Target Temperature (Tt), °C	Heat capacity flow rate (CP), kW/°C
1	Hot	150	60	2
2	Hot	90	60	8
3	Cold	20	125	2.5
4	Cold	25	100	3

Here the hot streams are referred to the streams that required cooling, i.e. the source temperature is higher than that of the target. While the cold streams are referred to those required heating, i.e. the target temperature is higher than the supply. Heat Capacity flow rate is defined as the multiple between specific heat capacity and mass flow rate as shown below.

$$CP = Cp * F \tag{3.1}$$

Where: CP = heat capacity flow rate (kW/°C)

Cp = Specific heat capacity of the stream (kJ/ °C.kg)

F = mass flow rate of the stream (kg/s)

The data used here is based on the assumption that the heat capacity flow rate is constant. In practice, this assumption is valid because every streams with or without phase change can easily be described in terms of linearization temperature-enthalpy data (i.e. CP is constant). The location of pinch and the minimum utility requirement can be calculated by using the problem table algorithm (Linnhoff and Flower, 1979) for a specified minimum temperature different, $\triangle T_{min}$. In the case of $\triangle T_{min} = 20^{o}C$, the results obtained from this method are shown in Table 3.2.

Table 3.2 The problem table for data given in Table 3.1

W				T hot (°C)	T cold (°C)	△W (kW/C)	△T (°C)	Required Heat (kW)	Interval (kW)	Cascade Heat (kW)	Sum Interval (kW)
H1	H2	C1	C2								
0	0	0	0	150	130	0		Qh		-105	
2	0	0	0	145	125	2	5	107.5	10	2.5	10
2	0	2.5	0	120	100	-0.5	25	117.5	-12.5	12.5	-2.5
2	0	2.5	3	90	70	-3.5	30	105	-105	0	-107.5
2	8	2.5	3	60	40	4.5	30	0	135	-105	27.5
0	0	2.5	3	45	25	-5.5	15	135	-82.5	30	-55
0	0	2.5	0	40	20	-2.5	5	52.5	-12.5	-52.5	-67.5
										Qc	

The pinch separates the problem into 2 thermodynamic regions, namely, hot end and cold end. The hot end is the region comprising all streams or part of stream above the pinch temperature. Only hot utility is required in this region but not cold utility. In contrast to the hot end, the cold end is the region comprising all streams or part of stream below the pinch temperature and only cold utility is instead desired regardless the hot utility. It is important to note that there is no heat transfer across the pinch therefore the minimum utility requirement is achieved.

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

3.2 Heat Exchanger Networks

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. Changing 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.

3.2.1 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.

In order to make Alternative 6 of HDA plant more economically appealing, the minimum number of auxiliary utilities is identified using the proposed design scheme adapted from Wongsri’s RHEN (for resilient heat exchanger network) design method.

3.2.2 Heuristics for HEN Synthesis

Several HEN matching rules with minimum energy and investment costs have been presented (Masso and Rudd, 1969, Ponton and Donalson, 1974 Rathore and Powers, 1975, Linnhoff and Hindmarsh, 1983, Jezowski and Hahne1986, Huang, Metha and fan, 1988, etc.), The following are heuristics from the literature classified according to the design criteria

The heuristics to minimize the capital cost (the number of heat exchangers):

Heuristic C1. To generate a network featuring the minimum number of heat exchanger units, let each match eliminate at least one of the two streams; a tick-off rule (Hohmann, 1971).

Heuristic C2. Prefer the matches that will leave a residual stream at its cold end for a heating problem, or its hot end for a cooling problem. A match of this type will feature the maximum temperature difference.

Heuristic C3. Prefer matching large heat load streams together. The significance of this rule is that the control problem (a capital cost) of a mach of this type (whether it is implemented by one or many heat exchangers) should be less than that of heating or cooling a large stream with many small streams.

The heuristics to minimize the energy cost (the minimum utility requirement):

Heuristic E1. Divide the problem at the pinch into subproblems, one a heat sink (heating subproblem or hot end problem) and the other a heat source (cooling subproblem or cold end problem), and solve them separately (Linnhoff and Hindmarsh, 1983).

Heuristic E2. Do not transfer heat across the pinch.

Heuristic E3. Do not cool above the pinch.

Heuristic E4. Do not heat below the pinch.

The laws of thermodynamics:

Heuristic T1. In a heating problem, if a supply temperature of a cold stream is less than a target temperature of a hot stream by ΔT_{min} or more and the heat capacity flow rate of a hot stream is less than or equal to the heat capacity flow rate of a cold stream, the match between these two streams is feasible. (Immediately above the pinch temperature, the heat capacity flow rate of a cold stream must be greater than or equal to that of a hot stream.)

Heuristic T2. In a cooling problem, if a supply temperature of a hot stream is greater than a target temperature of a cold stream by ΔT_{min} or more and the heat capacity flow rate of a hot stream is greater than equal to the heat capacity flow rate of a cold stream, the mach between these two streams is feasible. (Immediately below the pinch temperature, the heat capacity flow rate of a hot stream must be greater than or equal to that of a cold stream.)

Heuristic T3. For a situation different from the above rule, a match feasibility must be determined by checking whether the minimum temperature difference of a match violates the minimum approach, ΔT_{min}, specific by the design.

3.2.3 Math Classification

In order to make use of the heuristics we must classify matches. The following criteria are considered important in this research:

1. Position of a Match. One heuristic prefers a match at the cold end and another prefers a match at the hot end. Pinch heuristics prefers a match at the cold end in a heating subproblem and a match at the hot end in a cooling subproblem. However, there are other possibilities. By using the tick-off heuristic, there are four ways that two streams can match. This leads to the basic four match patterns (Wongsri, 1990).

2. Heat capacity flow rate (between hot and cold stream). See Heuristic T.1 and T.2.

3. Heat Load (between hot and cold streams). The heuristic that concerns heat load state that one must match large heat load hot and cold streams first. This leads to two additional heuristic:

<u>Heuristic N1.</u> For a heating subproblem, a match where the heat load of a cold stream is greater than that of a hot stream should be given higher priority than the other .The reason is that the net heat load heating subproblem is in deficit. The sum of heat loads of cold streams is greater than of hot streams. The purposed match will likely be part of a solution (Wongsri, 1990).

<u>Heuristic N2.</u> Conversely, we prefer a mach where the heat load of a hot stream is greater than that of a cold in a cooling subproblem (Wongsri, 1990).

4. Residual Heat Load. No heuristics for this quantity have thus far appeared in the literature. Two new heuristics are introduced.

For a match in a heating subproblem that satisfies the heat load preference heuristics N.1;

<u>Heuristic N3.</u> We prefer a match where the residual heat load is less than or equal to the minimum heating requirement (Wongsri, 1990).

For a match in a cooling subproblem that satisfies the heat load preference or heuristics N.2:

<u>Heuristic N4.</u> We prefer a match where the residual heat load is less than or equal to the minimum cooling requirement, (Wongsri, 1990).

The reason behind the above two heuristics N3 and N4 is that the residual may be matched to a utility stream. One has the possibility of eliminating two streams at once.

3.2.4 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 structural 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, and 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 flow rates between a pair of matched streams.

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 (heat load) 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 3.4, 3.5, 3.6 and 3.7 respectively. Any eligible match must belong to one of the four match pattern classes.

Definition 3.1 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 3.1)

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 hot end (Heuristic N1) and follows the pinch heuristics. (See Table 3.3)

Definition 3.2 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 3.2)

A match of this class is a second type match; a hot end match and the heat load of the hot stream 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 (Heuristic N2) and also follows the pinch heuristics. (See Table 3.3)

Definition 3.3 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 3.3)

A match of this class is a first type match; a cold end match and the heat load of the hot stream greater than that of the cold stream. This is a downstream match. (See Table 3.4)

Definition 3.4 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 3.4)

A match of this class is a second type match; a hot end match and the heat load of the cold stream greater than that of the hot stream. This is a downstream match. (See Table 3.4)

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 less than the minimum heating or cooling requirement then the chances that the match pattern will be matched to a utility stream is high. So we give a match pattern which it's residual less than the minimum heating or cooling requirement a high priority in match pattern.

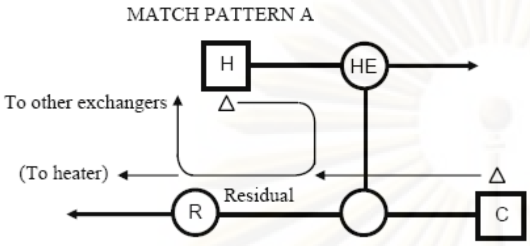


Figure 3.1 Class A Match Pattern

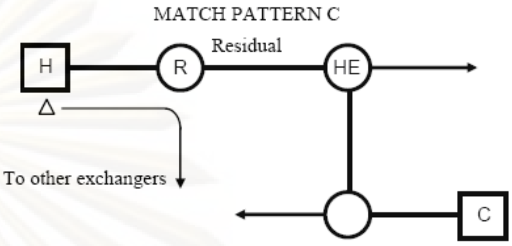


Figure 3.3 Class C Match Pattern

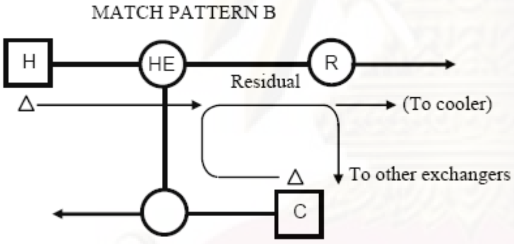


Figure 3.2 Class B Match Pattern

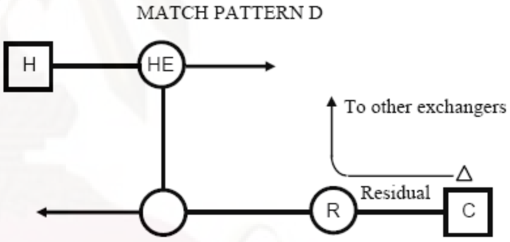


Figure 3.4 Class D Match Pattern

A match of Class A or Class C will leave a residual at the hot end, while a match of Class B or D will leave a residual at the cold end. Heuristics N.3 and N.4 will be use heuristics to further subclassify matches of Class A and B into matches of high priority.

We will make use of Heuristic N.3 and N.4 to further subclassify matches of Class A and B and give the following subclass matches high priorities.

Subclass AH. A match of this subclass is a member of Class A, a heating problem where the residual is less than or equal to the minimum heating requirement. (A letter H in the subclass name denotes that the residual is matched to a heating utility.)

Subclass BK. A match of this subclass is a member of Class B, a cooling problem where the residual is less than or equal to the minimum cooling requirement. (A letter K in the subclass name denotes that the residual is matched to a cooling utility.)

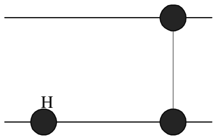
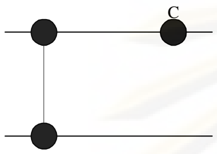
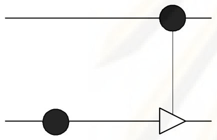
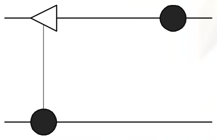
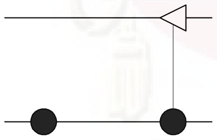
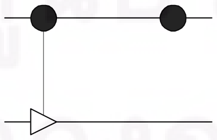
As it might be expected, we give a match of subclasses AH in a heating subproblem and BK in a cooling subproblem the highest priorities. See Table 3.4.

We further discriminate match patterns according to heat capacity flowrate. By following pinch heuristics, in a heating problem, we prefer a match where the heat capacity flowrate of a cold stream is greater than or equal to that of a hot stream. For example, A[H]H is a match in which the heat capacity flowrate of the cold stream is greater than that of the hot stream and the residual of the cold stream is matched to the heating utility.

Similarly in a cooling problem, we prefer a match where the heat capacity flowrate of the hot stream is greater than or equal to that of the cold stream. For example, B[C]K is a match in which the heat capacity flowrate of the hot stream is greater than that of the cold stream and the residual of the hot stream is matched to the cooling utility.

In summary, the rankings of the match patterns in a heating problem are AH, A[H], B[C], A[C], B[H], C[H], D[C], C[C] and D[H]. For a cooling problem, BK, B[C], A[H], B[H], A[C], D[C], C[H], D[H] and C[C].

Table 3.3 Match Pattern Operators of Class A and B

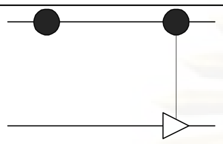
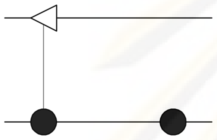
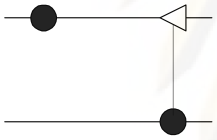
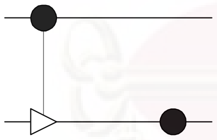
Match Operators	Conditions	Actions
 Pattern AH	$T_H^s{}^* \ge T_C^t{}^{**}$ $L_H \le L_C$ $T_H^s \ge T_C^s + L_H W_C^{-1}$ $L_C - L_H \le Q_{\min}^{heating}$	Match H and C Status of H $\Leftarrow$ Matched*** $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern BK	$T_H^s \ge T_C^t$ $L_C \le L_H$ $T_C^s \le T_H^s - L_C W_H^{-1}$ $L_H - L_C \le Q_{\min}^{cooling}$	Match H and C Status of C $\Leftarrow$ Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern A[H]	$T_H^t \ge T_C^s$ $L_H \le L_C$ $W_C \ge W_H$	Match H and C Status of H $\Leftarrow$ Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern B[C]	$T_H^s \ge T_C^t$ $L_C \le L_H$ $W_C \le W_H$	Match H and C Status of C $\Leftarrow$ Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern A[C]	$T_H^t \ge T_C^s$ $L_H \le L_C$ $W_C < W_H$ $T_H^s \ge T_C^s + L_H W_C^{-1}$	Match H and C Status of H $\Leftarrow$ Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern B[H]	$T_H^s \ge T_C^t$ $L_C \le L_H$ $W_H < W_C$ $T_C^s \le T_H^s - L_C W_H^{-1}$	Match H and C Status of C $\Leftarrow$ Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$

* T^t=target temp, T^s=supply temp, W=heat capacity flowrate, L, Q=heat load.

** Cold stream temperatures are shifted up by $\Delta T_{\min}$.

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set of process streams to be selected next.

Table 3.4 Match Pattern Operators of Class C and D

Match Operators	Conditions	Actions
 Pattern C[H]	$T_H^t \geq T_C^s$ $L_H > L_C$ $W_H \leq W_C$	Match H and C Status of C $\Leftarrow$ Matched $T_H^t \Leftarrow T_H^t - L_C\,W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern D[C]	$T_H^s \geq T_C^t$ $L_H < L_C$ $W_H \geq W_C$	Match H and C Status of H $\Leftarrow$ Matched $T_C^t \Leftarrow T_C^t + L_H\,W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern C[C]	$T_H^t \geq T_C^s$ $L_H > L_C$ $W_C < W_H$ $T_C^t \leq T_H^t + L_C\,W_H^{-1}$	Match H and C Status of C $\Leftarrow$ Matched $T_H^t \Leftarrow T_H^t - L_C\,W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern D[H]	$T_H^s \geq T_C^t$ $L_H \leq L_C$ $W_H < W_C$ $T_H^t \geq T_C^t - L_H\,W_C^{-1}$	Match H and C Status of H $\Leftarrow$ Matched $T_C^t \Leftarrow T_C^t + L_H\,W_C^{-1}$ $L_C \Leftarrow L_C - L_H$

* T^t=target temp, T^s=supply temp, W=heat capacity flow rate, L, Q=heat load.

** Cold stream temperatures are shifted up by ΔT_{min}.

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set of process streams to be selected next.

3.2.5 Disturbance Propagation Design Method

In order for a stream to be resilient with a specified disturbance load, the disturbance load must be transferred to heat sinks or heat sources within the network. With the use of the heuristic: To generate a heat exchanger network featuring the minimum number of heat transfer units, let each match eliminate at lease one of the two streams.

We can see that in a match of two heat load variable streams, the variation in heat load of the smaller stream S1 will cause a variation to the residual of the larger stream S2 by the same degree: in effect the disturbance load of S1 is shifted to the residual of S2. If the residual stream S2 is matched to S3 which has larger heat load, the same situation will happen. The combined disturbance load of S1 and S2 will cause the variation in the heat load to the residual S3. Hence, it is easy to see that the disturbance load in residual S3 is the combination of its own disturbance load and those obtained from S1 and S2. Or, if S2 is matched to a smaller heat load stream S4, the new disturbance load of residual S2 will be the sum of the disturbance loads of S1 and S4. Form this observation, in order to be resilient, a smaller process stream with specified disturbance load must be matched to a larger stream that can tolerate its disturbance. In other words, the propagated disturbance will not overshoot the target temperature of the larger process stream.

However, the amount of disturbance load that can be shifted from one stream to another depends upon the type of match patterns and the residual heat load. Hence, in design we must choose a pattern that yields the maximum resiliency. We can state that the resiliency requirement for a match pattern selection is that the entire disturbance load from a smaller heat load stream must be tolerated by a residual stream. Otherwise, the target temperature of the smaller stream will fluctuate by the unshifted disturbance. Of course, the propagated disturbance will be finally handled by utility exchangers. In short, the minimum heat load value of a larger stream must be less than a maximum heat load value of a smaller stream.

By choosing the minimum heat load condition for the design, the new input temperature of a residual stream to its design condition according to the propagated disturbance. The propagated disturbance will proportionally cause more temperature variation in the residual stream and the range of temperature variation of the residual stream will be larger than its original range.

Definition 3.5 Propagated Disturbance. The propagated disturbance of a stream is the disturbance caused by a variation in heat load of 'up-path' streams to which such a stream is matched. Only a residual stream will have a propagated disturbance. The new disturbance load of a residual stream will be the sum of its own disturbance (if any) and the propagated disturbance. See Figure 3.5 and 3.6.

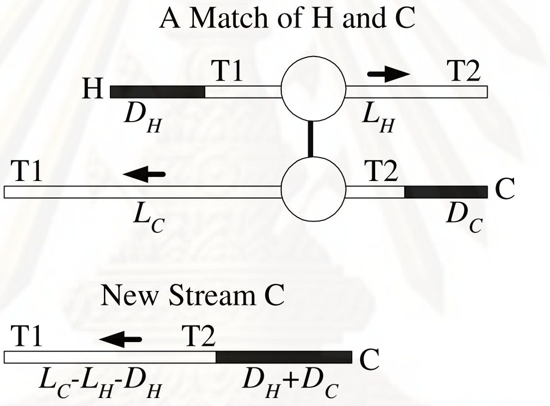


Figure 3.5 A Concept of Propagated Disturbance

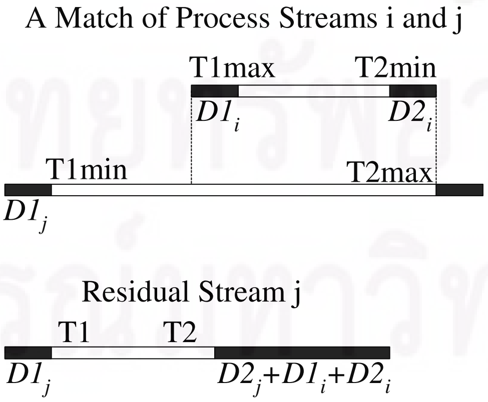


Figure 3.6 A General Concept of Propagated Disturbance

Hence, a stream with no original variation in heat load will be subjected to variation in heat load if it is matched to a stream with disturbance. Another design consideration is that the disturbance load travel path should be as short as possible, i.e. the lease number of streams involved. Otherwise, the accumulated disturbance will be at high level. From the control point of view, it is difficult to achieve good control if the order of the process and the transportation lag are high. From the design viewpoint, are may not find heat sinks or sources that can handle the large amount of propagated disturbance (Wongsri, 1990).

3.2.6 Synthesis Procedure

A procedure of HEN synthesis by using math operators and a notion of a design state can be carried in step as follow:

1. Push the match operators to a stack in proper order. This is a beginning of a new state.
2. While there is an operator on a stack.
    a. Pop a match operator form a stack to operate on process streams.
    b. If a match is found, exclude matched streams from a set of process stream. Change the condition of residual streams. Include the residual streams in to a set of process streams. Go to a new design state (the first step).
3. If there are only hot or cold process streams left in the set of stream, a solution is found. If there are other solutions, they can be found by backtracking to the previous states to try the unused operators in those states.
4. If no matches is found in a current design state, back track to a previous stare to try an available operator on the stack of that state. (Go to Step 2 in the previous loop.) It is a recursive procedure here. If a math still could not be found, backtrack again to the more previous.

The above sequences represent a loop of one design state. A total generation procedure a loop composing of these sequences.

3.3 Plantwide Control

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. Therefore, Plantwide Process Control involves the system and strategies required to control entire plant consisting of many interconnected unit operations.

3.3.1 Integrated Process

Figure 3.7 shows integrated process flowsheet. 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.

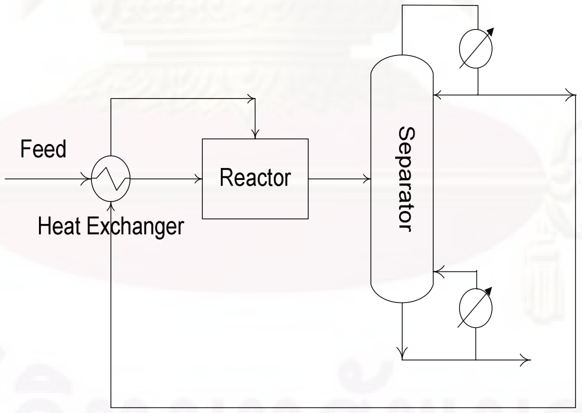


Figure 3.7 Integrated Process flowsheet

3.3.1.1 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.

3.3.1.2 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.

3.3.1.3 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.

3.3.2 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.

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.

3.3.3 Plantwide Control Design Procedures

The plantwide control design procedure satisfies the two fundamental chemical engineering principles, namely the overall conservation of energy and mass. Additionally, the procedure accounts for nonconserved entities within a plant such as chemical components (produced and consumed) and entropy (produced).

The goals for an effective plantwide process control system include.

1. Safe and smooth process operation.
2. Tight control of product quality in the face of disturbances.
3. Avoidance of unsafe process conditions.
4. A control system runs in automatic, not manual, requiring minimal operator attention.
5. Rapid rate and product quality transitions.

6. Zero unexpected environmental releases.

3.3.3.1 Basic Concepts of Plantwide Control

1. *Buckley Basic*

Page Buckley (1964) was the first to suggest the idea of separating the plantwide control problem into two parts:

(1) Material balance control.

(2) Production quality control.

He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loop is established, using the flowrates of liquid and gas process streams. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated as small as possible. The most level controllers should be proportional-only (P) to achieve flow smoothing.

2. *Douglas doctrines*

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Douglas points out that in the typical chemical plant the costs of raw materials and the value of the products are usually much greater than the costs of capital and energy. This leads to two Douglas doctrines.

(1) Minimize losses of reactants and products.

(2) Maximize flowrates through gas recycle systems.

The first implies that we need tight control of stream composition exiting the process to avoid losses of reactants and products. The second rests on the principle that yield is worth more than energy.

The control structure implication is that we do not attempt to regulate the gas recycle flow and we do not worry about what we control with its manipulation. We simply maximize its flow. This removes one control degree of freedom and simplifies the control problem.

3. *Downs drill*

Jim Downs (1992) pointed out the importance of looking at the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. We must ensure that all components (reactants, product, and inerts) have a way to leave or be consumed within the process. Most of the problems occur in the consideration of reactants, particularly when several chemical species are involved. Because we usually want to minimize raw material costs and maintain high-purity products, most of the reactants fed into the process must be chewed up in the reactions. And the stoichiometry must be satisfied down to the last molecule. Chemical plants often act as pure integrators in terms of reactants will result in the process gradually filling up with the reactant component that is in excess. There must be a way to adjust the fresh feed flowrates so that exactly the right amounts of the two reactants are fed in.

4. *Luyben laws*

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

(1) All recycle loops should be flow controlled.

(2) A fresh reactant feed stream cannot be flow-controlled unless there is essentially complete one-pass conversion of one of the reactants.

(3) If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). Even if steady-

state economics favor a liquid feed stream, the profitability of an operating plant with a product leaving the bottom of a column may be much better if the feed to column is vaporized.

5. *Richardson rule*

Bob Richardson suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel. (The bigger the handle you have to affect a process, the better you can control it).

6. *Shinskey schemes*

Greg Shinskey (1988) has produced a number of “advanced control” structures that permit improvements in dynamic performance.

7. *Tyreus tuning*

Use of P-only controllers for liquid levels, turning of P controller is usually trivial: set the controller gain equal to 1.67. This will have the valve wide open when the level is at 80 percent and the valve shut when the level is at 20 percent.

For other control loops, suggest the use of PI controllers. The relay-feedback test is a simple and fast way to obtain the ultimate gain (K_u) and ultimate period (P_u). Then either the Ziegler-Nichols setting or the Tyreus-Luyben (1992) settings can be used:

$$K_{ZN} = K_u/2.2 \quad \tau_{ZN} = P_u/1.2$$

$$K_{TL} = K_u/2.2 \quad \tau_{TL} = P_u/1.2$$

The use of PID controllers, the controlled variable should have a very large signal-to-noise ratio and tight dynamic control is really essential from a feedback control stability perspective.

3.3.3.2 Step of Plantwide Process Control Design Procedure

Step 1: 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 speci-fication, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine control degrees of freedom

Count the number of control values available.

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.

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

Select the best value to control each of the product-quality, safety and environmental variables.

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)

Fix a flow in every recycle loop and then select the manipulated variable to control inventories

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

Identify how components enter, leave, and are generated or consumed in the process

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

Establish the best way to use the remaining control degrees of freedom.

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

3.4 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provided we can independently manipulate the two inlet flowrates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Fig 3.8.a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig 3.8.b.

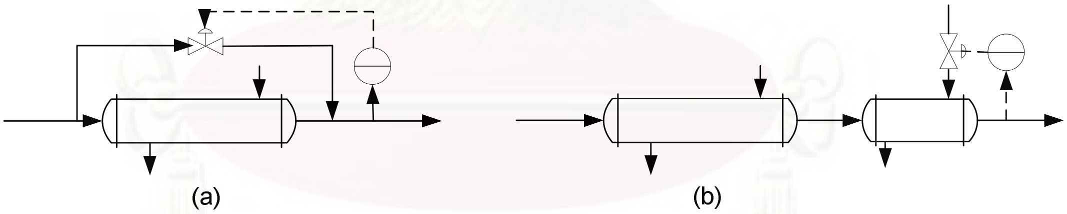


Figure 3.8 Control of P/P heat exchangers:
(a) use of bypass; (b) use of auxiliary utility exchanger.

3.4.1 Use of Bypass Control

When the bypass method is used for unit operation control, we have several choices about the bypass location and the control point. Figure 3.8(b) 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.

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 3.9 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.

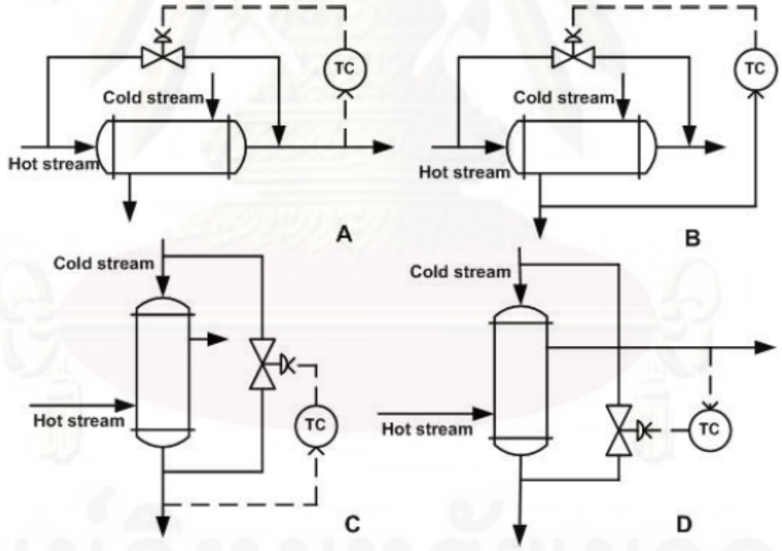


Figure 3.9 Bypass control of process-to process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

3.5 New Plantwide Control Structure Design Procedure

New design procedure of Wongsri (2009) presented our plantwide control structure design procedure based on heuristics and mathematical analysis. In our procedure, the precedence of control variables is established. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method (Wongsri, 1990) to cover the material disturbances. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

Normally, plantwide control design procedures consider decision about plant control structures in perspective. The plantwide control structure design is complex: hierarchical, structural, having mixed objectives, containing many units and layers, and therefore confusing. One easy way to deal with this complexity is compartmentalizing it. However, the plant is not merely the units combined, it has it own properties. The whole is greater than the sum of its parts. There are properties (or behavior) of a system as a whole emerge out of the interaction and the relationship of the components comprising the system. Therefore, a designer must deal with both parts and system.

New design procedure of Wongsri (2009):

1. Establishment of control objectives.
2. Selection of controlled variables to maintain product quality and to satisfy safety operational and environmental constrains. The selected CVs are ranked using the Fixture Point theorem.
3. Selection of manipulated variables and measurements via DOF analysis.
4. Energy management via heat exchanger networks.
5. Selection of control configuration using various tools available.

6. Completing control structure design by checking the component balance.

7. Selection of controller type: single loops or MPC

8. Validation via rigorous dynamic simulation

Fixture Point Theorem

The fixture point theorem is provided by Wongsri (2008) to define the control variable that the most sensitivity. Defined control variable should consider to control and pairing with manipulate variable (MV) in the first.

Fixture point theorem analysis

1. Consideration in dynamic mode of simulation until process set up to steady state.

2. Control variable (CV) can be arranged to follow the most sensibility of the process variable by step change the MV (change only one MV, the other should be fixed then alternate to other until complete). Study the magnitude of integral absolute error (IAE) of all process variables that deviates form steady state.
3. Consider CV that give the most deviation from steady state (high IAE score) to match with MV. CV and MV should be directing interactive together, after that will consider the next CV to match with other MV.

CHAPTER IV

PHENOL HYDROGENATION TO CYCLOHEXANONE PROCESS

4.1 Process Description

Cyclohexanone is a key intermediate in the production of ε-caprolactam and adipic acid, which are basic materials for nylon type polymers. This process uses phenol and hydrogen as reactants .There is two steps of reactions in the process. First step is hydrogenation of phenol to cyclohexanone (eq. 4.1) which gives cyclohexanol as a byproduct by hydrogenation of cyclohexanone (eq. 4.3). Second step is dehydrogenation of cyclohexanol to cyclohexanone (eq. 4.5). Then cycohexanone from two steps are combined and separated from other components as showed in figure 4.1.

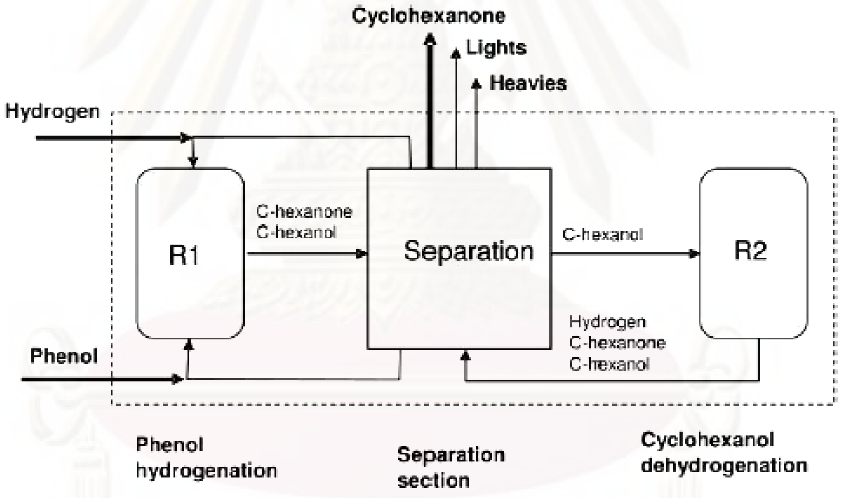


Figure 4.1 Overall materials – balance flowsheet

The reactions and reaction rate equations are:

Hydrogenation of phenol to cyclohexanone:

$$C_6H_5\text{-}OH + 2H_2 \rightarrow C_6H_{10} = O \qquad (4.1)$$

$$-r_1 = \frac{k_1 K_A p_A (K_B p_B)^2}{(1 + K_A p_A + K_B p_B + K_C p_C + K_D p_D)^3} \qquad (4.2)$$

Hydrogenation of cyclohexanone to cyclohexanol:

$$C_6H_{10} = O + H_2 \rightarrow C_6H_{11} - OH \tag{4.3}$$

$$-r_2 = \frac{k_2 K_C p_C (K_B p_B)}{(1 + K_A p_A + K_B p_B + K_C p_C + K_D p_D)^2} \tag{4.4}$$

Table 4.1 Rate constants for LHHW kinetics by the hydrogenation of phenol

Quantity	Reaction (4.1)	Reaction (4.3)
k_i $(\mathrm{mol\,kg^{-1}h^{-1}})^{a)}$	877	28.7
K_A $(\mathrm{atm^{-1}})^{a)}$	9.3	15
K_B $(\mathrm{atm^{-1}})^{a)}$	1.1	0.91
K_C $(\mathrm{atm^{-1}})^{a)}$	19	7.7
K_D $(\mathrm{atm^{-1}})^{a)}$	8	2.6
A_i $(\mathrm{mol\,kg^{-1}s^{-1}})^{a)}$	1234.28	40.40
E_i $(\mathrm{kJ\ kmol^{-1}})^{b)}$	30,000	30,000

Observations: $^{a)}$ kinetic data at 423 K and 1 bar; $^{b)}$ Arrhenius – type expression for k_i.

Dehydrogenation of cyclohexanol to cyclohexanone:

$$C_6H_{11} - OH \rightarrow C_6H_{10} = O + H \tag{4.5}$$

$$-r_3 = \frac{kK_D \left(y_D - {y_B y_C}/{K_y} \right)}{(1 + K_B y_B + K_C y_C + K_D y_D)^2} \tag{4.6}$$

Table 4.2 shows the values of a six-parameter model. The overall kinetic constant is formulated by the Arrhenius law $k = A \times \exp(-E/RT)$. The adsorption constants are given as $K = K_{j0} \times \exp(-\Delta H_a/RT)$ with the heat of adsorption equal for all species. Note that in the cited study the equilibrium constant is $K_y = 6.0416 \times 10^6 \times \exp(-7{,}953.5/T)$.

Table 4.2 Parameters in LHHW kinetic model for cyclohexanol dehydrogenation

A, frequency factor	E, activation energy	K_C	K_B	K_D	Adsorption heat of species
$(mol/g\,h)$	(kJ/mol)	-	-	-	(kJ/mol)
9.40×10^{-8}	108	2.68×10^{-9}	3.43×10^{-9}	34.7×10^{-9}	-96.9

where A, B, C, D = phenol, hydrogen, cyclohexanone and cyclohexanol respectively

k = the reaction rate constant

K_i = the adsorption rate constant for component i

K_y = the equilibrium constant

p_i = partial pressure for component i

y_i = mole fraction for component i

4.1.1 Phenol Hydrogenation

Figure 4.2 presents the flowsheet for phenol hydrogenation. Fresh and recycled phenol is preheated by the hot reactor effluent in the feed-effluent-heat-exchanger (FEHE). Then it is evaporated and mixed with hydrogen in the evaporator at about 2 bar. The gas mixture enters the catalytic hydrogenation reactor. The inlet temperature should be kept strictly constant, in this case at 150 °C, to avoid the occurrence of a “hot spot”. The hydrogenation reactor has cooling system to control the exothermic reactions and prevent hot spot. The reaction mixture is separated in gas and liquid streams in the flash after cooling at 33 °C by passing through the exchanger. The gas containing hydrogen is recycled to the reactor via the compressor, while the liquid phase is sent to separation.

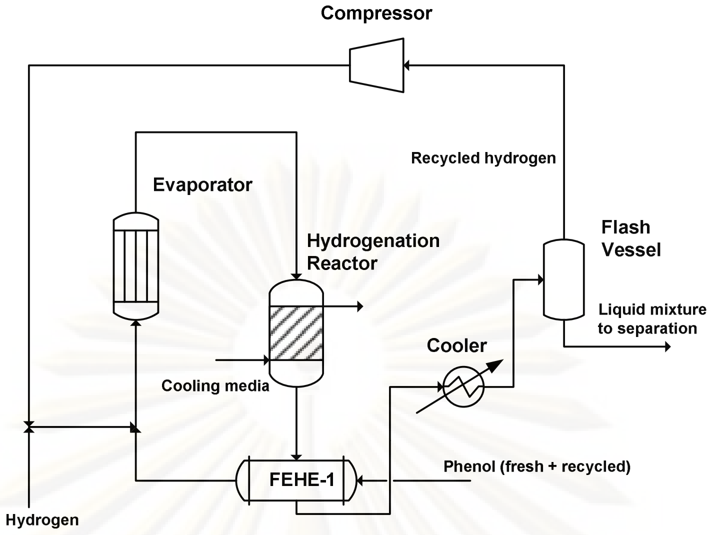


Figure 4.2 Flowsheet for the phenol hydrogenation step

4.1.2 Dehydrogenation of Cyclohexanol

Figure 4.3 presents the flowsheet for cyclohexanol dehydrogenation. Cyclohexanol from the separation section is preheated by exchange with the product in the FEHE, and heated further to 330 °C in the heat exchanger. The dehydrogenation reactor has heating utility to supply the heat of reaction. The hot reactor effluent is cooled in countercurrent with the feed in FEHE, and finally for phase separation in the heat exchanger at 33 °C. The simple flash can ensure a sharp split between hydrogen, recycled to hydrogenation reactor, and a liquid phase sent to separation.

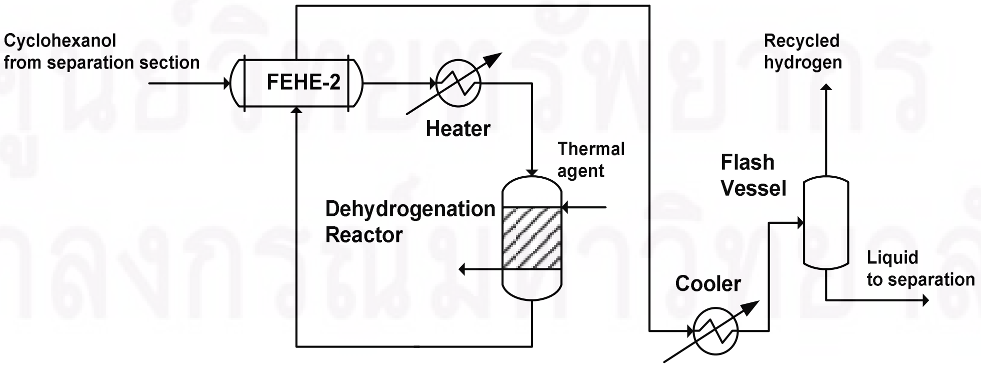


Figure 4.3 Flowsheet for the cyclohexanol dehydrogenation step

4.1.3 Separation Section

The separation section receives liquid streams from both reactors. Two columns are necessary for the separation of the ternary mixture cyclohexanone / cyclohexanol / phenol. The azeotropic phenol mixture is a bottom product from the first split. Then, in the second split cyclohexanone (98 mole %) is obtained as the top distillate, while cyclohexanol is taken off as the bottom product as presented in the Figure 4.4. Because the volatility of cyclohexanone increases considerably at low pressure, the separations in both columns should take place under vacuum. By combining the reaction and separation sections the final flowsheet is obtained, as pictured in the Figure 4.5. The dash lines represent the way of heat transfer in the energy integration process.

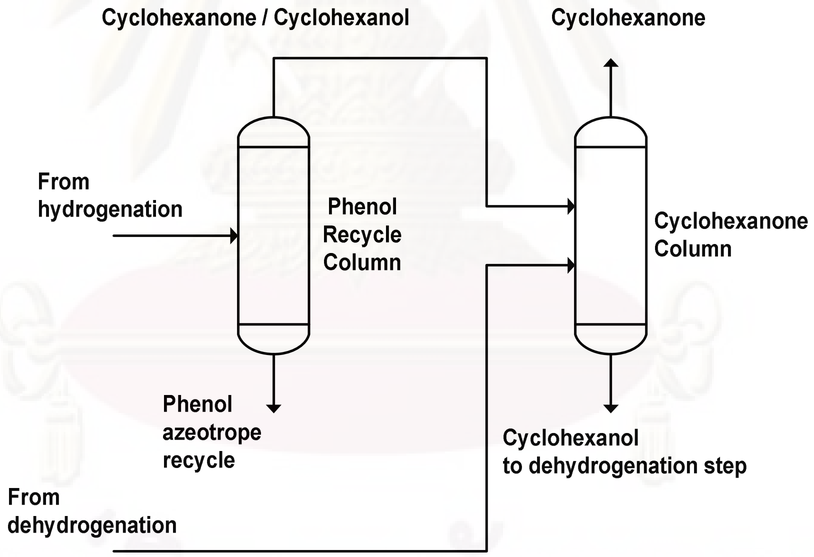


Figure 4.4 Flowsheet for the liquid – separation system

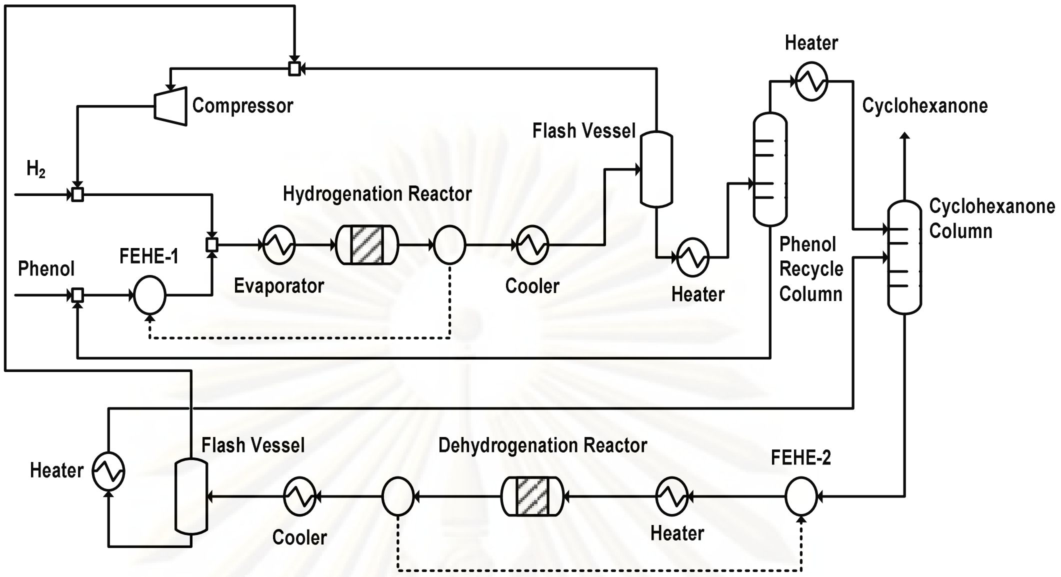


Figure 4.5 Phenol hydrogenation to cyclohexanone process (Dimian and Bildea, 2008)

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 network for phenol hydrogenation to cyclohexanone process. The design procedures and definitions from previous chapters will be an accessory to design in conceptual design. The information for used in design is shown in Table 4.3.

Table 4.3 The information of phenol hydrogenation to cyclohexanone process

	Stream Name	*Tin* °C	*Tout* °C	W (*kW*/°*C*)	Duty (kW)
H1 :	Product stream of hydrogenation reactor	154.6	33	38.46	4,676.92
H2 :	Product stream of dehydrogenation reactor	344.2	33	9.14	1,812.26
C1 :	Phenol (fresh + recycled) stream	102.91	144	14.48	603.61
C2 :	Liquid stream of hydrogenation step	33.13	70	13.90	512.61
C3 :	Top stream of first column	92.18	115	9.45	215.77

Table 4.3 (Continued)

Stream Name		*Tin* °C	*Tout* °C	W (*kW*/°C)	Duty (kW)
C4 :	Bottom stream of second column	127.64	207.5	20.11	1,638.65
C5 :	Liquid stream of dehydrogenation step	33.21	90	5.02	285.14

4.2.1 HEN Base Case

According to Table 4.3, it can be simply translated to a heat exchanger network for phenol hydrogenation to cyclohexanone process (Base Case) in Figure 4.6.

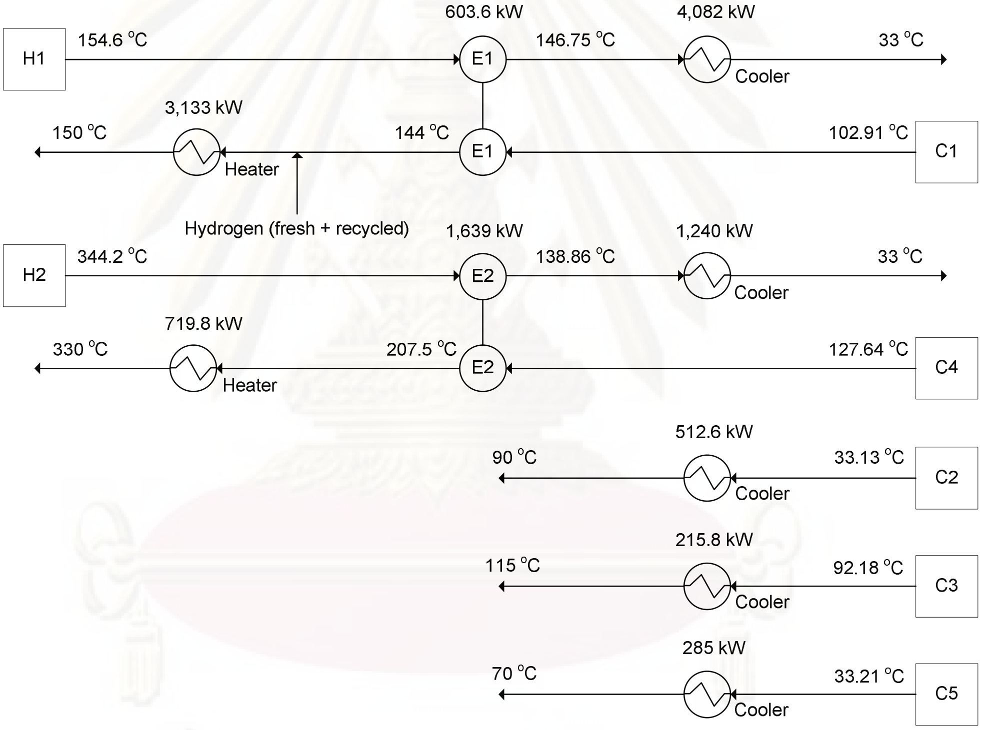


Figure 4.6 The heat exchanger network, Base case

4.2.2 HEN using the disturbance propagation method

There are two hot streams and three cold streams in the network. Pinch temperature using Problem table method is not found. The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.4 and Table 4.5. Figure 4.7 shows a design of resilient heat exchanger network for phenol hydrogenation to cyclohexanone process. In this design, the minimum temperature difference in the process-to-process-heat-exchanger is set to 10 °C. The Phenol hydrogenation to cyclohexanone process with resilient heat exchanger network is shown in Figure 4.8

Table 4.4 Synthesis table for hot stream H1

Stream	Load	W	T1	T2	D1	D2	DT	Action
(a)	State 1							
H1	4,484.61	38.46	149.60	33.00	384.62	0.00	384.62	Selected B[C]
C1	522.53	14.48	144.00	107.91	0.00	144.78	144.78	Selected
C2	443.10	13.90	70.00	38.13	0.00	139.03	139.03	
(b)	State 2							
H1	3817.30	38.46	132.25	33.00	0.00	0.00	529.40	Selected B[C]
C1								Matched to H1
C2	443.10	13.90	70.00	38.13	0.00	139.03	139.03	Selected
(c)	State 3							
H1	3235.17	38.46	117.11	33.00	0.00	0.00	668.43	To cooler
C1								Matched to H1
C2								Matched to H1

Table 4.5 Synthesis table for hot stream H2

Stream	Load	W	T1	T2	D1	D2	DT	Action
(a)	State 1							
H2	2,799.77	9.14	339.20	33.00	91.44	0.00	91.44	Selected B[C]
C4	1,538.12	20.11	207.50	131.00	0.00	201.06	201.06	Selected
C5	159.62	5.02	70.00	38.21	0.00	50.21	50.21	
(b)	State 2							
H1	1060.59	9.14	148.99	33.00	0.00	0.00	292.50	Selected B[C]
C4								Matched to H2
C5	159.62	5.02	70.00	38.21	0.00	50.21	50.21	Selected

Table 4.5 (Continue)

(c)	State 3							
H1	850.77	9.14	126.05	33.00	0.00	0.00	0.00	To cooler
C4								Matched to H2
C5								Matched to H2

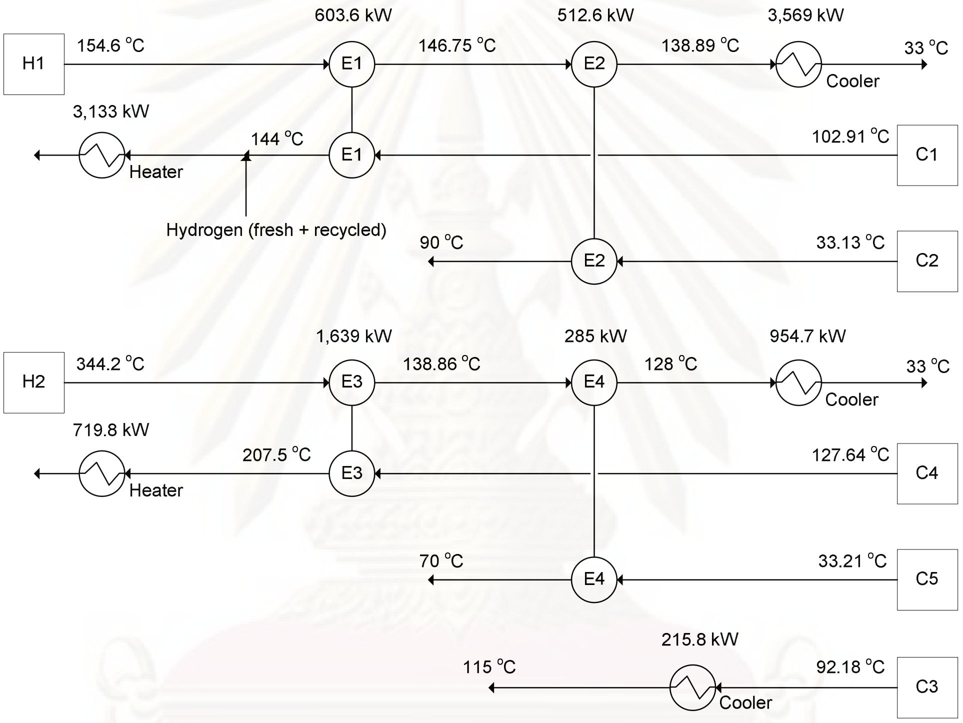


Figure 4.7 The heat exchanger network using the disturbance propagation method

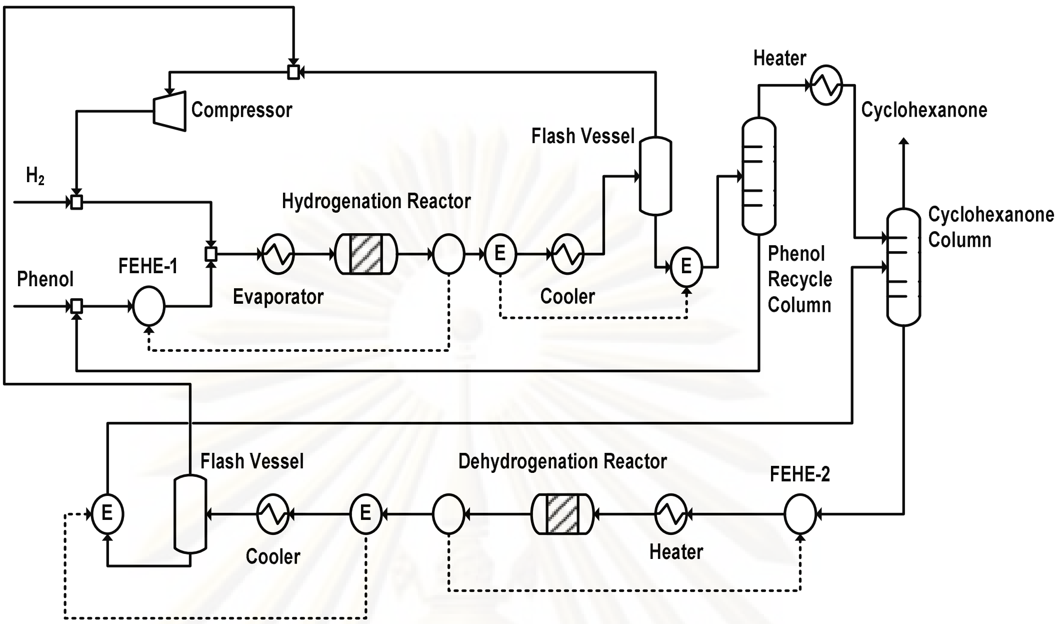


Figure 4.8 Phenol hydrogenation to cyclohexanone process with resilient heat exchanger network

4.3 Steady State Modeling

The steady state model is built in HYSYS. The flowsheet information is obtained from Dimian and Bildea (2008). The Wilson model is selected for liquid activity with Redlich – Kwong EOS for vapor phase in thermodynamic calculation. The kinetic reactions are LHHW model expressions available in HYSYS which all parameters data is taken from Dimian and Bildea (2008).

4.3.1 Steady State Simulation

All of two columns are simulated using the 'distillation column' module. In steady state, the specification of inlet stream, pressure profiles, number of trays and feed tray need for model. Besides, 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. Reflux rate and bottom component mole fraction for two columns are chosen in simulation. In the part of hydrogenation reactor, two plug flow reactors are used to model in order to control temperature of this reactor at 1 m length in order to prevent hot spot occurs since HYSYS cannot do it directly. Figure 4.9 present the steady state flowsheet with resilient heat exchanger network built in HYSYS.

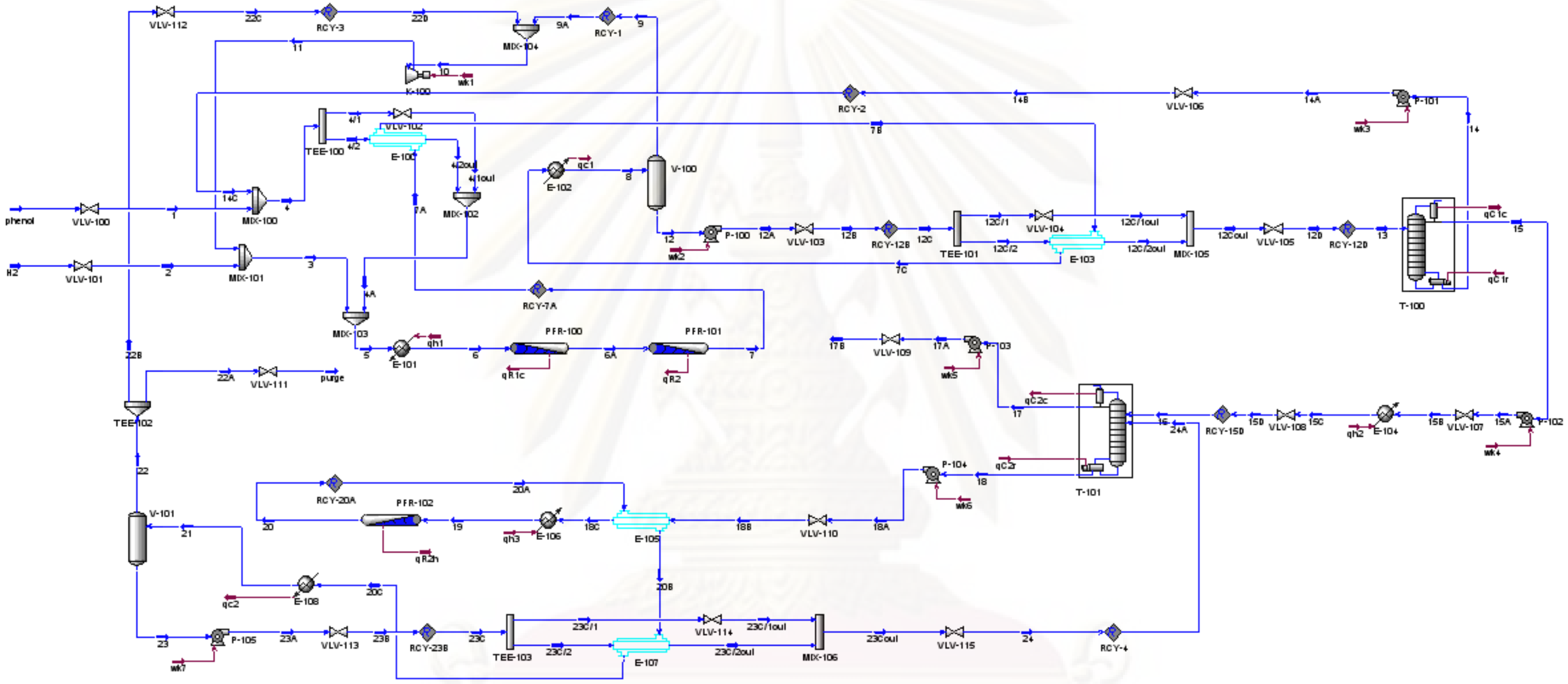


Figure 4.9 Phenol hydrogenation to cyclohexanone process

with resilient heat exchanger network flowsheet via HYSYS

CHAPTER V

CONTROL STRUCTURE DESIGN AND DYNAMIC SIMULATION

5.1 Plantwide Control Design Procedures

In this work, control structure is designed by using Luyben heuristic design method (1997) for control structure 1 and new plantwide control structure design procedure (Wongsri, 2009) for control structure 1, 2, 3 and 4.

5.1.1 Nine – Step Approach of Luyben

The design procedures are carried out as follows:

Step1. Establish Control Objective

The steady state design of the process is assessed and the dynamic control objectives are formulated. The objectives typically include reaction and separation yields, product quality specifications, environmental restrictions, and safety concerns. The control objectives for the phenol hydrogenation to cyclohexanone process are as follows.

1. Good purity product, of minimum 98 % cyclohexanone.
2. Process constraints:
    a) The temperature at the hydrogenation reactor inlet should be 150 ^{o}C in order to prevent hot spot occurs.
    b) The two distillation columns should operate under vacuum.
    c) The ratio of Hydrogen to Phenol molar flow rates at the entrance of the hydrogenation reactor is set at 3.6.
    d) The temperature of the both separators should be at 33 ^{o}C.

Step2. Determine Control Degrees of Freedom (CDOF)

Table 5.1 Degree of freedom of phenol hydrogenation to cyclohexanone process

Unit Operation	Position of Valves	Degree of Freedom
Hydrogenation reactor	fresh feed valves of phenol (VLV-100) and hydrogen (VLV-101), cooling duty of reactor (qR1c1)	3
Vessel (V-100)	separator base valve (VLV-103),	1
Phenol recycle column	bottom (VLV-106), distillate (VLV-107), reflux, condenser duty, reboiler duty	5
Cyclohexanone column	bottom (VLV-110), distillate (VLV-109), reflux, condense duty, reboiler duty	5
Dehydrogenation reactor	heating duty of reactor (qR2h)	1
Vessel (V-101)	separator base valve (VLV-1113), purge valve (VLV-111)	2
Compressor	work input (wk1)	1
Coolers and Heaters	duty: qh1, qh2, qh3, qc1, qc2	5
	Sum	23

Degree of freedom = 23.

Step3. Establish Energy Management System

Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system. The control system must ensure that exothermic heats of reaction are removed from the process. In the current application, the hydrogenation reactor contains two exothermic reactions which have shown in process description. Hence, the temperature of the first reactor needs to control at 1 m length of reactor where the peak temperature occurs. The second reactor contains one endothermic reaction which is favored at high temperatures so the outlet reactor temperature is controlled. The inlet temperature of both the reactors needs to be controlled at the desired values. The management of heat exchanger network is described in energy management of heat-integrated process section.

Step4. Set Production Rate

There are not constrained to set production either by supply or demand. The process variables that dominate the reactor productivity are typically reactor conditions such as temperature, pressure, reactant concentrations, and holdups. The most dominant variable should be used to set throughput. The selected variable should have 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. In the phenol hydrogenation to cyclohexanone process, temperature cannot be selected since the hydrogenation reactor should operate at desire value in order to prevent side reaction occurs too much and hot spot occurs. Hence, the total flow (fresh feed plus recycle) of phenol is used for setting the production rate. The most suitable manipulator to control total phenol flow is the fresh feed flow of phenol.

Step5. Control Product Quality and Address Safety, Operational and Environmental Concerns.

The main product in this case is cyclohexanone coming from the top stream of the product column. To achieve the product quality control, cyclohexanol impurity composition of the top stream from the product column is controlled using the reflux flow rate. The important operational constraints on the two reactor inlet temperatures have already been handled in step 3. A ratio controller is installed to maintain the ratio of hydrogen to phenol of the first reactor inlet stream at the desired value by adjusting the flow rate of fresh hydrogen stream. The operating pressures of the both vacuum columns have to be controlled. Condenser duty is chosen as the manipulator. The temperatures of two flash vessels are controlled using the cooling duties of the cooler preceding the separators.

Step6. Control Inventories and Fix a Flow in Every Recycle Loop

There are three recycle streams which are phenol, hydrogen and cyclohexanone in the process. Phenol fresh feed valve, hydrogen fresh feed valve and bottom valve of cyclohexanone column are manipulated to control these three recycle streams respectively.

. There are two separators and two distillations in the process. For the pressure, the work input to the compressor is selected in vessel (V-100), purge valve is selected in vessel (V-101) and condenser duties are selected in both columns. For the liquid levels, the most direct way to control is the liquid flow leaving the separators, the reflux drums and the reboilers.

Step7. Check Component Balances

Component balances are particularly important in process with recycle streams because of their integration effect. The specific mechanism or control loop must be identified to guarantee that there will be no uncontrollable build up of any chemical component within the process (Downs drill). In process, the reactant components should not be left in the product stream because of the yield loss and the specification of the desired product purity. Hence we are limited to use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. Table 5.2 shows the checking of all components in the process by overall mass balance equation.

Table 5.2 Component balance

Component	Input	+ Generation	-Output	-Consumption	Accumulation
					Controlled by
Hydrogen	Fresh feed	Dehydrogenation	Purge stream	Hydrogenation	Total flow (fresh + recycle)
Phenol	Fresh feed	0	0	Hydrogenation	Total flow (fresh + recycle)

Table 5.2 (Continued)

Component	Input	+ Generation	-Output	-Consumption	Accumulation
					Controlled by
Cyclohexanone	0	Hydrogenation, Dehydrogenation	Product stream	0	Temperature control in product column
Cyclohexanol	0	Hydrogenation	0	Dehydrogenation	H2:Phenol ratio, Temperature control in dehydrogenation reactor

Step8. Control Individual Unit Operations

The control loops which are necessary to operate each of the individual unit operations are established. The reflux in the recycle column is flow controlled. The bottom composition of the recycle column is controlled by manipulating reboiler duty.

Step9. Optimize Economics or Improve Dynamic Controllability

The remaining one control degree of freedom is still unused. However, there is no particular necessity to establish any additional control loops.

5.1.2 New Plantwide Control Strategies

For CS1, CS2, CS3 and CS4 control structures, the new plantwide control structure design procedure (Wongsri, 2009) is used.

Step1. Establishment of control objectives

The steady state design of the process is assessed and the dynamic control objectives are formulated. The objectives typically include reaction and separation yields, product quality specifications, environmental restrictions, and safety concerns. The control objectives for the phenol hydrogenation to cyclohexanone process are as follows.

1. Good purity product, of minimum 98 % cyclohexanone.
2. Process constraints:
    a) The temperature at the hydrogenation reactor inlet should be 150 °C in order to prevent hot spot occurs.
    b) The two distillation columns should operate under vacuum.
    c) The ratio of Hydrogen to Phenol molar flow rates at the entrance of the hydrogenation reactor is set at 3.6.
    d) The temperature of the both separators should be at 33 °C.

Step2. Selection of controlled variables to maintain product quality and to satisfy safety operational and environmental constrains. The selected CVs are ranked using the Fixture Point theorem.

Plantwide Level: Consider material recycle loop because it causes a system to be born “snowball effect”. Phenol hydrogenation process has three recycle streams which are phenol, hydrogen and cyclohexanone. Therefore to avoid snowball effect, phenol fresh feed valve, hydrogen fresh feed valve and bottom valve of cyclohexanone column are manipulated to control these three recycle streams respectively.

Unit Level: The Fixture Point theorem is used to rank the selected CVs to maintain product quality, to satisfy safety operational and to environmental constrains. The most disturbed points must be satisfactorily controlled by giving them consideration before other variables. Table 5.3 shows the ranked CVs and the IAE summation result.

Table 5.3 Ranked CVs and IAE summation result

	Variables	SUM
Dehydrogenation reactor outlet stream	Temperature	160.17
Dehydrogenation reactor inlet stream	Temperature	127.14
Flash vessel V-101	Liquid level	115.26
Reboiler of cyclohexanone column	Liquid level	82.39
Reboiler of phenol recycle column	Liquid level	82.13
Flash vessel V-101	Pressure	35.62
Flash vessel V-101	Temperature	34.60
Flash vessel V-100	Temperature	32.52
Flash vessel V-100	Pressure	26.49
Flash vessel V-100	Liquid level	24.54
Feed stream of phenol recycle column	Temperature	22.70
Condenser of phenol recycle column	Liquid level	19.44
Feed (recycle) stream of cyclohexanone column	Temperature	17.61
Feed stream of cyclohexanone column	Temperature	8.96
Condenser of cyclohexanone column	Liquid level	6.67
Hydrogenation reactor at 1 m length	Temperature	5.77
Hydrogenation reactor inlet stream	Temperature	5.35
Condenser of phenol recycle column	Pressure	4.56
Condenser of cyclohexanone column	Pressure	2.25

Table 5.4 shows the IAE summation result of tray temperature deviation for phenol recycle column. From this table, tray 21 which has max deviation is selected to control the operation of phenol recycle column. This selected tray is the same tray that changes significantly from tray to tray as shown in Figure 5.1. Furthermore, Figure

5.1 shows that tray 16 gives quite high gradient too. So, two point controls is the one choice for design control structures.

Table 5.4 IAE summation result of tray temperature deviation for phenol recycle column

Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE
1	5.7816	11	3.8362	21	7.1531
2	5.3482	12	3.7595	22	6.8247
3	5.0237	13	3.6924	23	5.1711
4	4.7750	14	3.6363	24	4.0119
5	4.5742	15	3.6097	25	3.3723
6	4.4056	16	3.6745	26	3.0257
7	4.2605	17	3.6669	27	2.8274
8	4.1343	18	3.7079	28	2.7048
9	4.0222	19	4.0894	29	2.6191
10	3.9231	20	5.4375	30	2.5527

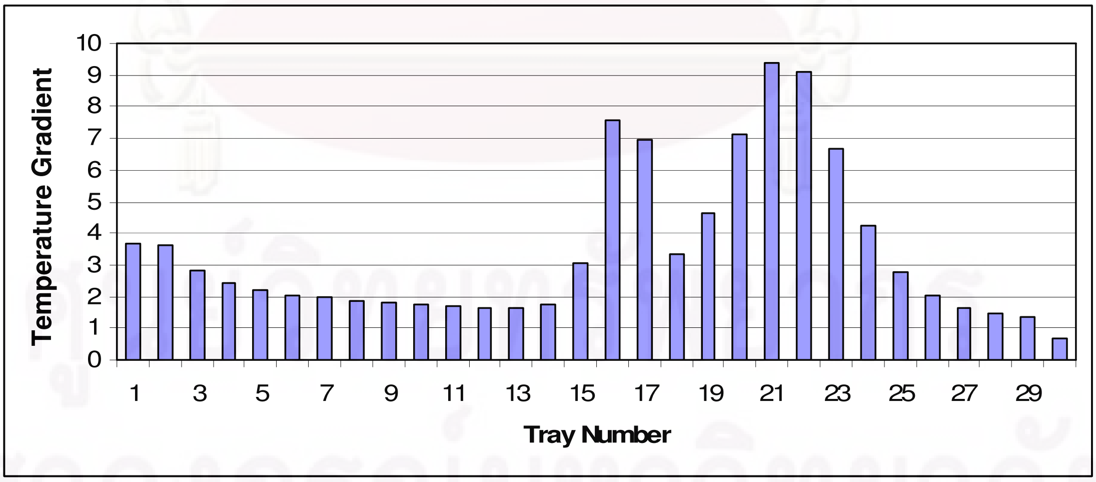


Figure 5.1 Temperature Gradient of phenol recycle column

Table 5.5 IAE summation result of tray temperature deviation for cyclohexanone column

Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE
1	3.1111	11	1.9506	21	1.4597	31	1.3059
2	2.9202	12	1.8931	22	1.4209	32	1.3146
3	2.7547	13	1.8432	23	1.3831	33	1.3142
4	2.6092	14	1.8020	24	1.3454	34	1.3133
5	2.4810	15	1.7404	25	1.3075	35	1.3038
6	2.3665	16	1.6843	26	1.3000	36	1.2811
7	2.2644	17	1.6328	27	1.2956	37	1.2472
8	2.1724	18	1.5856	28	1.2937	38	1.2040
9	2.0900	19	1.5410	29	1.2950	39	1.1480
10	2.0163	20	1.4994	30	1.2985	40	1.0882

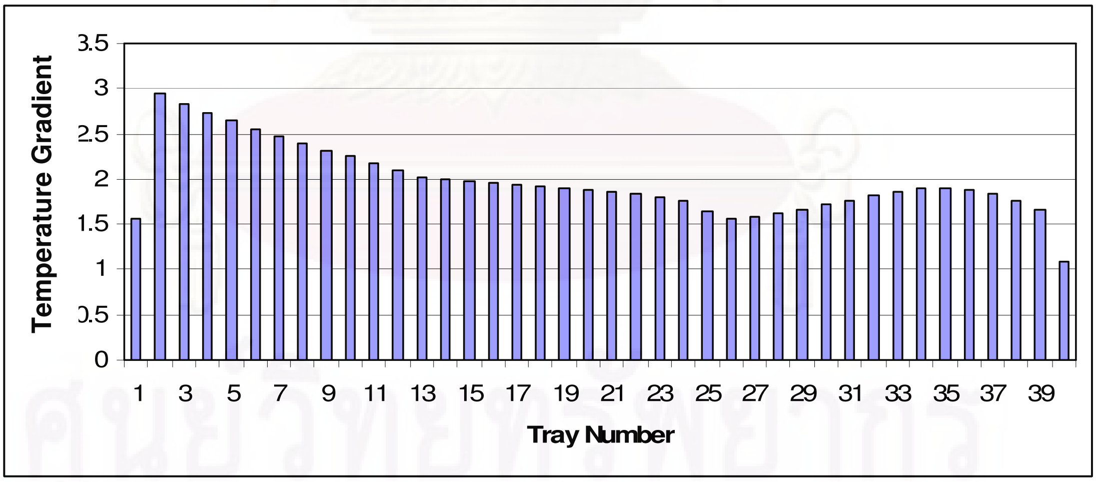


Figure 5.2 Temperature Gradient of cyclohexanone column

Table 5.5 shows the IAE summation result of tray temperature deviation for cyclohexanone column. From this table, tray 1 gives max deviation. From Figure 5.2, tray 2 gives max gradient. However, there is not dominant tray from both results and it is hard to kept tray temperature constant by reflux flow rate which is not direct manipulated variable for controlling tray temperature. Hence, it is properly to control product stream composition directly in this product column.

Step3. Selection of manipulated variables and measurements via DOF analysis

The manipulated variables and measurements which is selected via DOF analysis has already been shown in Table 5.1.

Step4. Energy management via heat exchanger networks

The Energy management via heat exchanger network is described in energy management of heat-integrated process section.

Step5. Selection of control configuration using various tools available

Selection of control configuration use heuristic knowledge. The criteria for selecting an adjustable variable include: causal relationship between the valve and controlled variable, automated valve to influence the selected flow, fast speed of response, ability to compensate for large disturbances and ability to adjust the manipulated variable rapidly and with little upset to the remainder of the plant.

Table 5.6 Matching CVs with MVs

		MVs			
CVs		CS1	CS2	CS3	CS4
Dehydrogenation reactor outlet stream	T	qR2h	qR2h	qR2h	qR2h
Dehydrogenation reactor inlet stream	T	qh3	qh3	qh3	qh3
Flash vessel V-101	L	VLV-113	VLV-113	VLV-113	VLV-113
Reboiler of cyclohexanone column	L	qC2r	qC2r	qC2r	qC2r
Reboiler of phenol recycle column	L	VLV-106	VLV-106	VLV-106	VLV-106
Flash vessel V-101	P	VLV-111	VLV-111	VLV-111	VLV-111
Flash vessel V-101	T	qc2	qc2	qc2	qc2
Flash vessel V-100	T	qc1	qc1	qc1	qc1

Table 5.6 (Continued)

		MVs			
CVs		CS1	CS2	CS3	CS4
Flash vessel V-100	P	wk1	wk1	wk1	wk1
Flash vessel V-100	L	VLV-103	VLV-103	VLV-103	VLV-103
Feed stream of phenol recycle column	T	VLV-104	VLV-104	VLV-104	VLV-104
Condenser of phenol recycle column	L	VLV-107	VLV-107	VLV-107	VLV-107
Feed (recycle) stream of cyclohexanone column	T	VLV-114	VLV-114	VLV-114	VLV-114
Feed stream of cyclohexanone column	T	qh2	qh2	qh2	qh2
Condenser of cyclohexanone column	L	VLV-109	Reflux	VLV-109	Reflux
Hydrogenation reactor at 1 m length	T	qR1c	qR1c	qR1c	qR1c
Hydrogenation reactor inlet stream	T	qh1	qh1	qh1	qh1
Condenser of phenol recycle column	P	qC1c	qC1c	qC1c	qC1c
Condenser of cyclohexanone column	P	qC2c	qC2c	qC2c	qC2c
Tray 21 of phenol recycle column	T	qC1r	qC1r	qC1r	qC1r
Production stream	C	Reflux	VLV-109	Reflux	VLV-109
Tray 16 of phenol recycle column	T	-	-	Reflux	Reflux

Note: C refers to composition, L refers to liquid level, P refers to pressure and T refers to temperature.

For controlling liquid level at condenser of cyclohexanone column, bottom flow rate and reflux flow rate can also used as manipulated variable since both of them are direct effect to this controlled variable, and it is the same case for controlling composition of production stream. Therefore, the different control structures are designed for controlling these two manipulated variables in order to find the appropriate control structures. Temperature at tray 16 of phenol recycle column is controlled in CS3 and CS4 by reflux flow rate which is the remaining manipulated variable. In sum, the four appropriate control structures are designed by the new plantwide control structure design procedure (Wongsri, 2009) as shown in Table 5.6. By the way, using Luyben heuristic can also result these four control structures too depending on designer's judgment in matching the CVs and MVs. However, the new design procedure gives the priority of CVs, so in principle the new design procedure will give designer the important information of what CV to be considered first if there are conflicts of matching two or more CVs with appropriate MVs.

Step6. Completing control structure design by checking the component balance

Checking the component balance with overall mass balance has already been shown in Table 5.2.

Step7. Selection of controller type: single loops or MPC

In this research, all controller type is single-input-single-output loop.

Step8. Validation via rigorous dynamic simulation

Using software HYSYS to evaluate performance for phenol hydrogenation to cyclohexanone process of all designed control structures at dynamic simulation.

5.2 Design of Plantwide Control Structures

In all control structures: CS1, CS2, CS3 and CS4 the same loops are used as follows:

<u>Plantwide level</u>

- Valve VLV-100 is manipulated to control the phenol recycle flow rate
- Valve VLV-101 is manipulated to control the hydrogen recycle flow rate as the H_2: Phenol ratio equals 3.6.

- Valve VLV-110 is manipulated to control the bottom flow rate of cyclohexanone column.

Unit level

Hydrogenation reactor (PFR-100)

- Heating duty (qh1) is manipulated to control the reactor inlet temperature.
- Cooling duty (qR1c) is manipulated to control the reactor temperature at 1m length.

Dehydrogenation reactor (PFR-102)

- Heating duty (qh3) is manipulated to control the reactor inlet temperature.
- Heating duty (qR2h) is manipulated to control the reactor outlet temperature.

Flash vessel (V-100)

- Cooling duty (qc1) is manipulated to control the vessel inlet temperature.
- Work input to the compressor (wk1) is manipulated to control the vessel pressure.
- Valve VLV-103 is manipulated to control the liquid level in the vessel.

Flash vessel (V-101)

- Cooling duty (qc2) is manipulated to control the vessel inlet temperature.
- Purge valve (VLV-111) is manipulated to control the vessel pressure.
- Valve VLV-113 is manipulated to control the liquid level in the vessel.

Phenol recycle column (T-100)

- Bypass valve (VLV-104) is manipulated to control the feed stream temperature.
- Condenser duty (qC1c) is manipulated to control the condenser pressure.
- Valve VLV-107 is manipulated to control the condenser level.
- Valve VLV-106 is manipulated to control the reboiler level.
- Reboiler duty (qC1r) is manipulated to control tray 21 temperature.

Cyclohexanone column (T-100)

- Heating duty (qh2) is manipulated to control the feed stream temperature.
- Bypass valve (VLV-114) is manipulated to control the recycle stream temperature.
- Condenser duty (qC2c) is manipulated to control the condenser pressure.
- Reboiler duty (qC2r) is manipulated to control the reboiler level.

5.2.1 Summary of All Control Structures Design

Table 5.7 shows the different of each control structure and matching of controlled variables with manipulated variables. Figure 5.5, Figure 5.6, Figure 5.7 and Figure 5.8 shows the applications for control structure 1 (CS1), control structure 2 (CS2), control structure 3 (CS3) and control structure 4 (CS4) respectively.

Table 5.7 Summary of all designed control structures design

	CS1				CS2			
CVs	MV1	MV2	MV3	MV4	MV1	MV2	MV3	MV4
Phenol recycle column								
Tray 21 temperature	√				√			
Tray 16 temperature								
Cyclohexanone column								
Product composition				√			√	
Condenser level			√					√

	CS3				CS4			
CVs	MV1	MV2	MV3	MV4	MV1	MV2	MV3	MV4
Phenol recycle column								
Tray 21 temperature	√				√			
Tray 16 temperature		√				√		
Cyclohexanone column								
Product composition				√			√	
Condenser level			√					√

Note: MV1 refers to reboiler duty of phenol recycle column, **MV2** refers to reflux flow rate of phenol recycle column, **MV3** refers to top flow rate of cyclohexanone column and **MV4** refers to reflux flow rate of cyclohexanone column.

5.3 Energy Management of Heat-Integrated Process

The design of heat pathways for resilient heat exchanger network is shown in Figure 5.3. In the network of hot stream H1, there are two cold streams C1 and C2. Considering H1 exchange heat with C1, it is not necessary to control the both exit temperature so the disturbance still exists in both. Then C1 is combined with Hydrogen (fresh + recycled) stream and heated to inlet temperature condition of hydrogenation reactor. Next considering H1 exchange heat with C2, C2 temperature is controlled using bypass stream of C2 in order to maintain temperature feed condition of phenol recycle column. Finally, the target temperature of H1 is achieved by cooler.

In the network of hot stream H2, there are two cold streams C4 and C5. Considering H2 exchange heat with C4, it is difficult to control H1 and C4 outlet temperature since phase change occur both in H1 and C4 so there is no control loop for this match. Next considering H1 exchange heat with C5, C5 temperature is controlled using bypass stream of C5 in order to maintain temperature feed condition of cyclohexanone column. Finally, the target temperature of H2 is achieved by cooler.

However, large change of the H1 and H2 inlet temperatures do not occur since they are already controlled in the process. Summary, both positive and negative disturbance loads of all streams in H1 network are directed to cooler. In H2 network, both positive and negative disturbance loads of H2 and C4 are directed to heater and cooler. For C5, positive and negative disturbance loads are directed to cooler. Figure 5.4 present the control configurations of resilient heat exchanger network.

Selective controllers with low selector switches (LSS) which perform to select an appropriate heat pathway through the network to direct the disturbance load to a heating or cooling utility unit in order to achieve dynamic maximum energy recovery are also considered in this work. However, it is difficult to control temperature of hot streams in order to transfer disturbance load to cold streams because of phase changing. So low selector switches are not employed in this work.

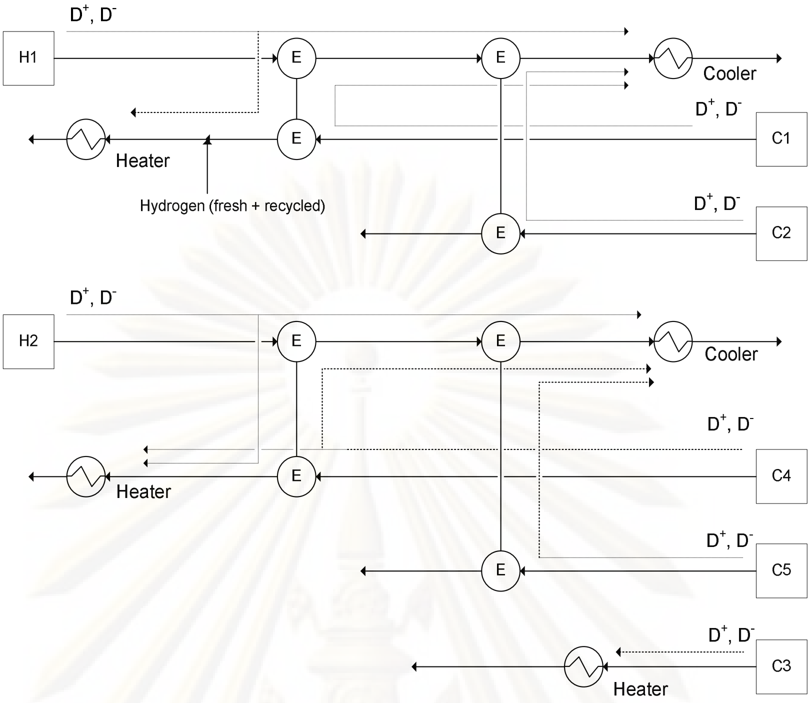


Figure 5.3 Heat pathways of resilient heat exchanger network

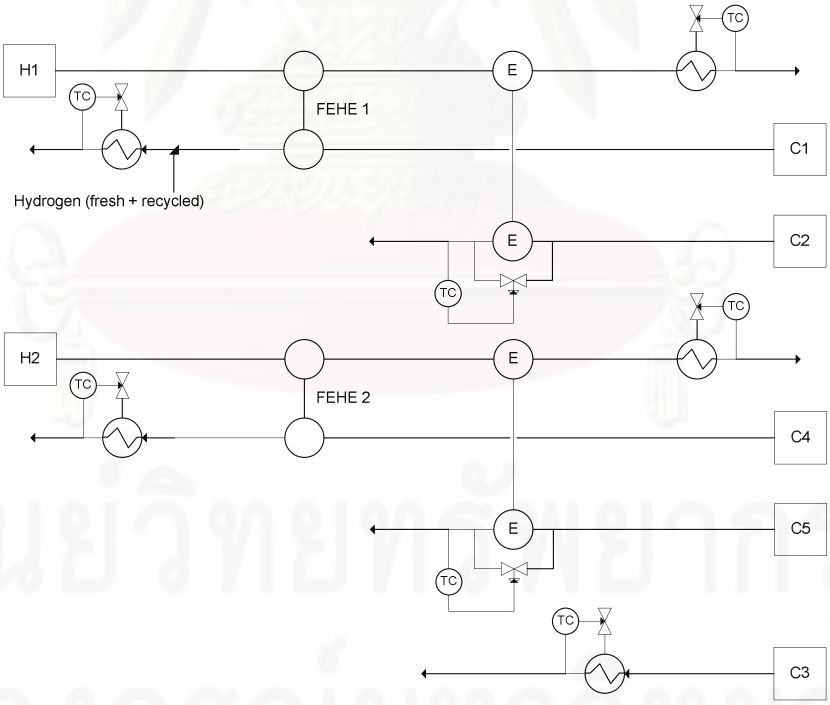


Figure 5.4 Control configurations of resilient heat exchanger network

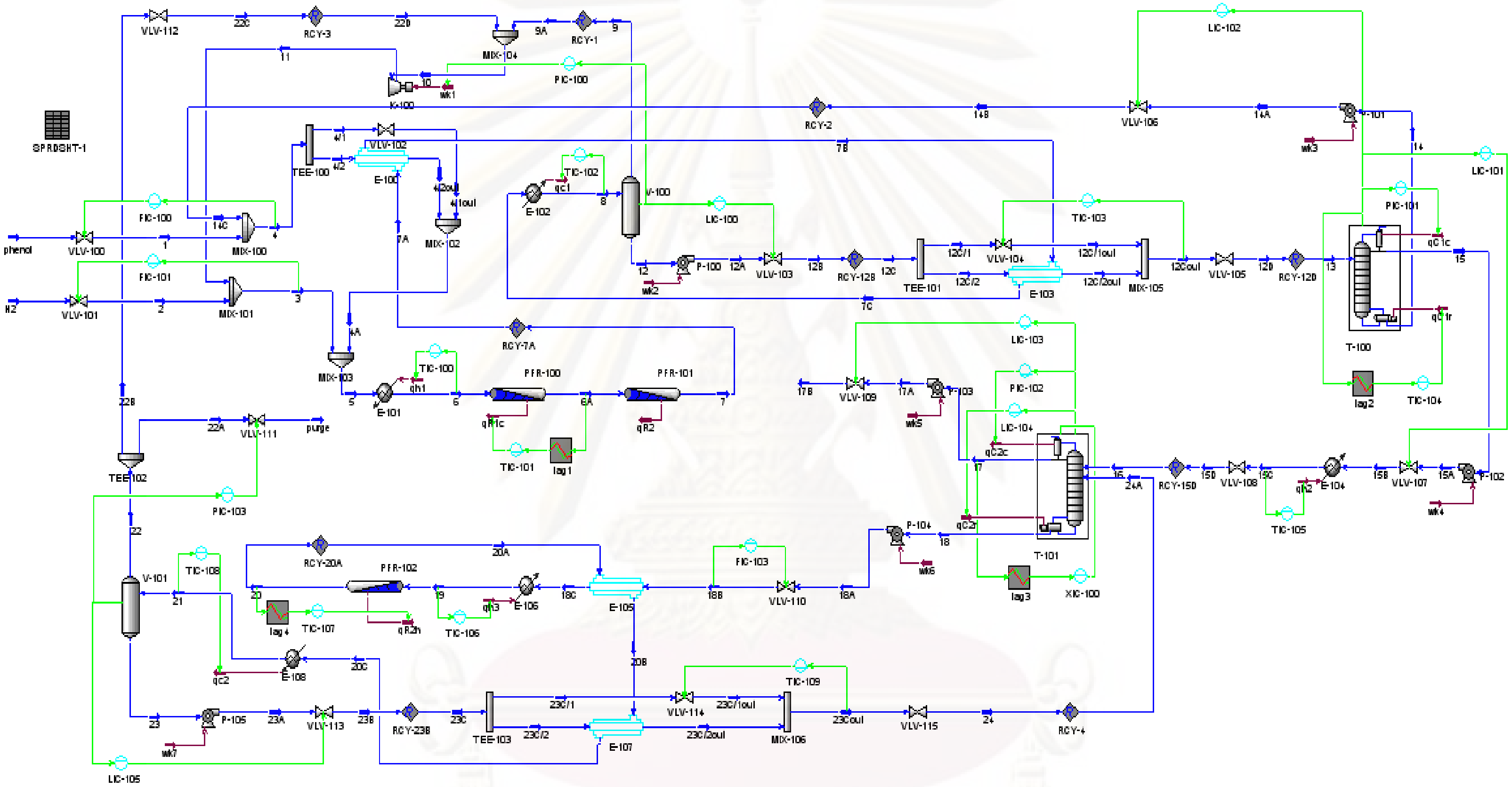


Figure 5.5 Application of control structure 1 (CS1)

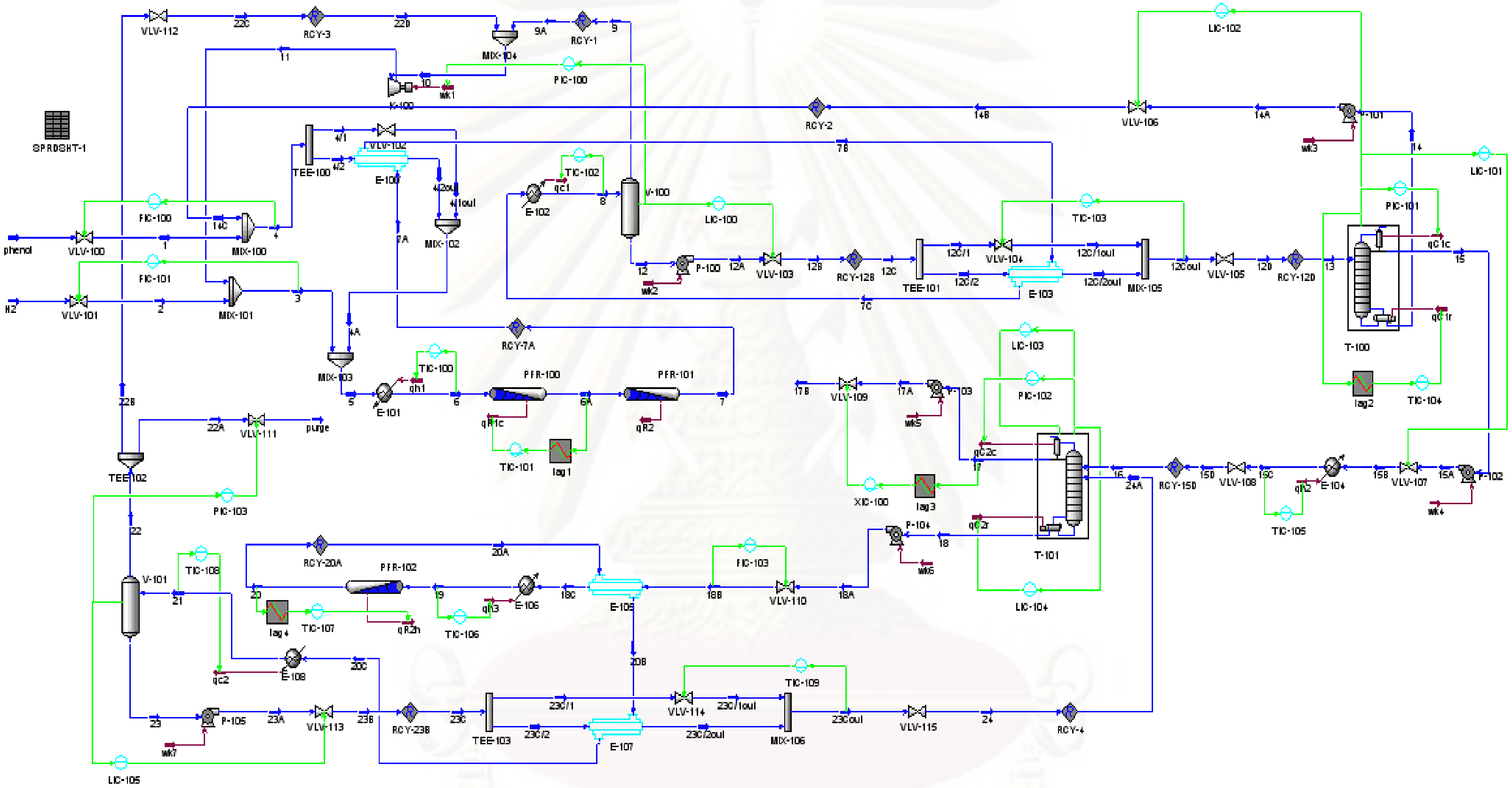


Figure 5.6 Application of control structure 2 (CS2)

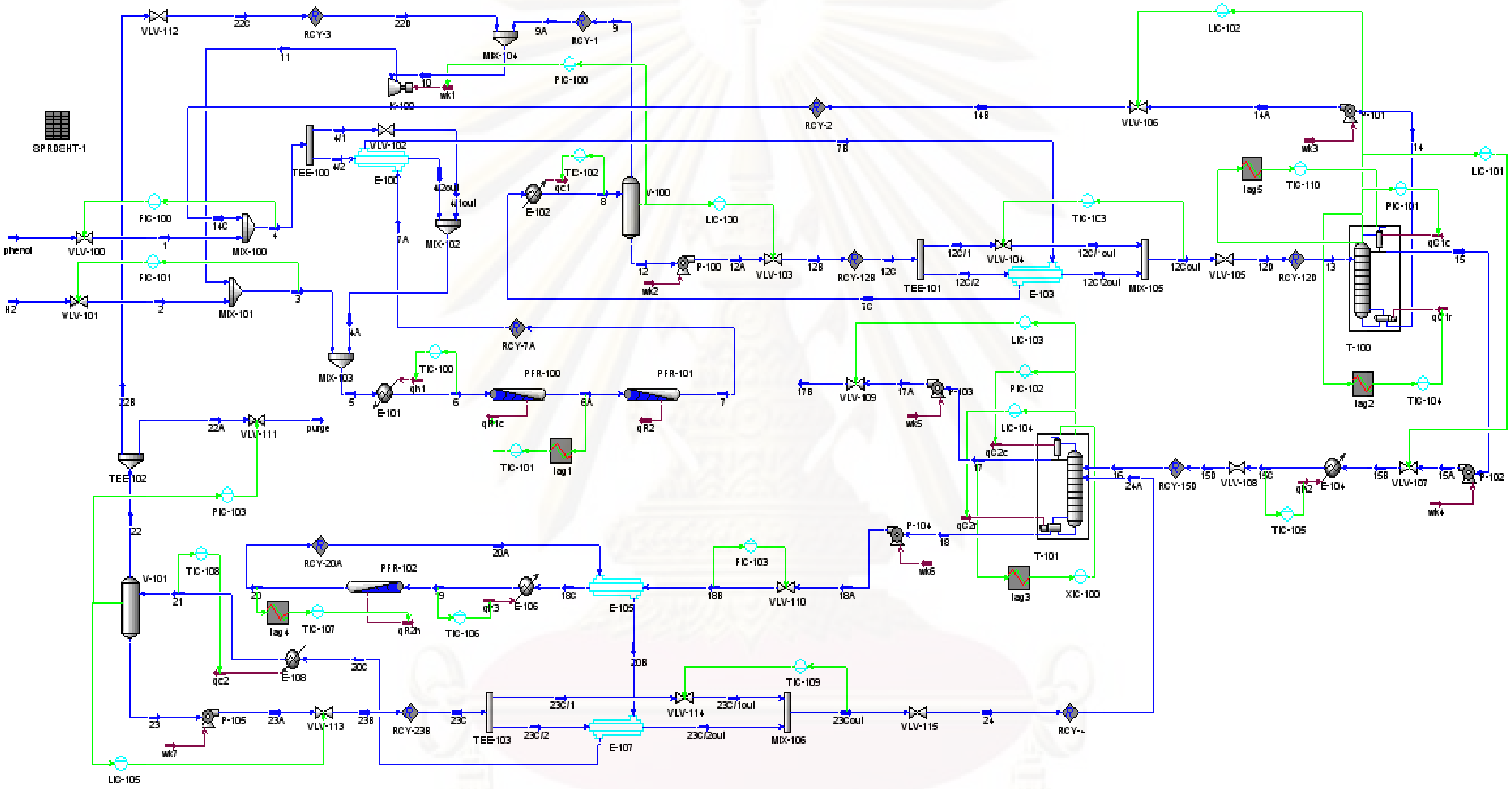


Figure 5.7 Application of control structure 3 (CS3)

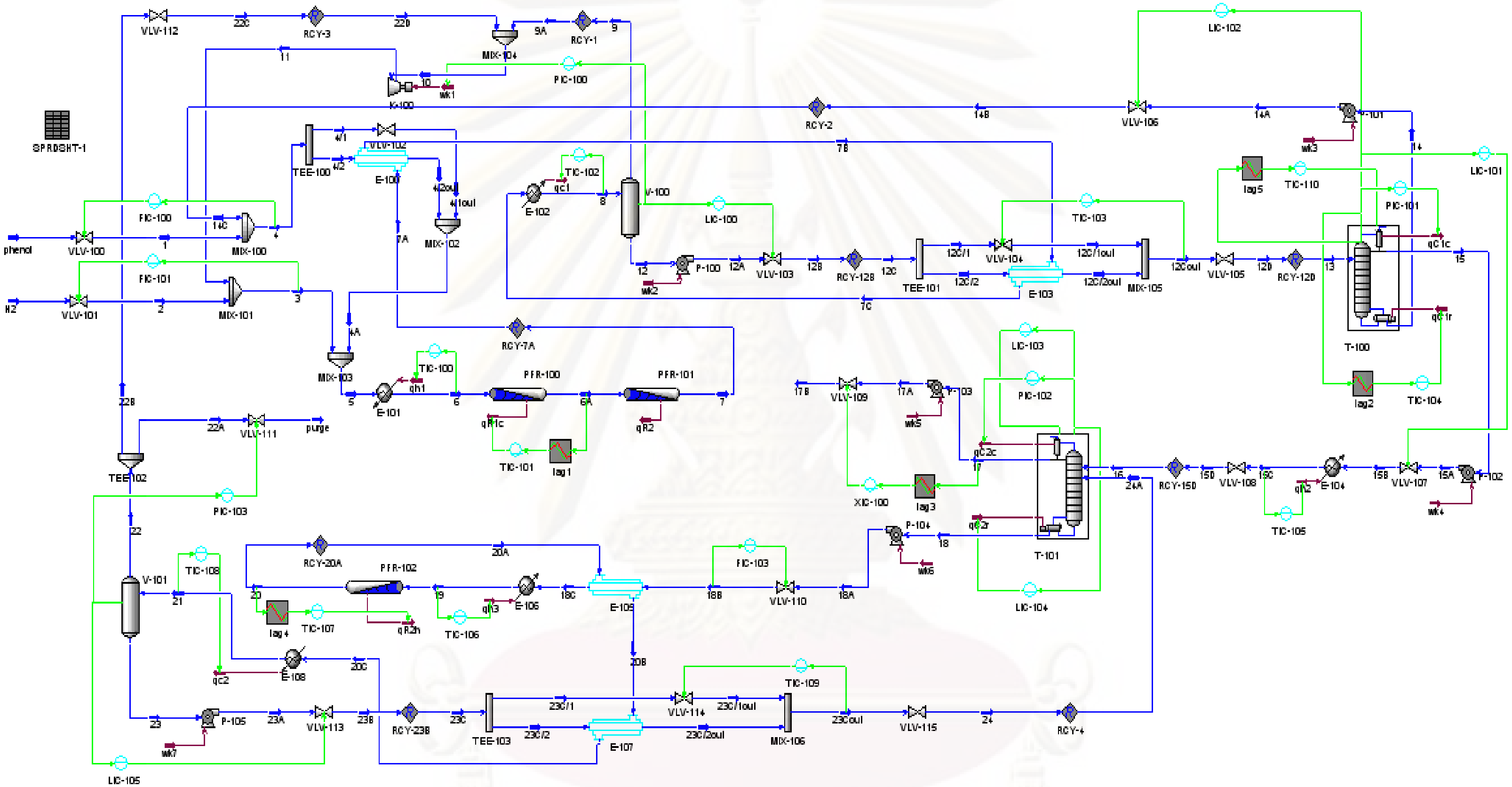


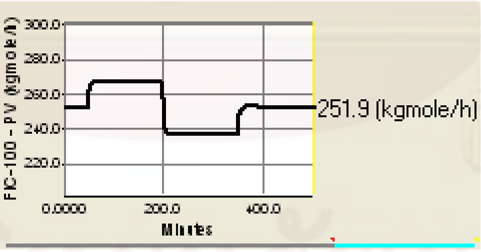
Figure 5.8 Application of control structure 4 (CS4)

5.4 Dynamics Simulation Results

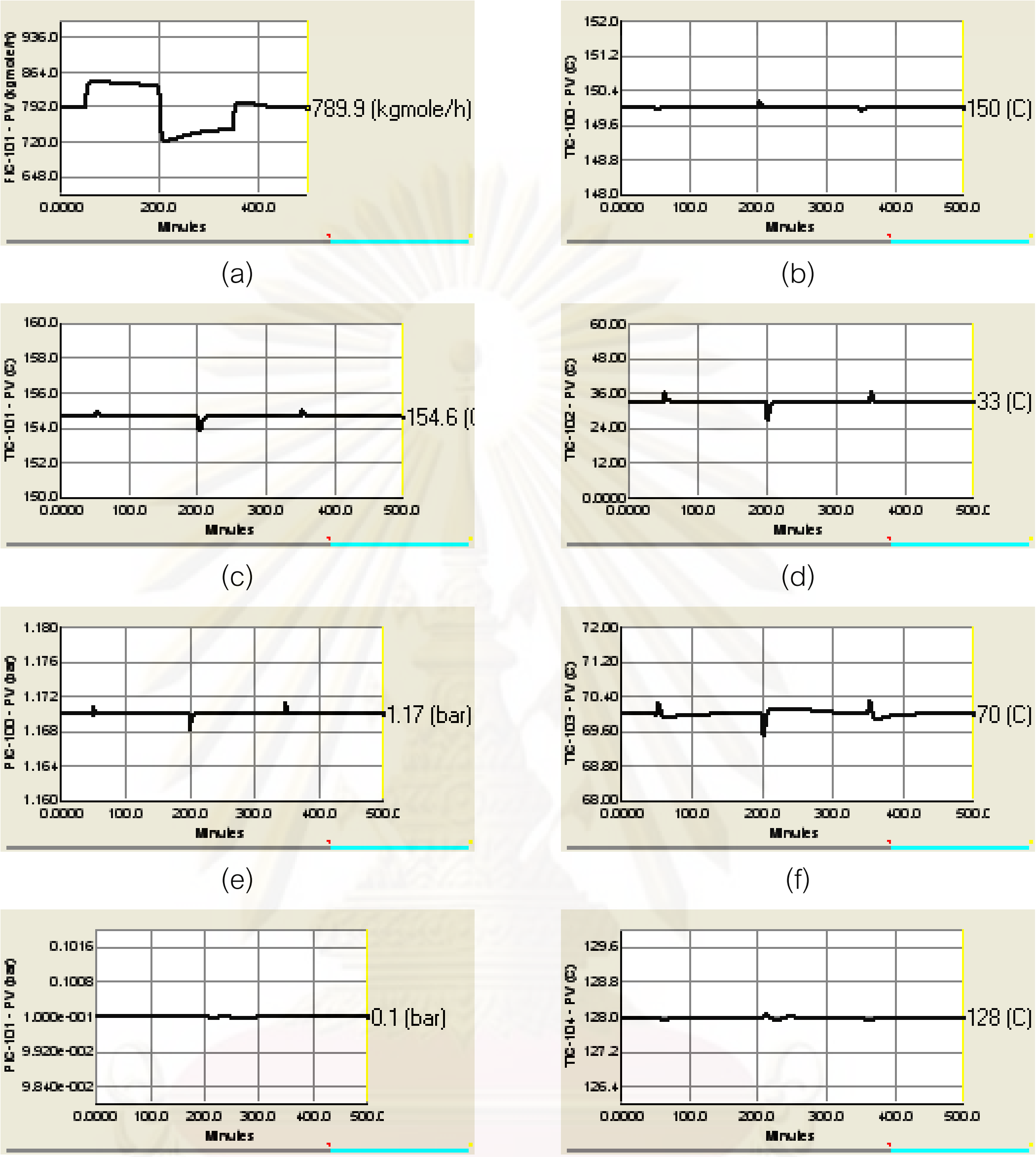
In order to illustrate the dynamic behaviors of our control structures, two types of disturbance: thermal and material disturbances are used to test response of the system. Temperature controllers and composition controllers are PIDs which are tuned using autotuner in HYSYS. Temperature measurement lags of 0.5 minute are included in the temperature loops. A 3 minute deadtime is assumed in the composition measurement. 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 phenol (fresh + recycled) flow

Figure 5.9 to 5.12 show the dynamic response of the phenol hydrogenation to cyclohexanone process in the material disturbance of phenol (fresh + recycled) stream. The disturbance made as follows: The stream flow is increased from 251.9 kgmole / h to 267 kgmole / h at time equals 50 minutes and decreased from 267 kgmole / h to 237 kgmole / h at time equals 200 minutes and then return to its set point at time equals 350 minutes.

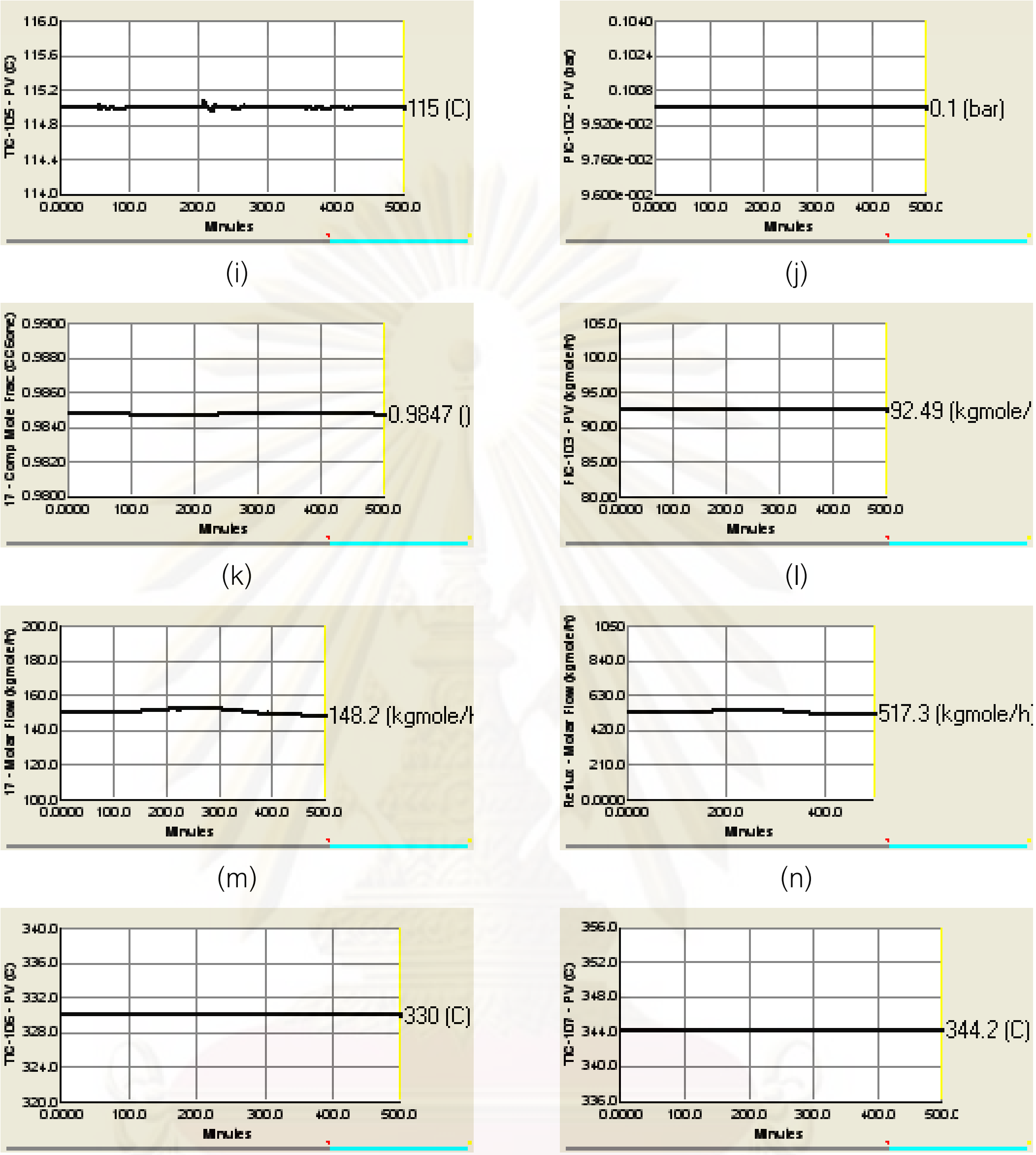


In all control structures give the same trend result to reject material disturbance which can reject disturbance and return to their set point as shown in the figures. From all graphs of dehydrogenation section, we can notice that the material disturbance in hydrogenation section does not effect to dehydrogenation section since the bottom flow rate of cyclohexanone column which is the feed stream of dehydrogenation section is controlled. Besides, all process constraint variables are achieved when material disturbance occur in all designed control structure.



(a) (b) (c) (d) (e) (f) (g) (h)

Figure 5.9 Dynamic responses of CS1 when change in phenol (fresh + recycled flow): (a) hydrogen (fresh + recycle) flow, (b) hydrogenation reactor inlet temperature, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature



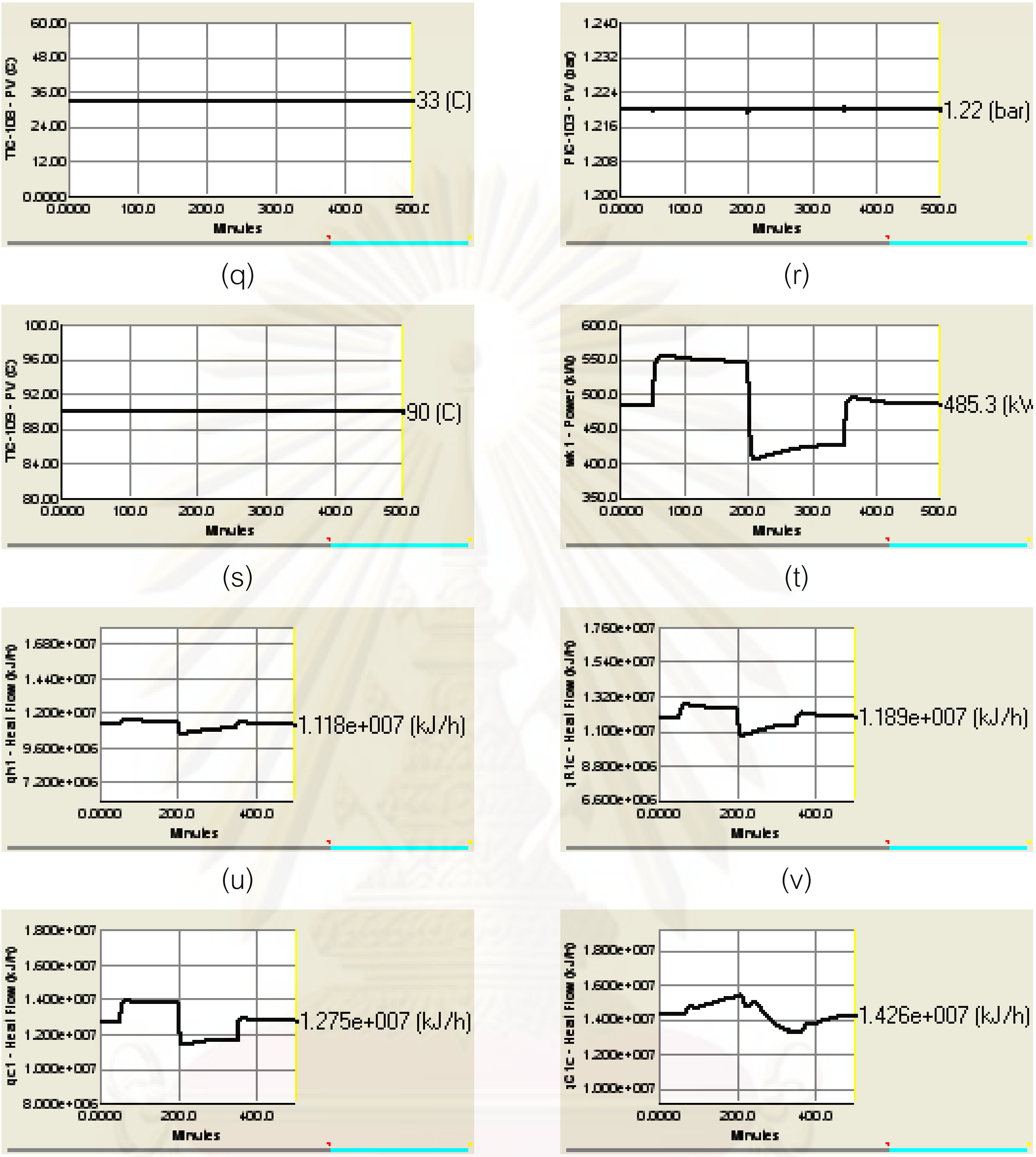
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.9 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



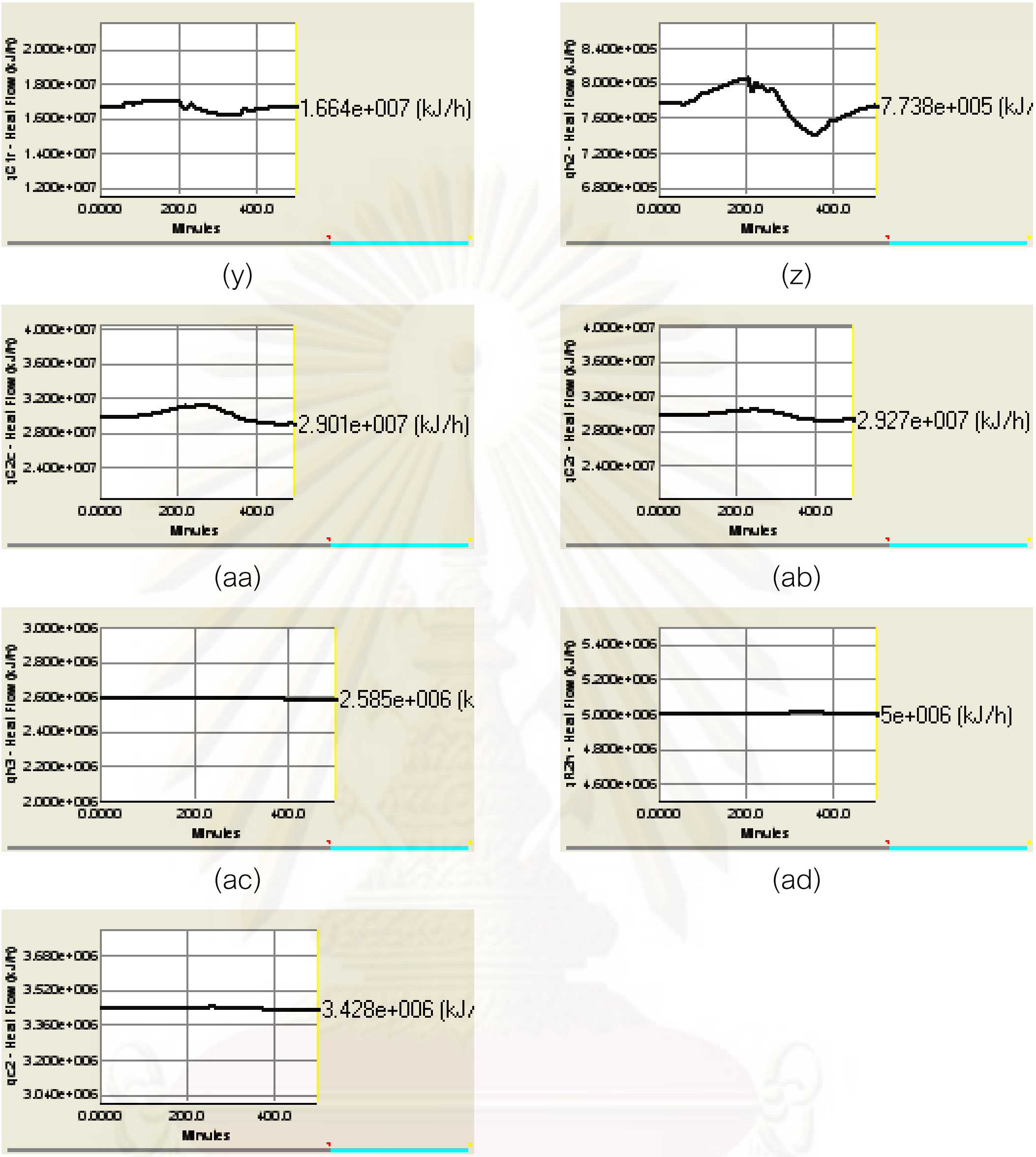
(q) (r)

(s) (t)

(u) (v)

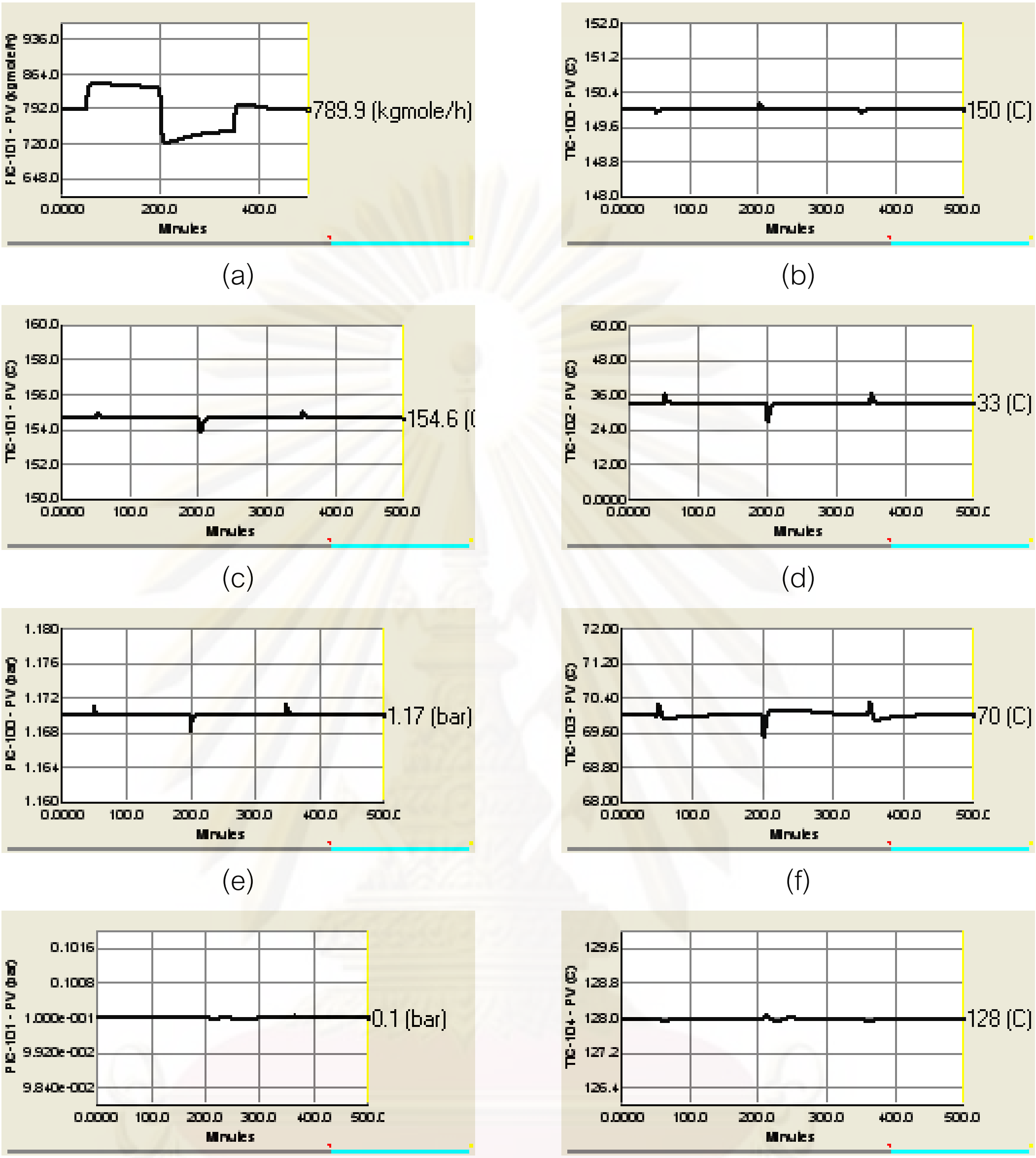
(w) (x)

Figure 5.9 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y)
(z)
(aa)
(ab)
(ac)
(ad)
(ae)

Figure 5.9 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



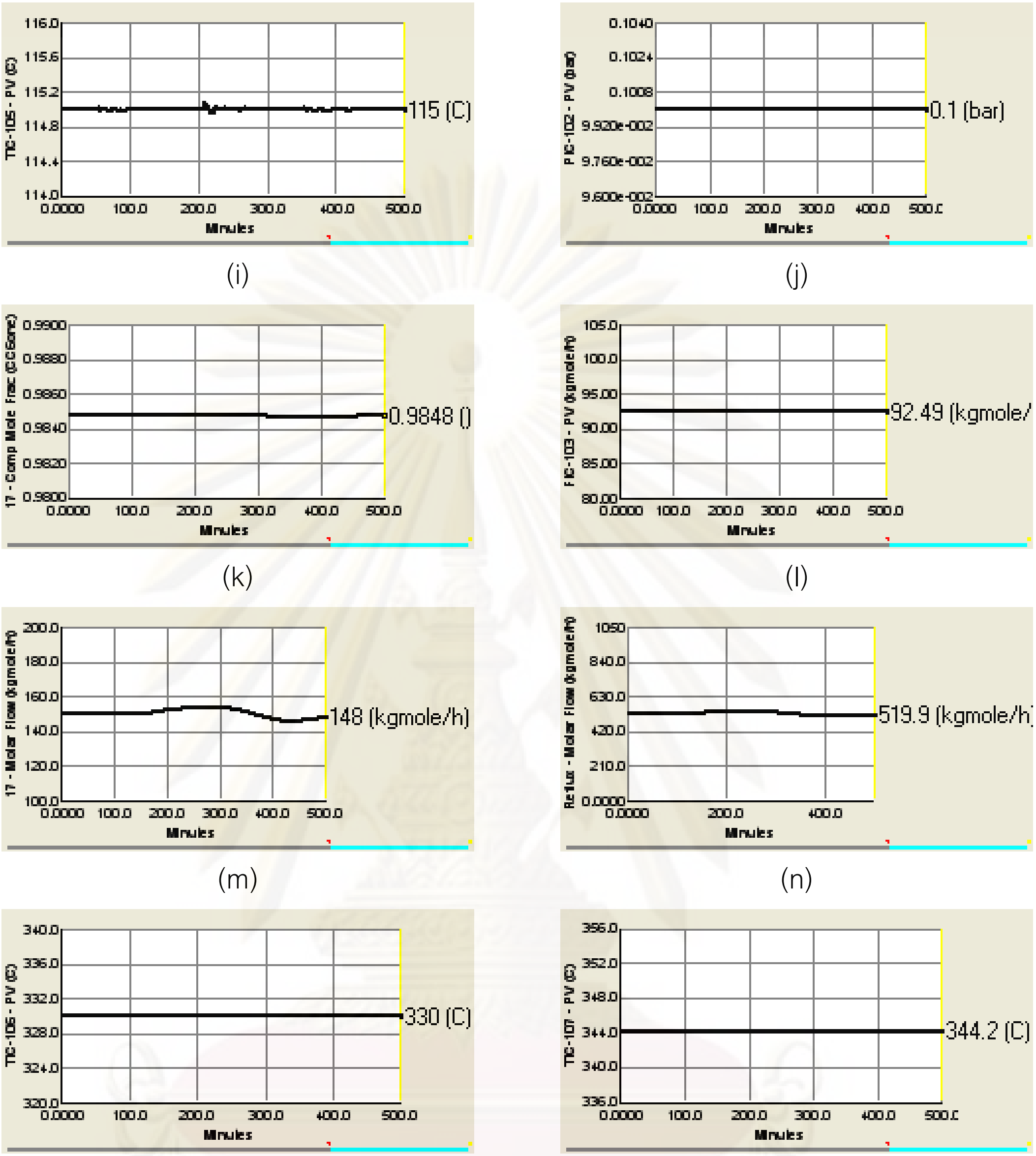
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.10 Dynamic responses of CS2 when change in phenol (fresh + recycled flow): (a) hydrogen (fresh + recycle) flow, (b) hydrogenation reactor inlet temperature, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature



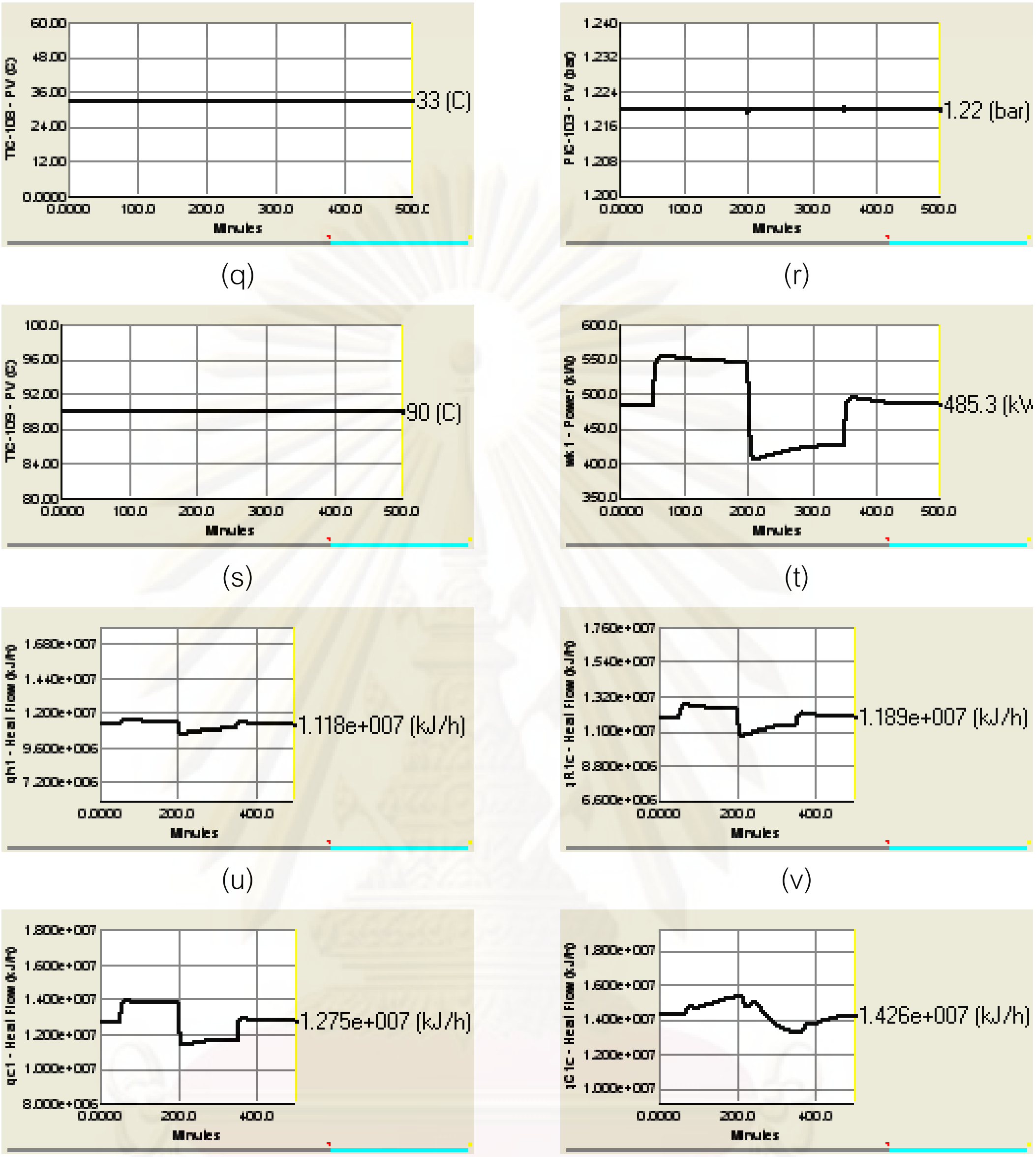
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.8 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



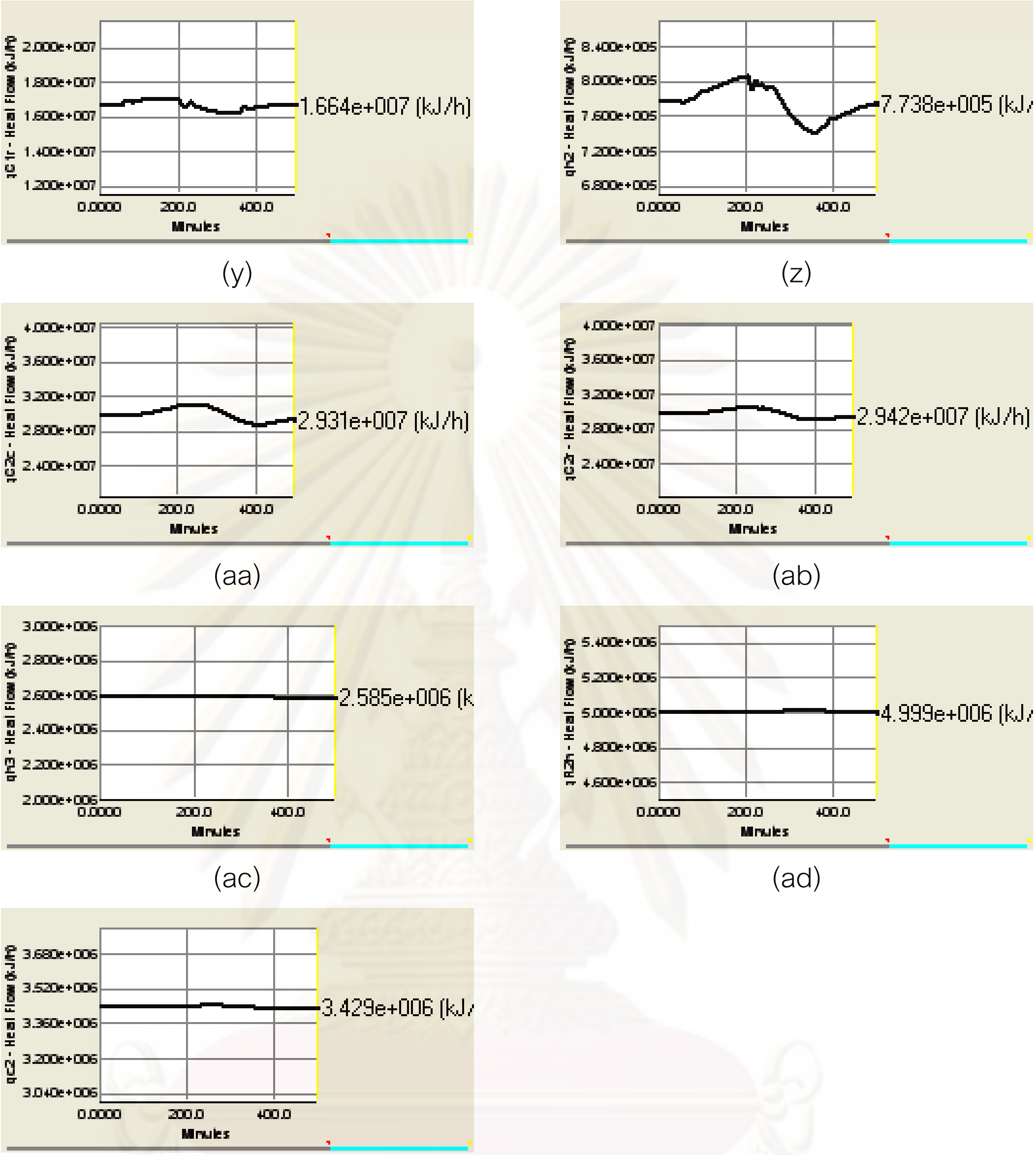
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.8 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



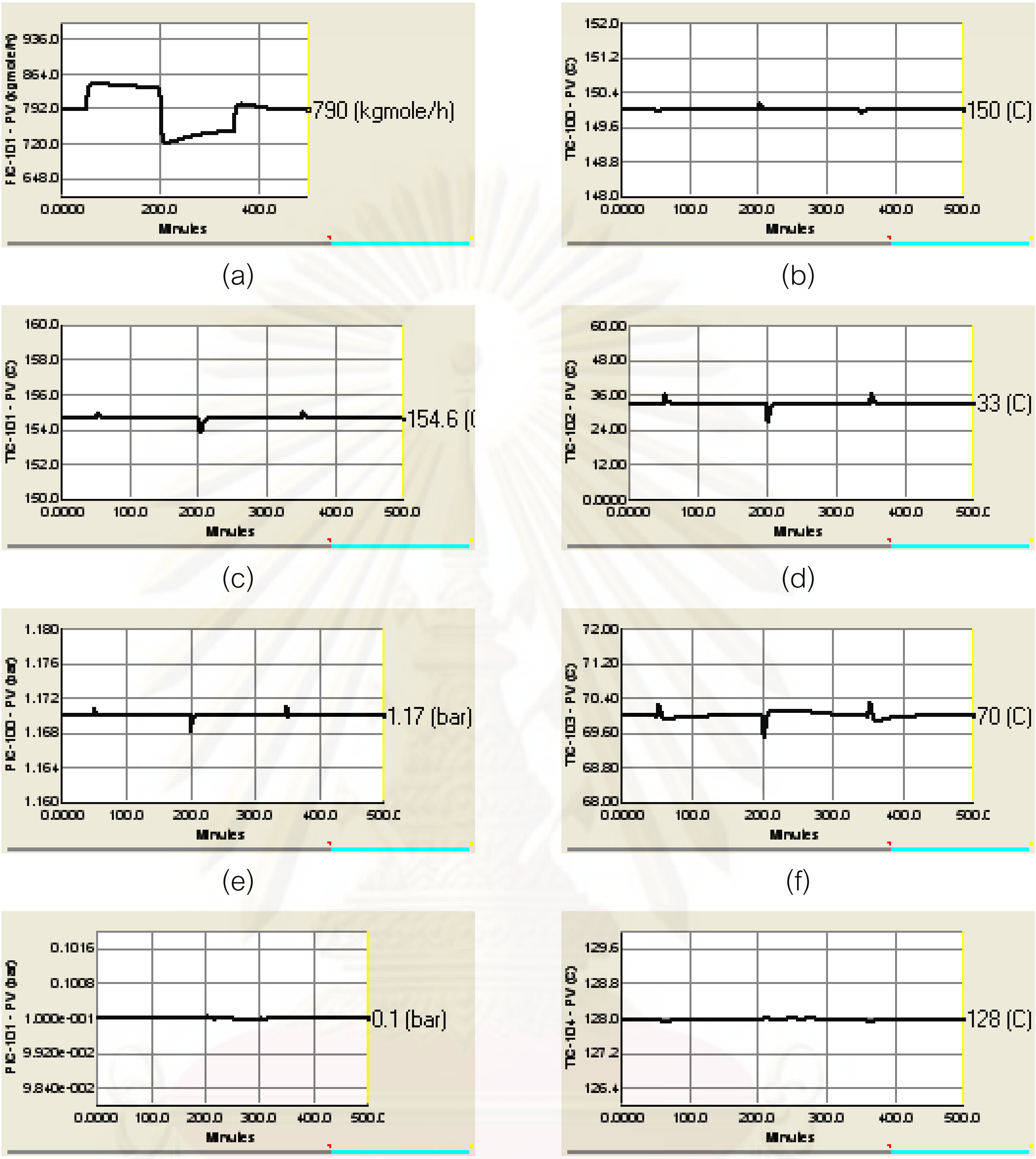
(y) (z)

(aa) (ab)

(ac) (ad)

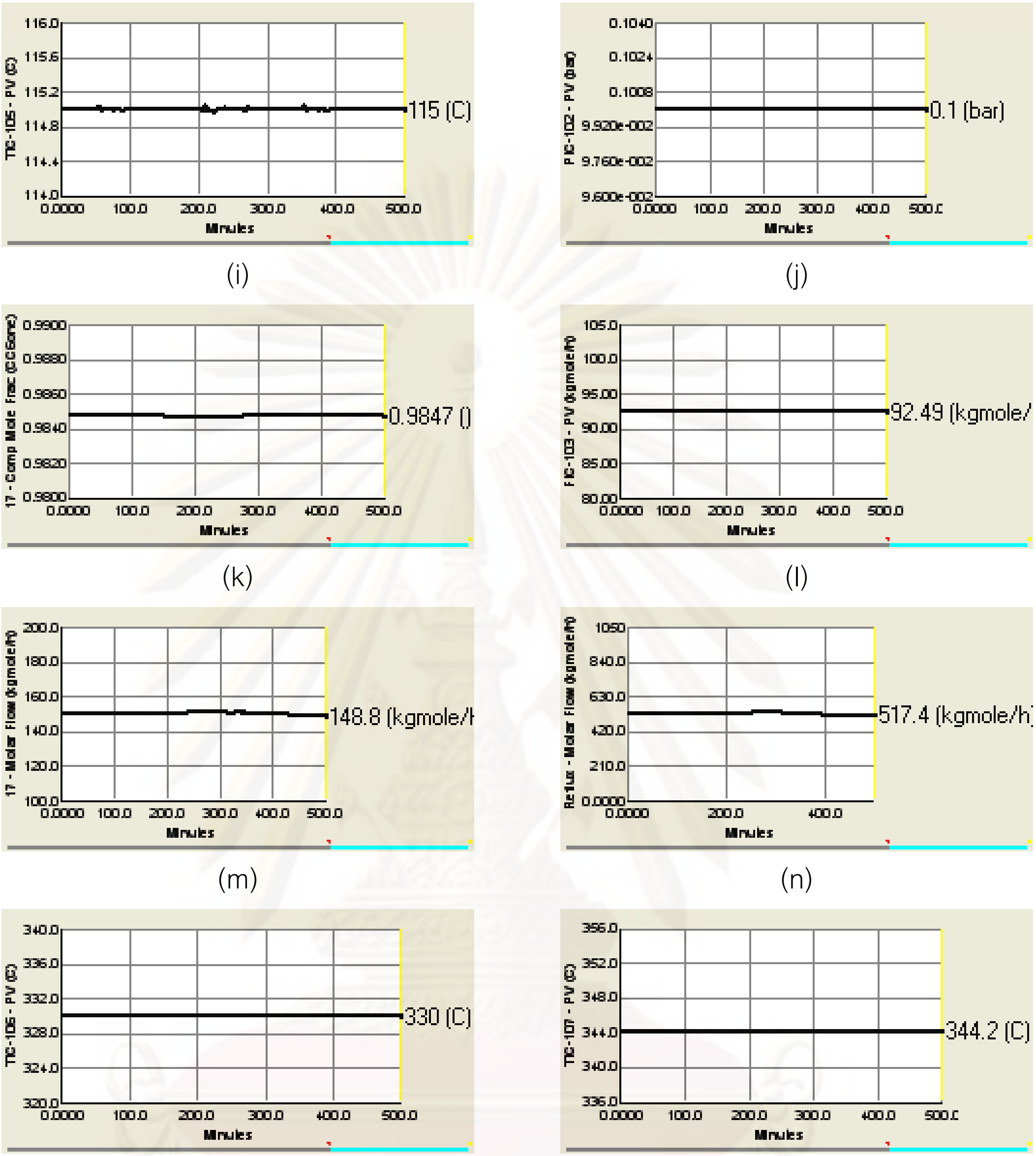
(ae)

Figure 5.8 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



(a) (b) (c) (d) (e) (f) (g) (h)

Figure 5.11 Dynamic responses of CS3 when change in phenol (fresh + recycled flow): (a) hydrogen (fresh + recycle) flow, (b) hydrogenation reactor inlet temperature, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature



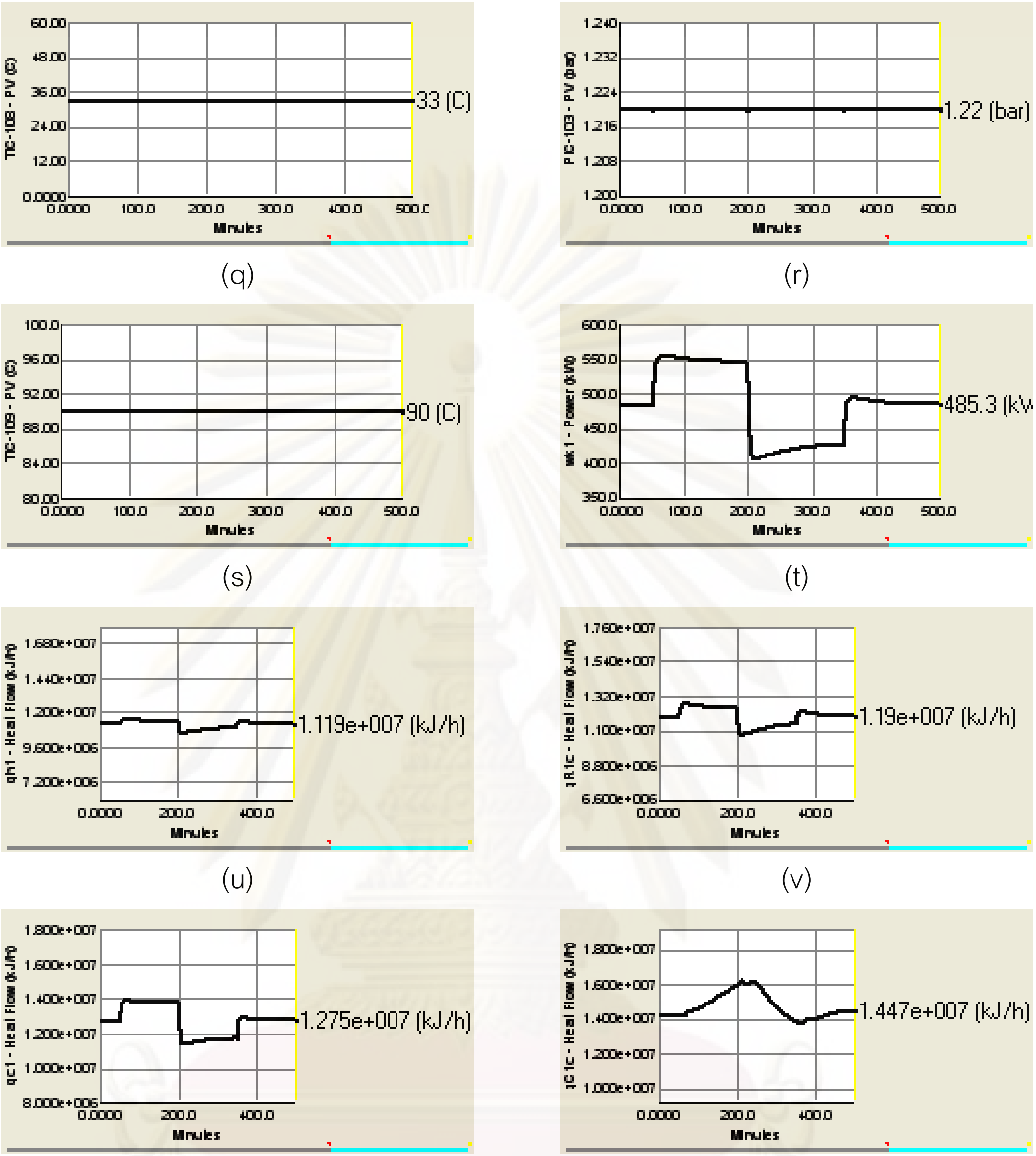
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.11 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



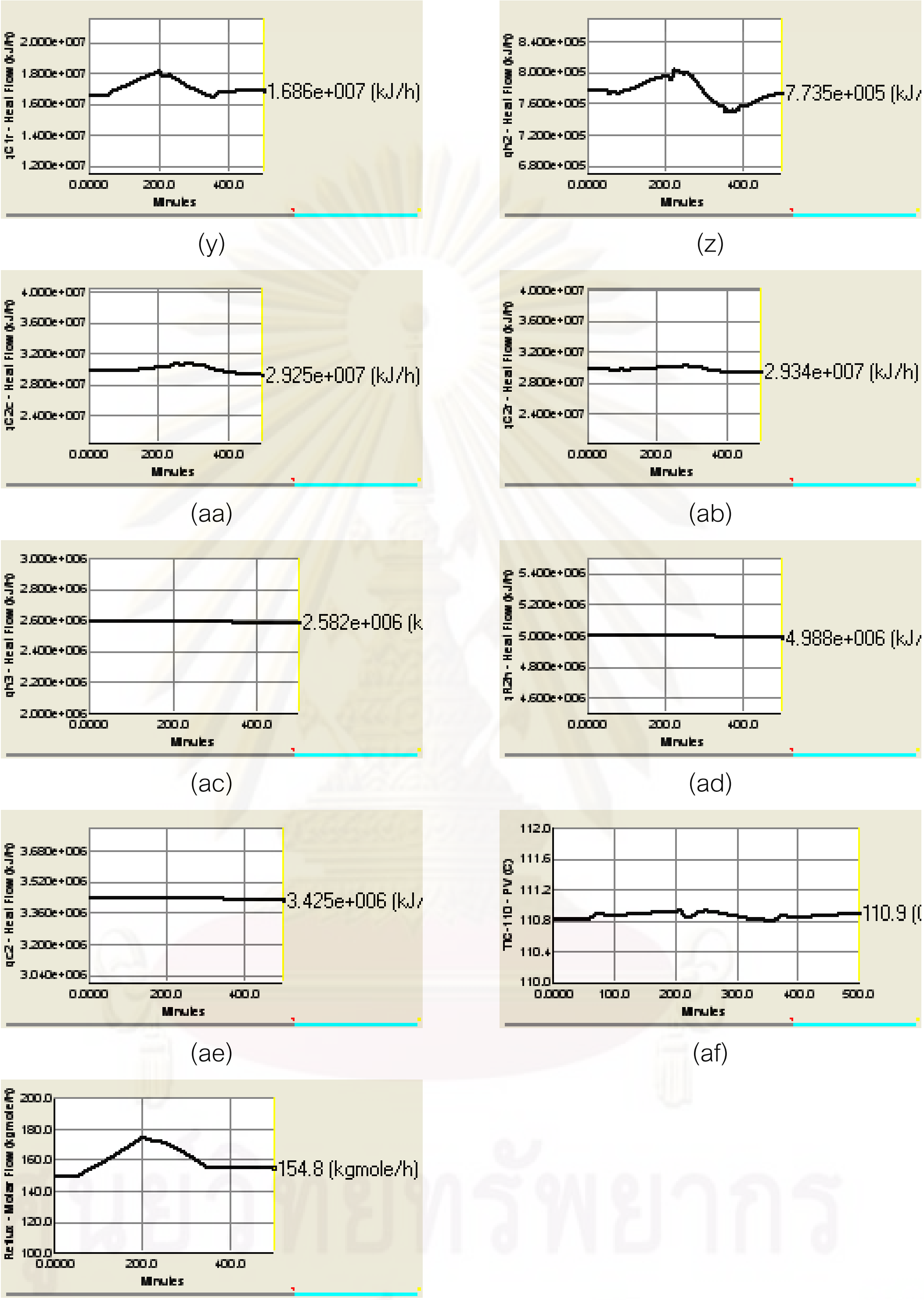
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.11 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

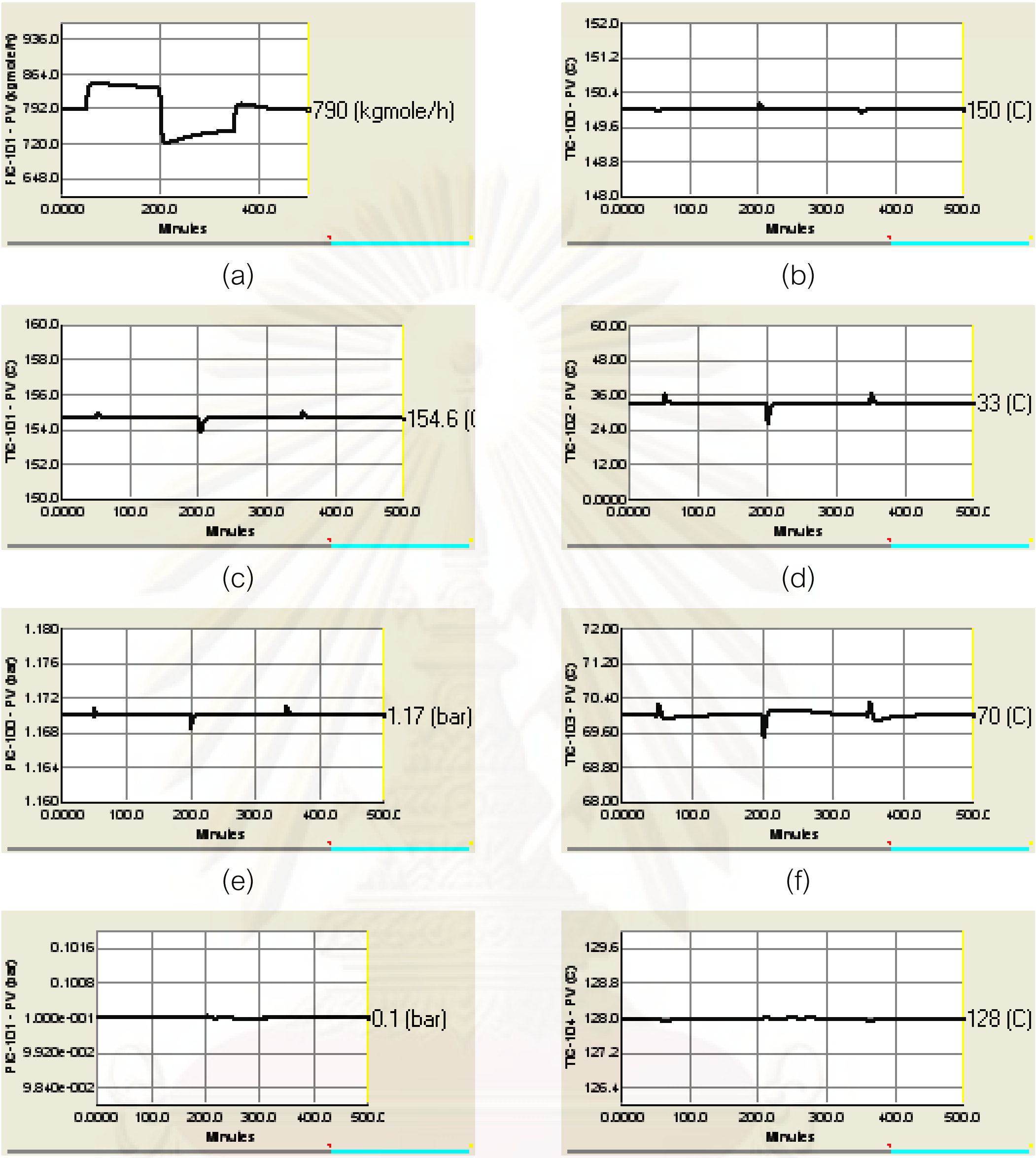
(aa) (ab)

(ac) (ad)

(ae) (af)

(ag)

Figure 5.11 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow



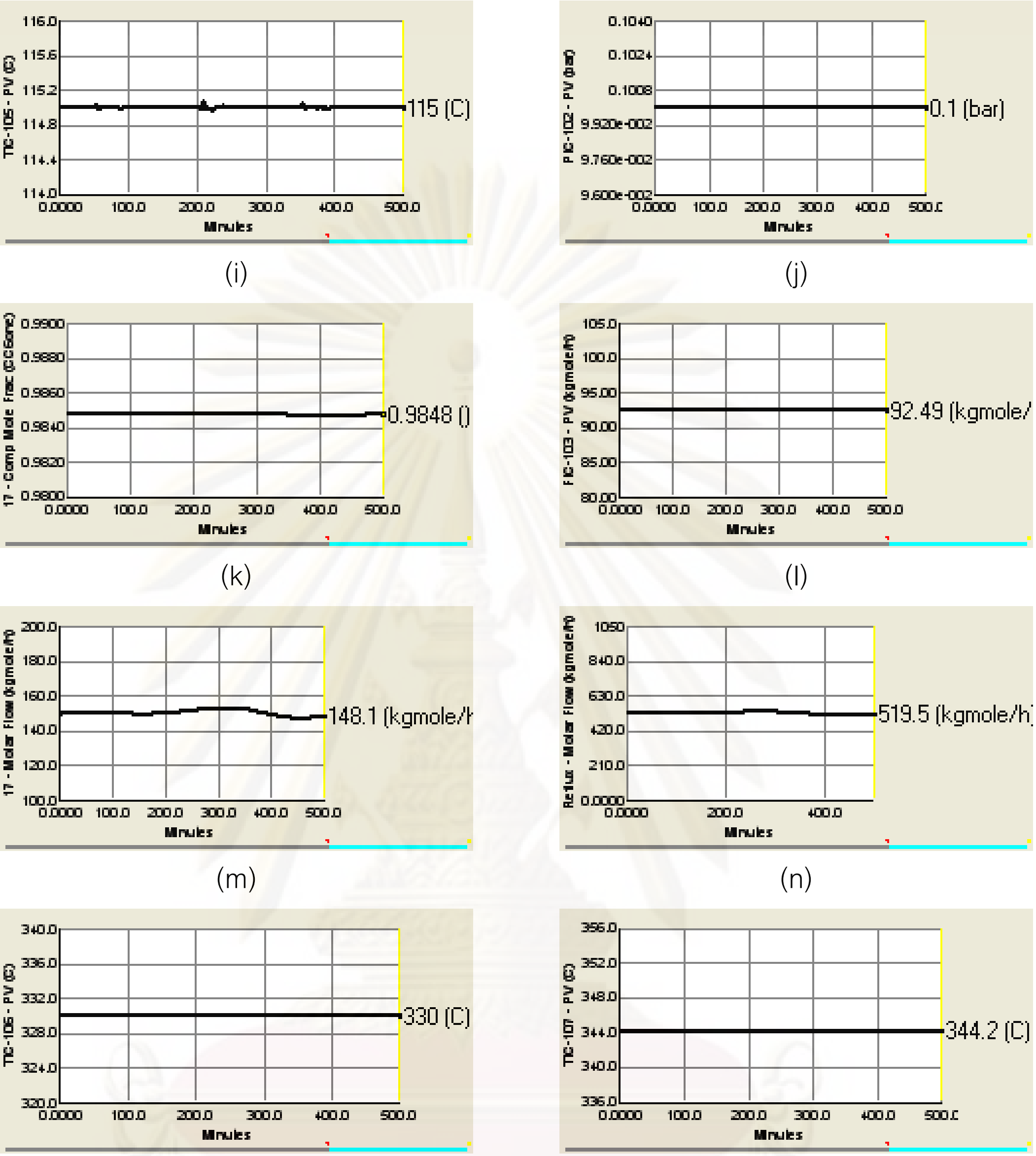
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.12 Dynamic responses of CS4 when change in phenol (fresh + recycled flow): (a) hydrogen (fresh + recycle) flow, (b) hydrogenation reactor inlet temperature, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature



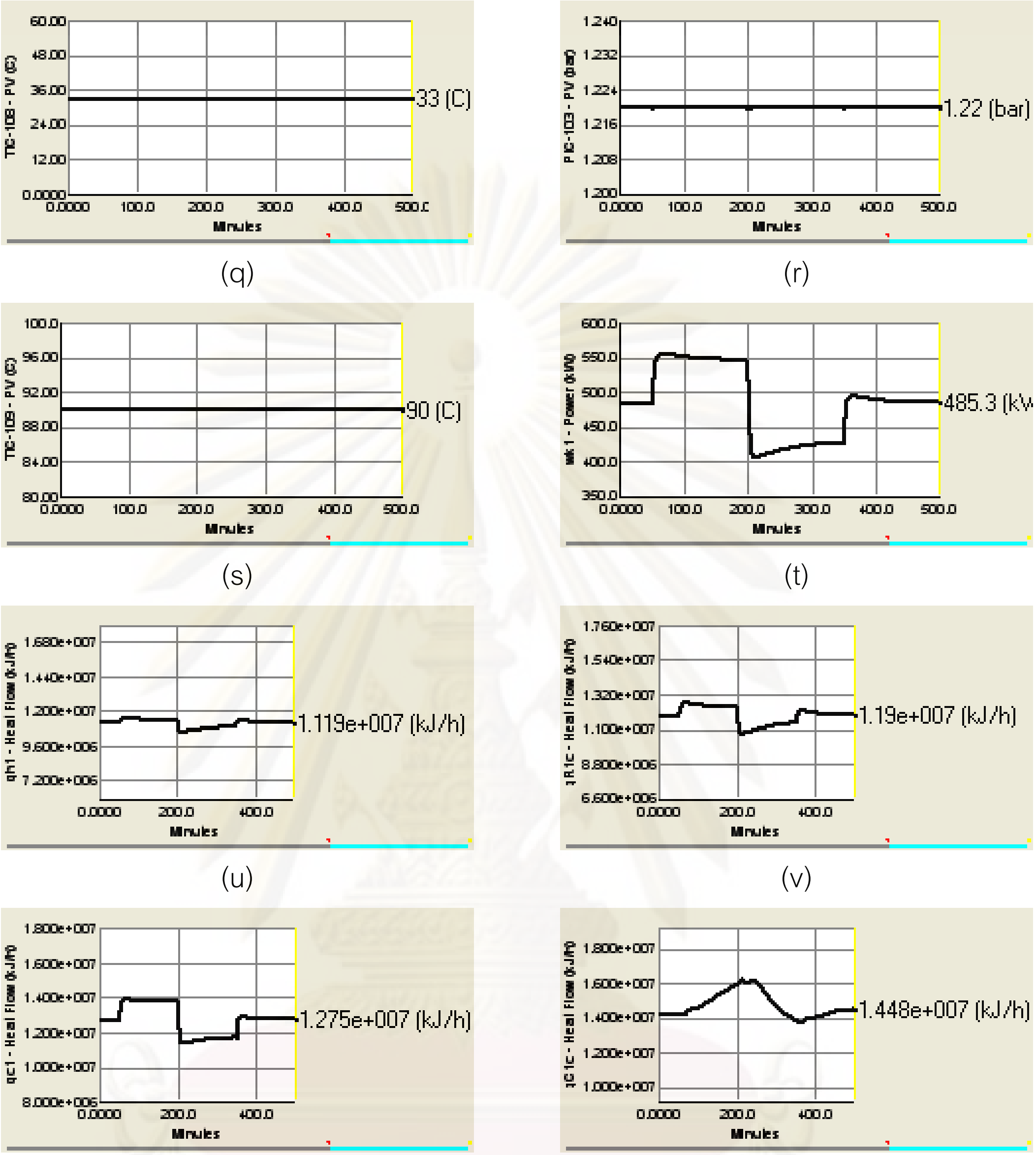
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.12 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



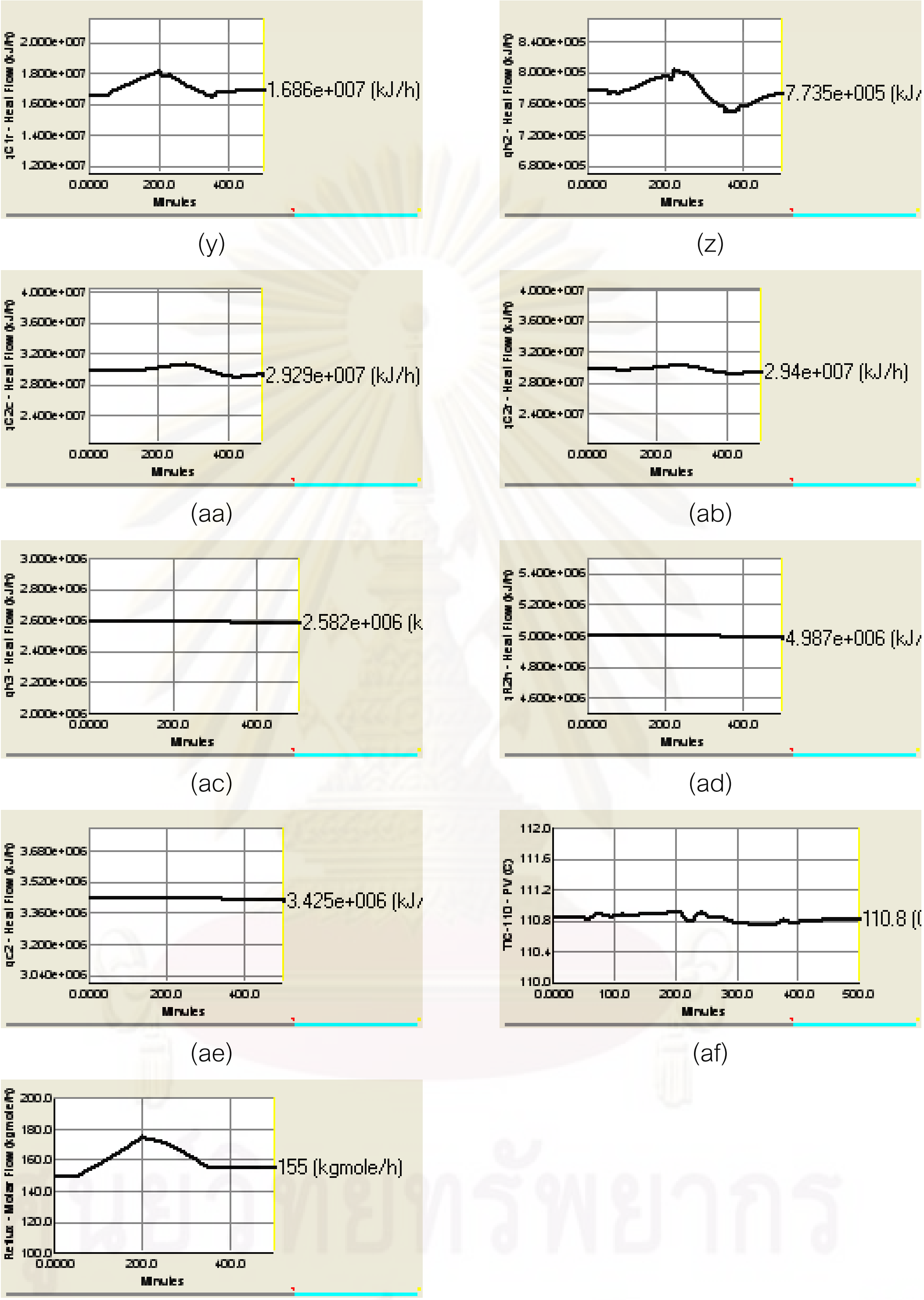
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.12 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

(aa) (ab)

(ac) (ad)

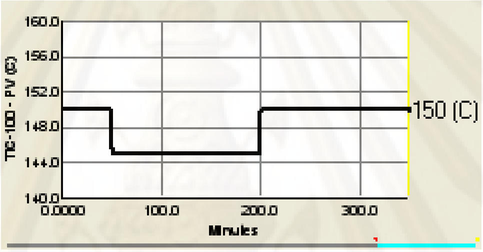
(ae) (af)

(ag)

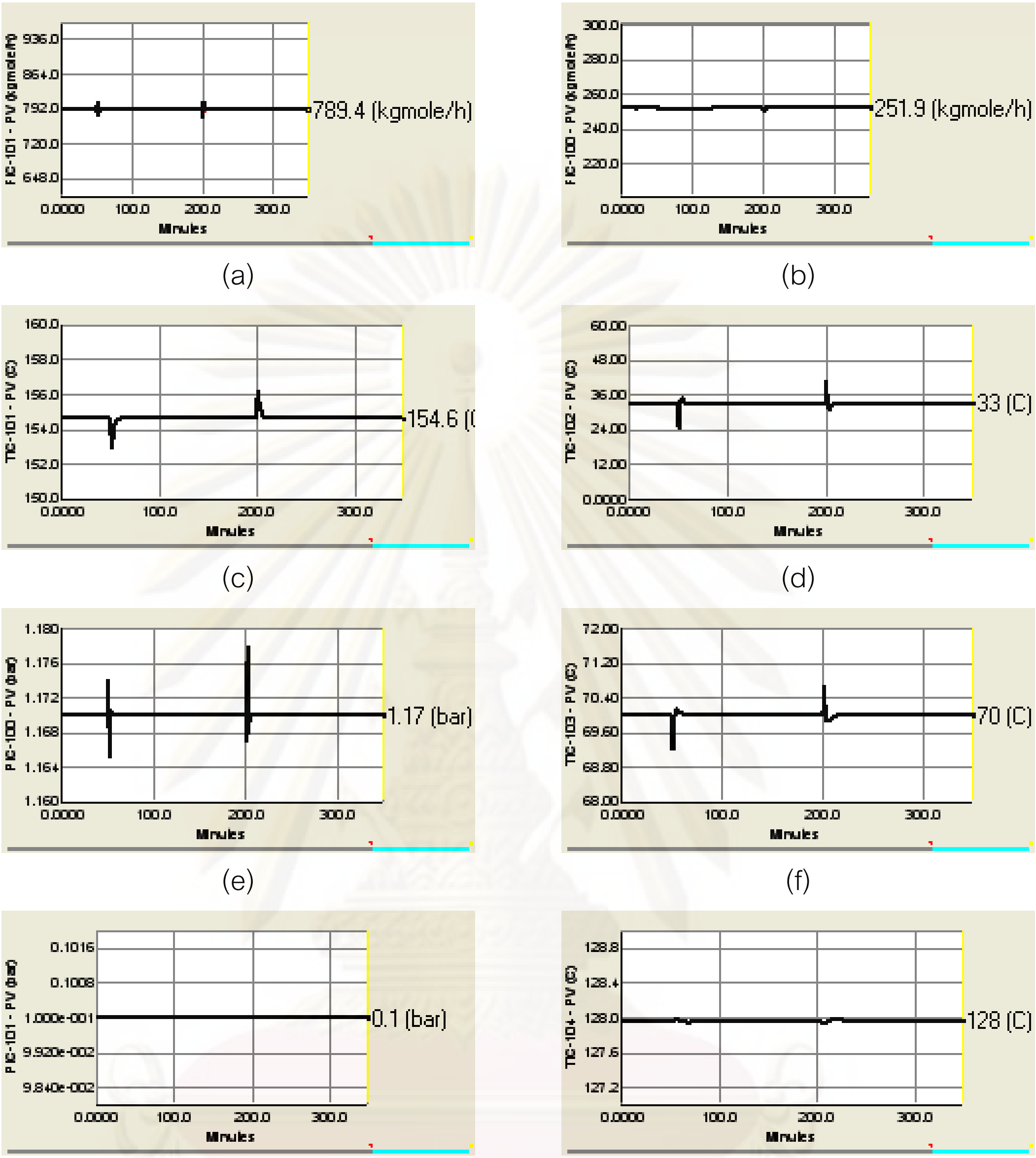
Figure 5.12 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow

5.4.2 Change in hydrogenation reactor inlet temperature

Figure 5.13 to 5.16 show the dynamic response of the phenol hydrogenation to cyclohexanone process in the thermal disturbance of hydrogenation reactor inlet temperature. The disturbance made as follows: The inlet temperature is decreased from 150 °C to 145 °C at time equals 50 minutes and return to its set point at time equals 200 minutes. Increased inlet temperature is not tested in the work because it is sensitive to the hydrogenation reactions. The hydrogenation reactor will run out of control when the inlet temperature is increased.



In all control structures give the same trend result to reject thermal disturbance which can reject disturbance and return to their set point as shown in the figures. From considering graphs, all process constraint variables are achieved when this thermal disturbance occur in all designed control structure.



(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.13 Dynamic responses of CS1 when change in hydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycled) flow, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature

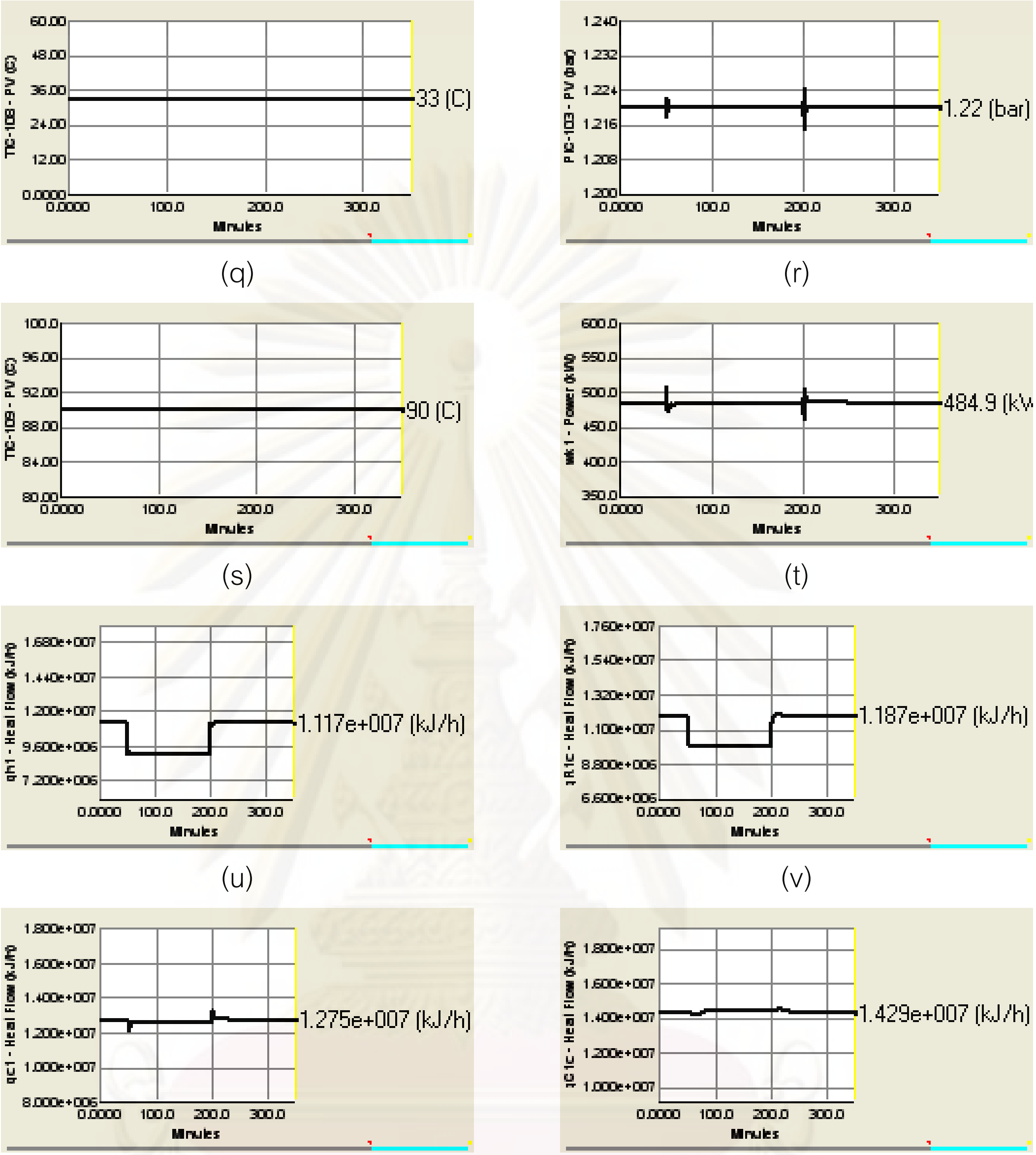
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.13 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



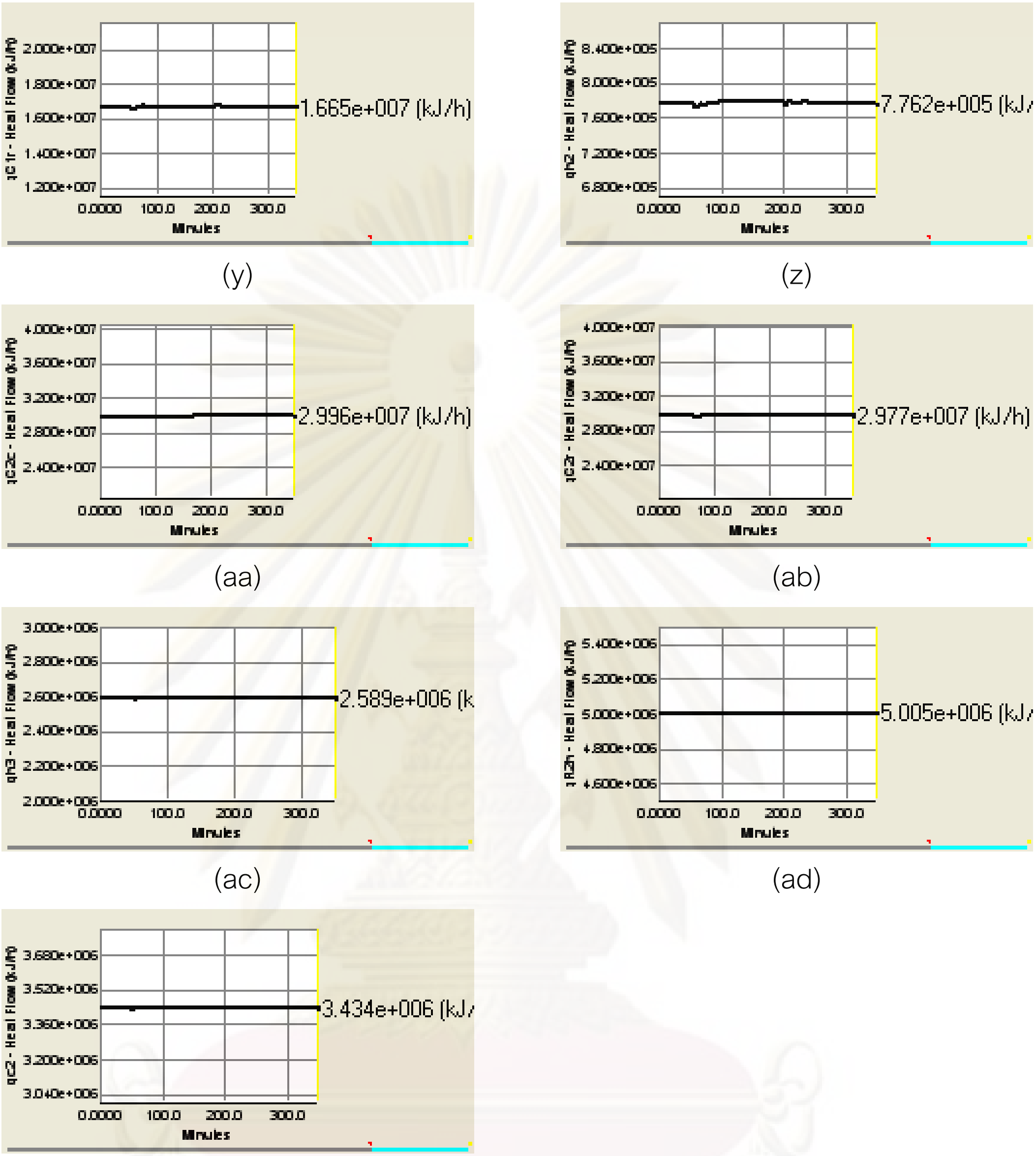
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.13 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



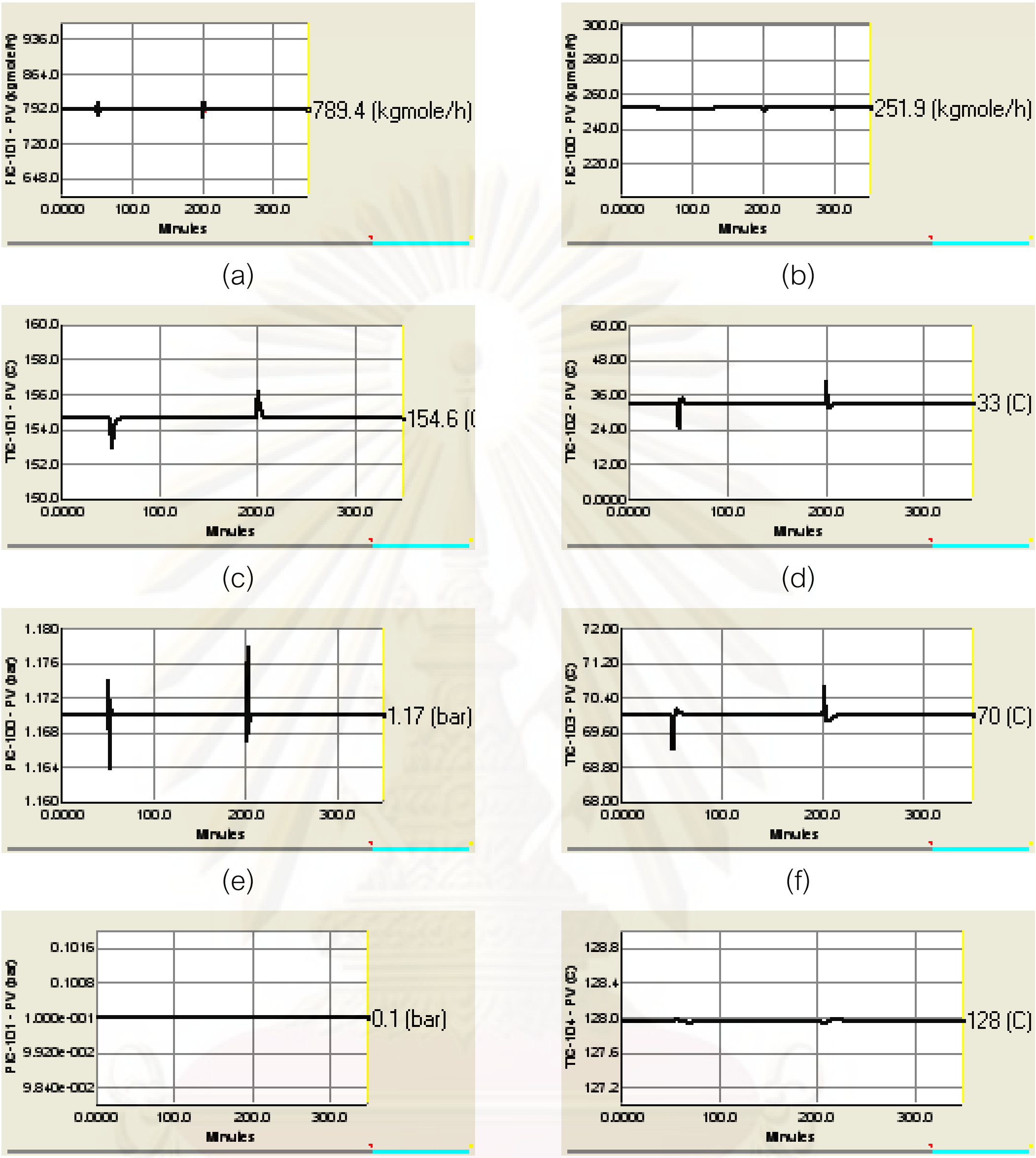
(y) (z)

(aa) (ab)

(ac) (ad)

(ae)

Figure 5.13 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.14 Dynamic responses of CS2 when change in hydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycled) flow, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature

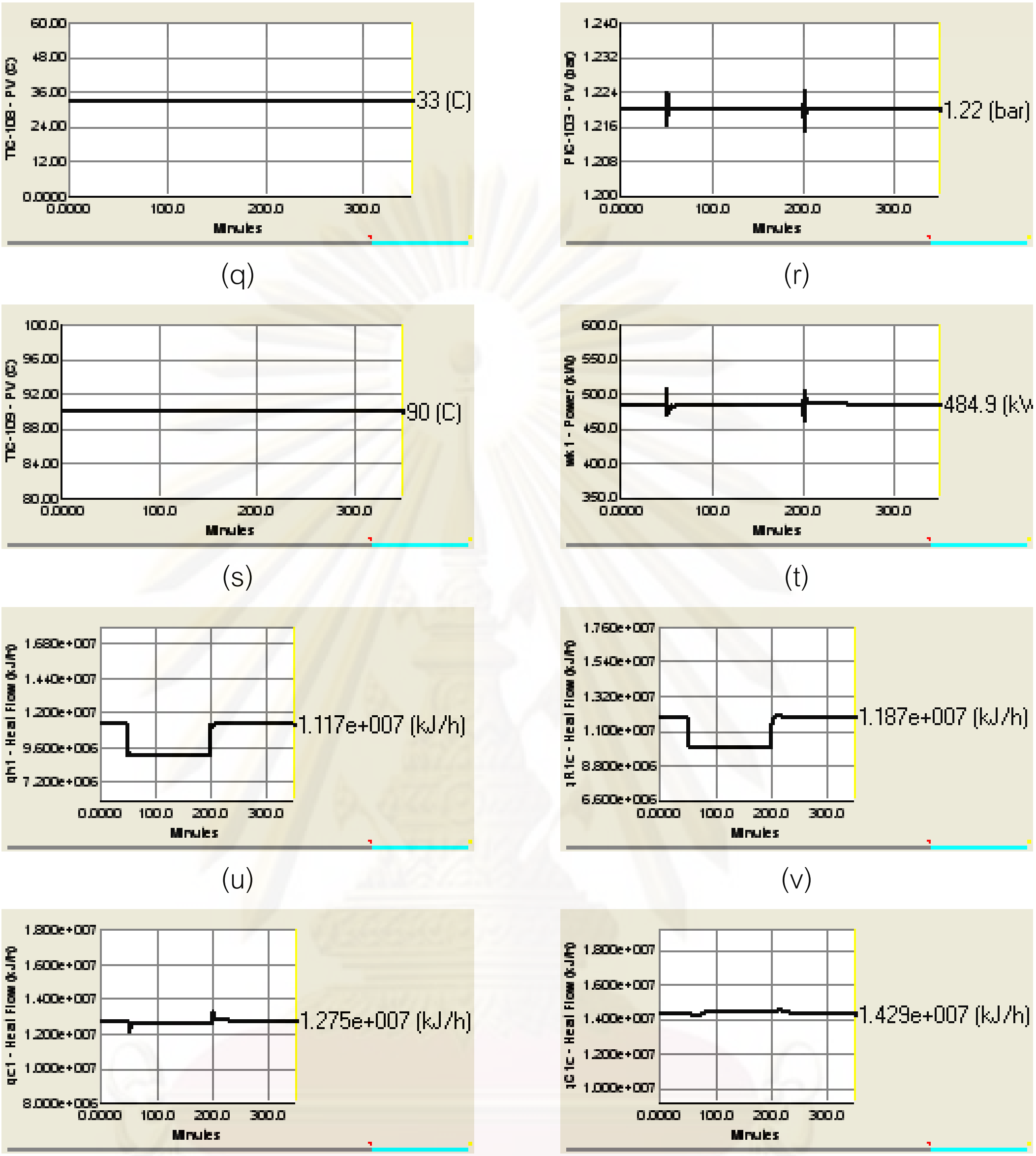
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.14 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



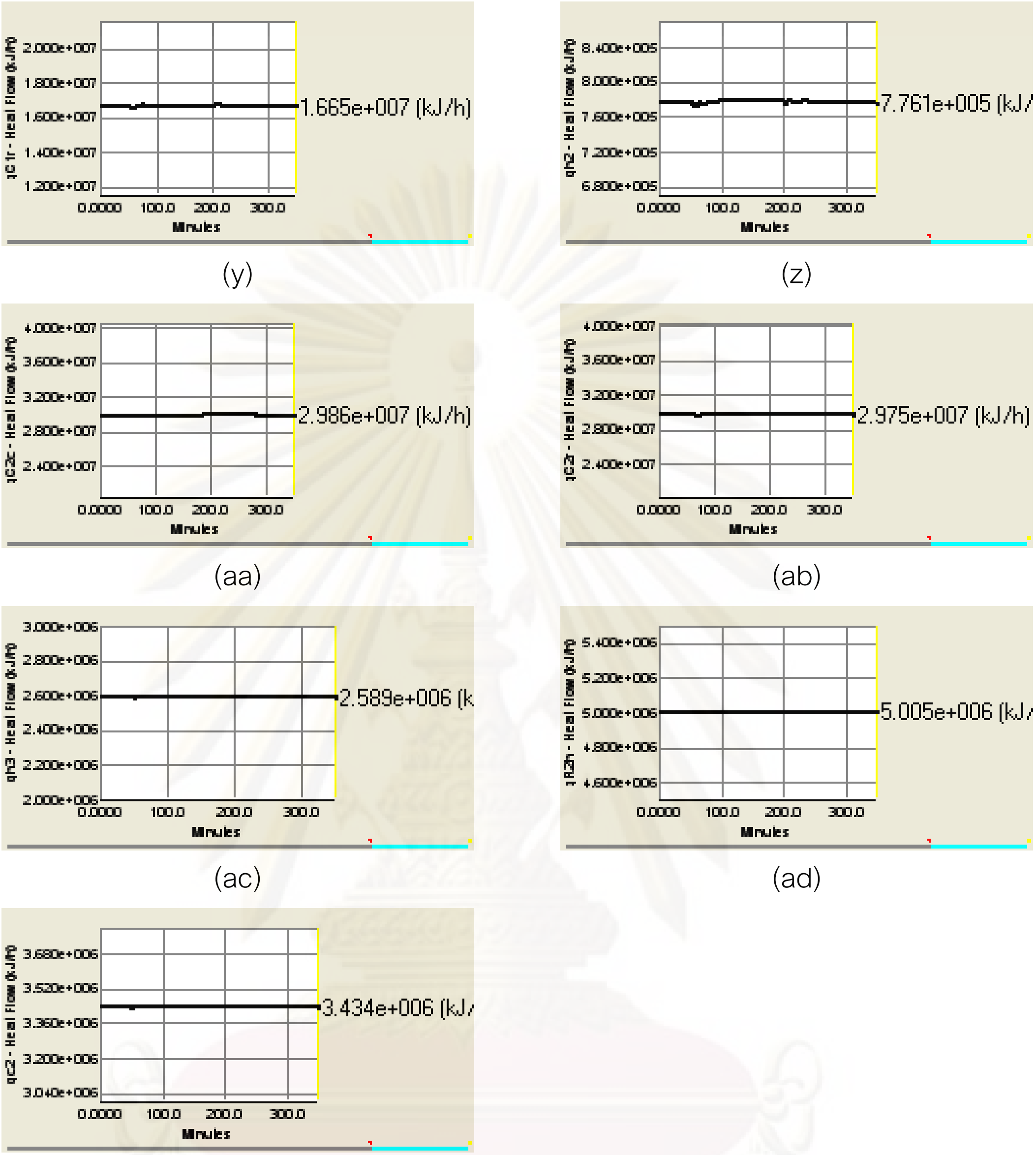
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.14 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



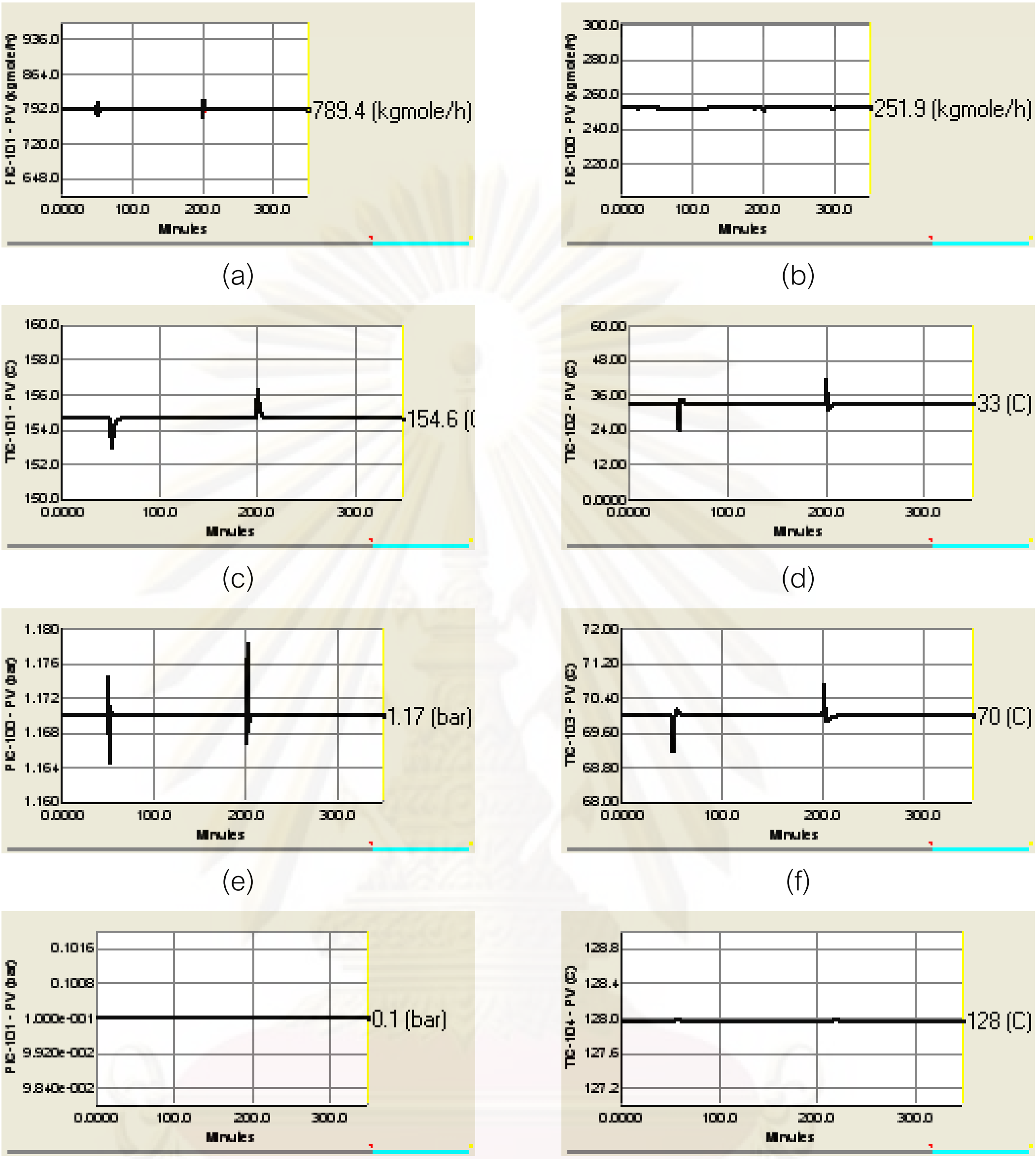
(y) (z)

(aa) (ab)

(ac) (ad)

(ae)

Figures 5.14 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.15 Dynamic responses of CS3 when change in hydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycled) flow, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature

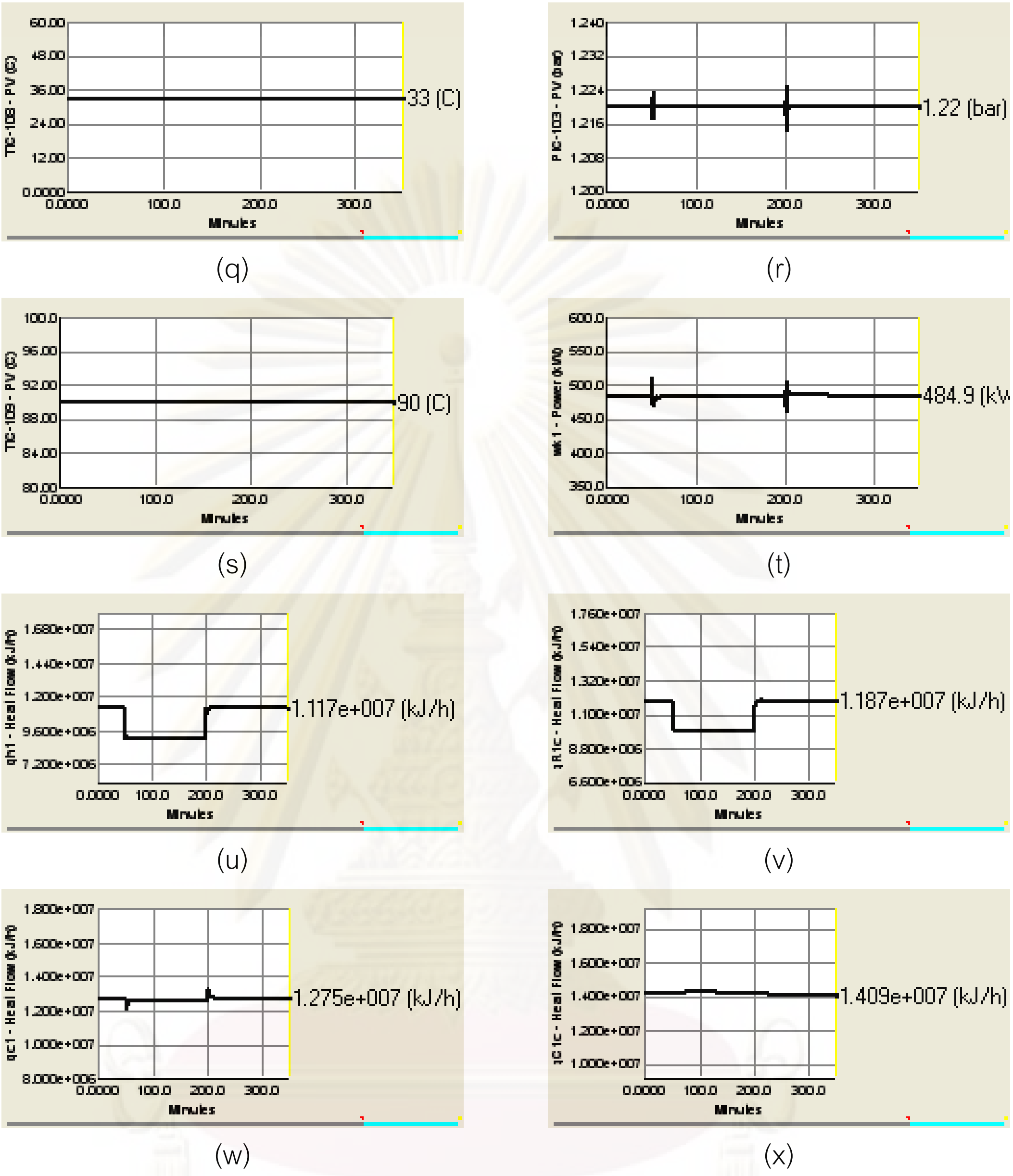
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.15 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



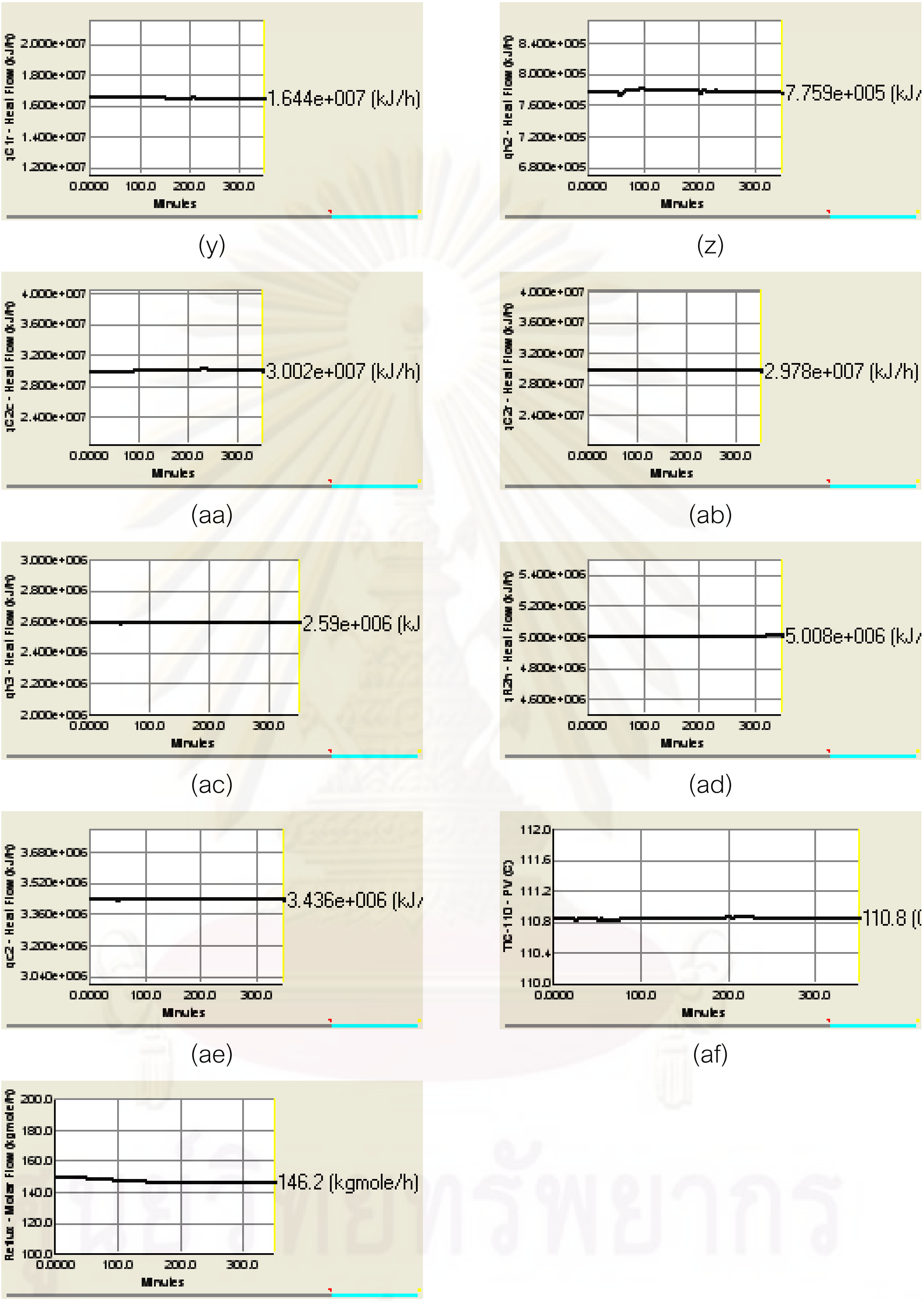
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.15 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

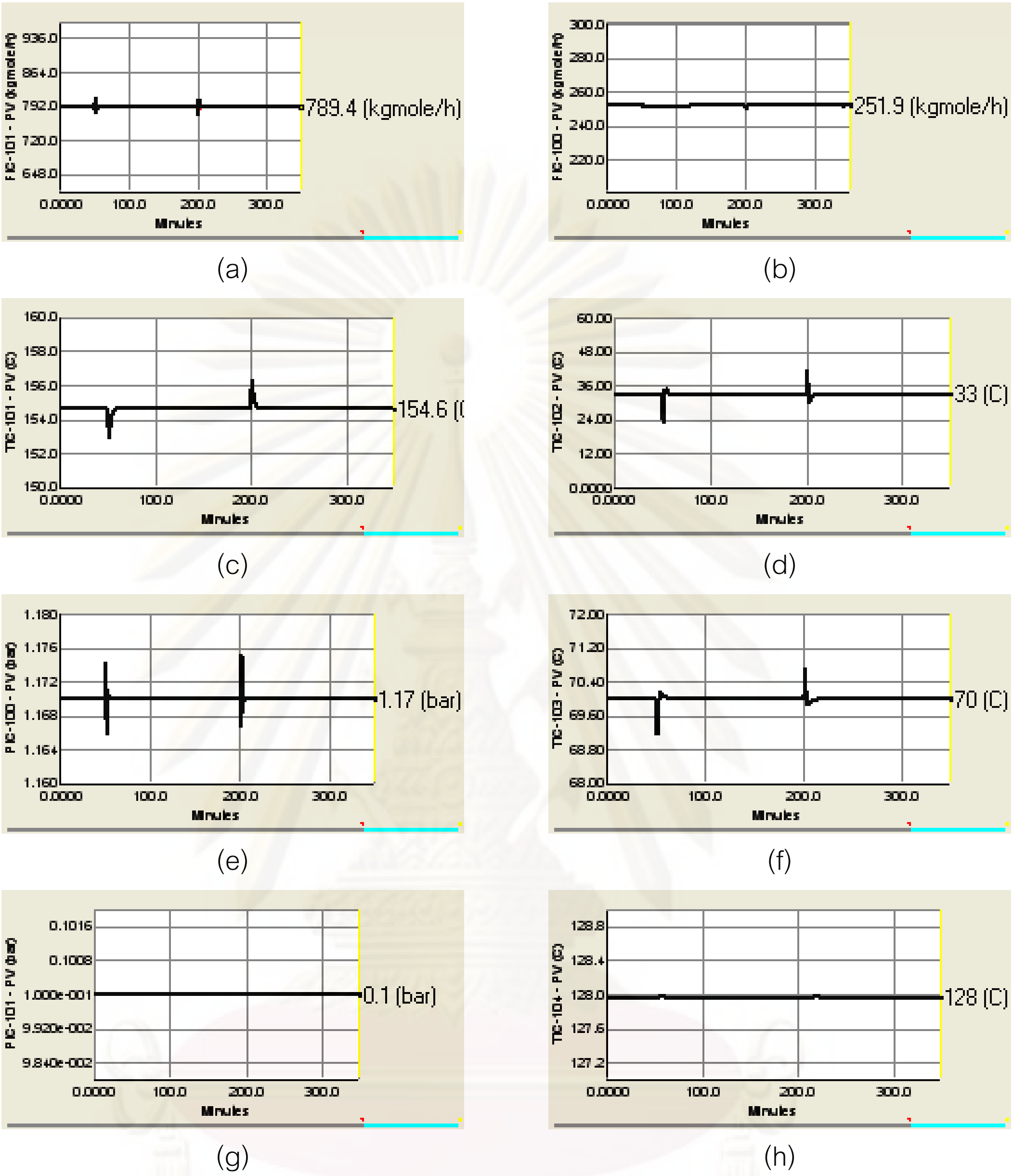
(aa) (ab)

(ac) (ad)

(ae) (af)

(ag)

Figure 5.15 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow



(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.16 Dynamic responses of CS4 when change in hydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycled) flow, (c) hydrogenation reactor temperature at 1 m length, (d) separator V-100 inlet temperature, (e) separator V-100 pressure, (f) phenol recycle column feed temperature, (g) phenol recycle column – condenser pressure, (h) phenol recycle column – stage 21 temperature

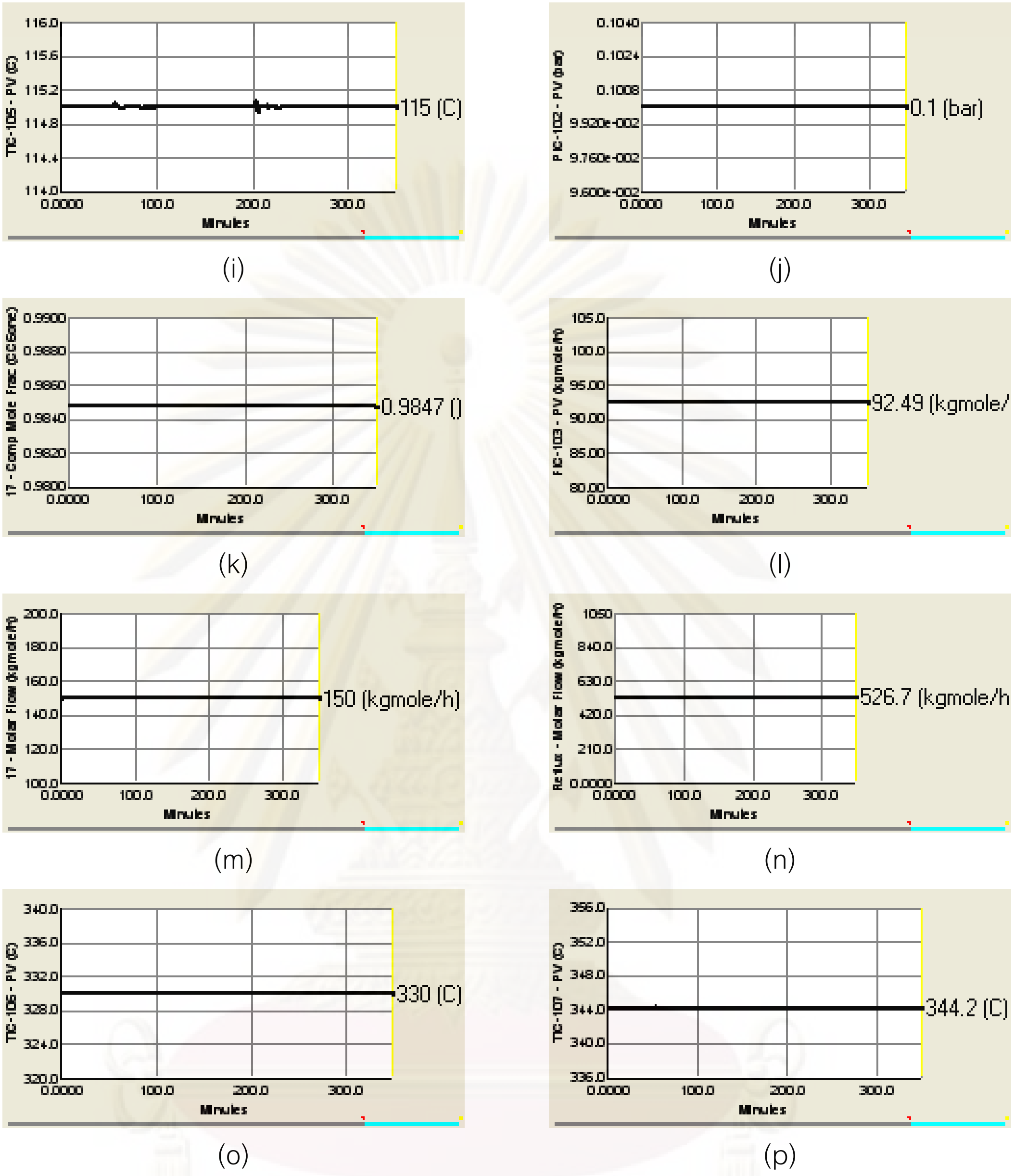
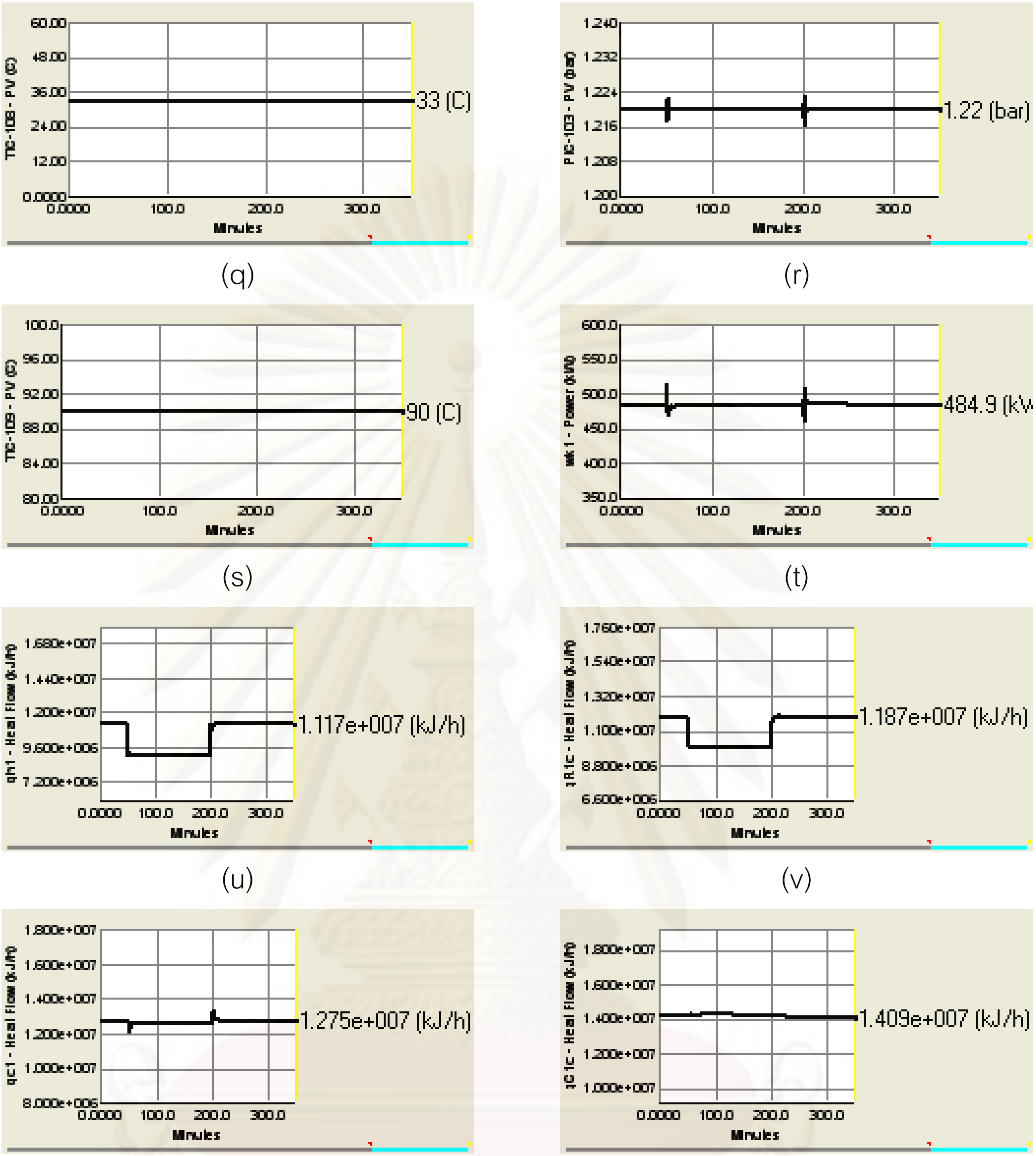


Figure 5.16 (Cont.) (i) cyclohexanone column feed temperature, (j) cyclohexanone column – condenser pressure, (k) cyclohexanol product composition, (l) cyclohexanone column – bottom flow, (m) cyclohexanone production flowrate, (n) cyclohexanone column – reflux flow (o) dehydrogenation reactor inlet temperature, (p) dehydrogenation reactor outlet temperature



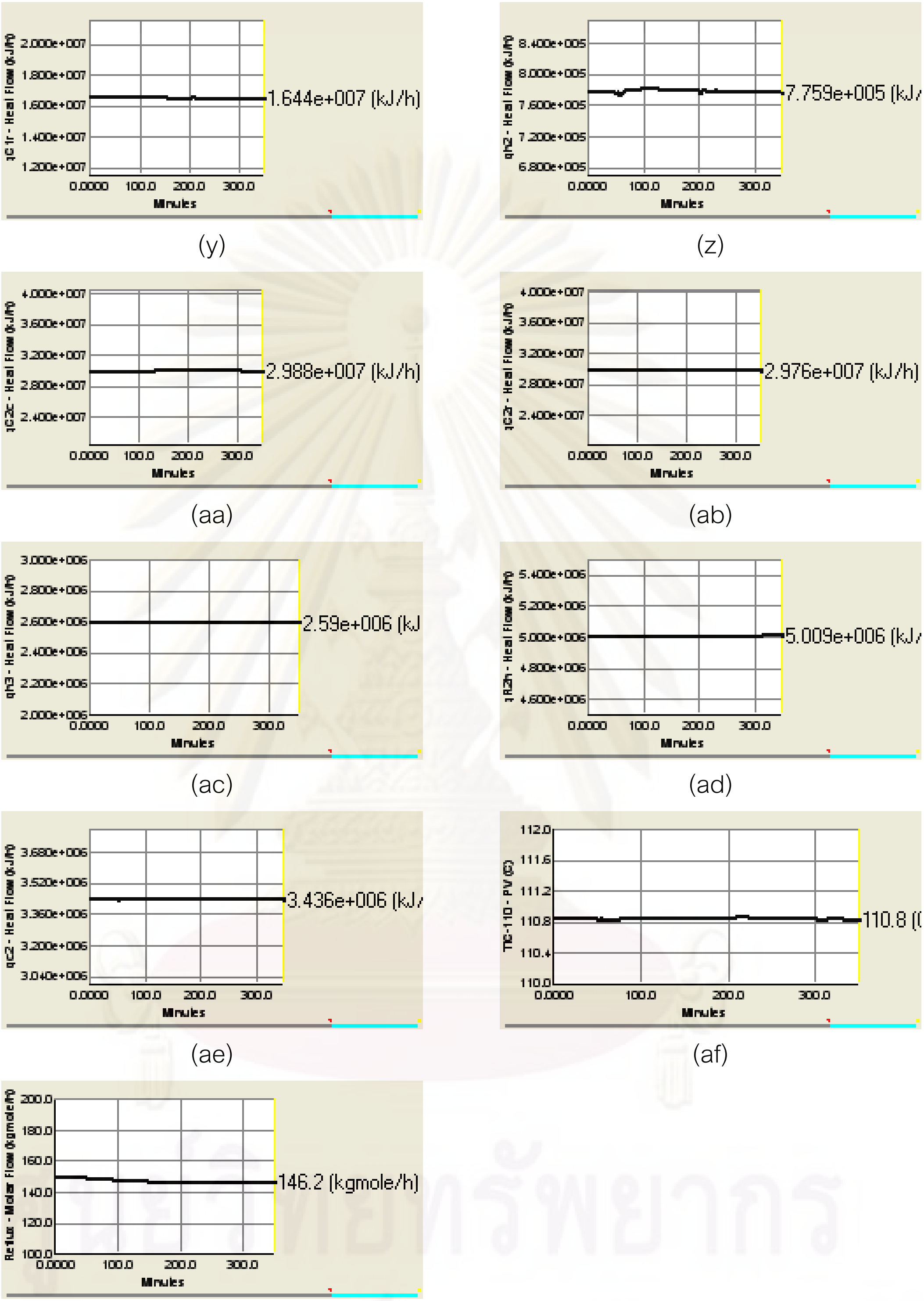
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.16 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

(aa) (ab)

(ac) (ad)

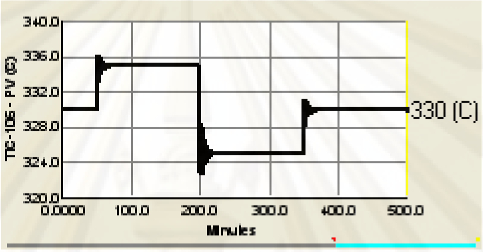
(ae) (af)

(ag)

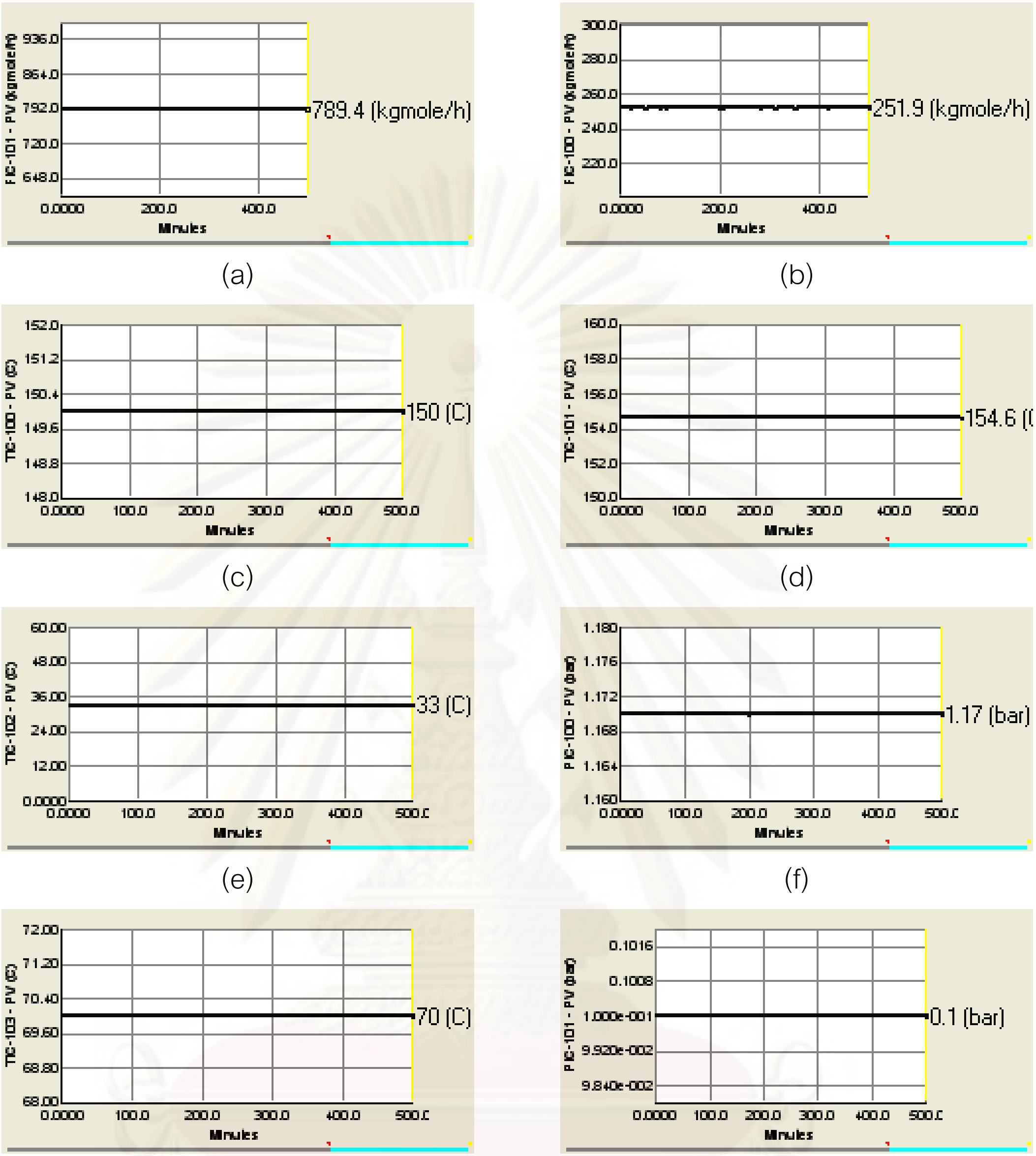
Figure 5.16 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow

5.4.3 Change in dehydrogenation reactor inlet temperature

Figure 5.17 to 5.20 show the dynamic response of the phenol hydrogenation to cyclohexanone process in the thermal disturbance of dehydrogenation reactor inlet temperature. The disturbance made as follows: The inlet temperature is increased from 330 °C to 335 °C at time equals 50 minutes and decreased from 335 °C to 325 °C at time equals 200 minutes and then return to its set point at time equals 350 minutes.



In all control structures give the same trend result to reject thermal disturbance which can reject disturbance and return to their set point as shown in the figures. From all graphs of hydrogenation section, we can notice that the thermal disturbance in dehydrogenation section does not much effect to hydrogenation section since the effect of this disturbance is passed to hydrogenation section by small hydrogen recycle stream which can eliminate intermediately using total hydrogen (fresh + recycle) flow rate controller. Besides, all process constraint variables are achieved when this thermal disturbance occur in all designed control structure.



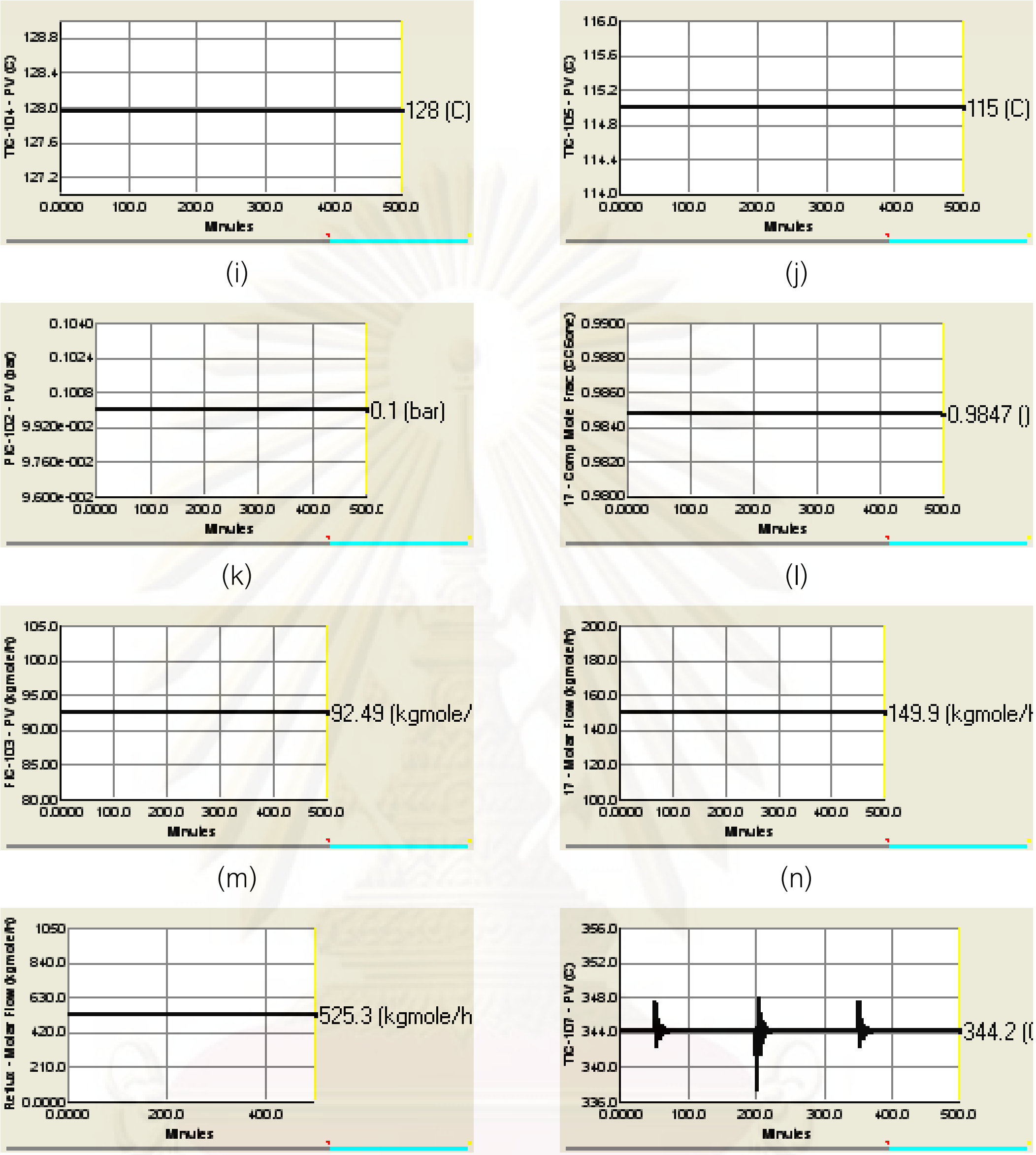
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.17 Dynamic responses of CS1 when change in dehydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycle) flow (c) hydrogenation reactor inlet temperature, (d) hydrogenation reactor temperature at 1 m length, (e) separator V-100 inlet temperature, (f) separator V-100 pressure, (g) phenol recycle column feed temperature, (h) phenol recycle column – condenser pressure



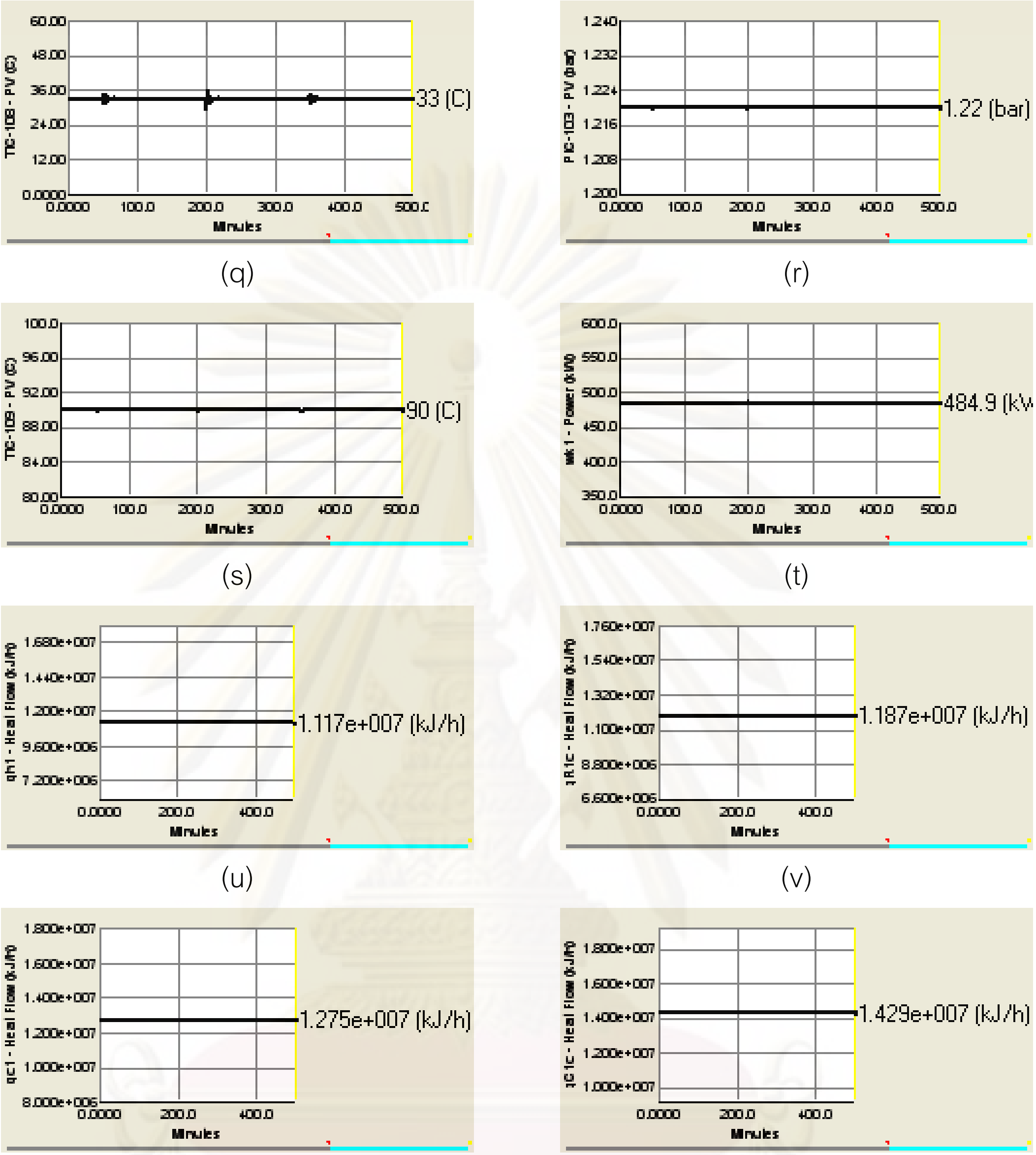
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.17 (Cont.) (i) phenol recycle column – stage 21 temperature, (j) cyclohexanone column feed temperature, (k) cyclohexanone column – condenser pressure, (l) cyclohexanol product composition, (m) cyclohexanone column – bottom flow, (n) cyclohexanone production flowrate, (o) cyclohexanone column – reflux flow, (p) dehydrogenation reactor outlet temperature



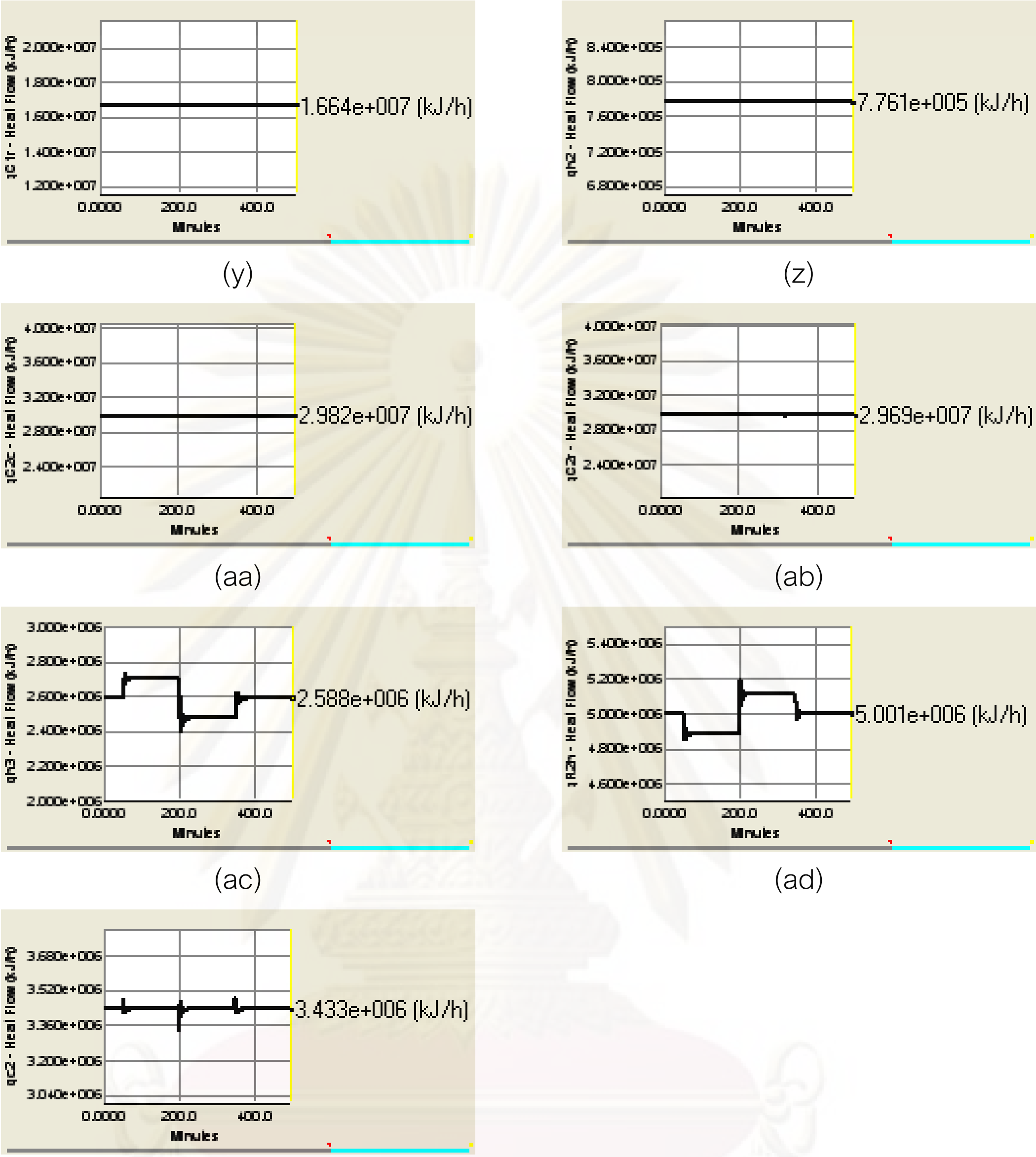
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.17 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



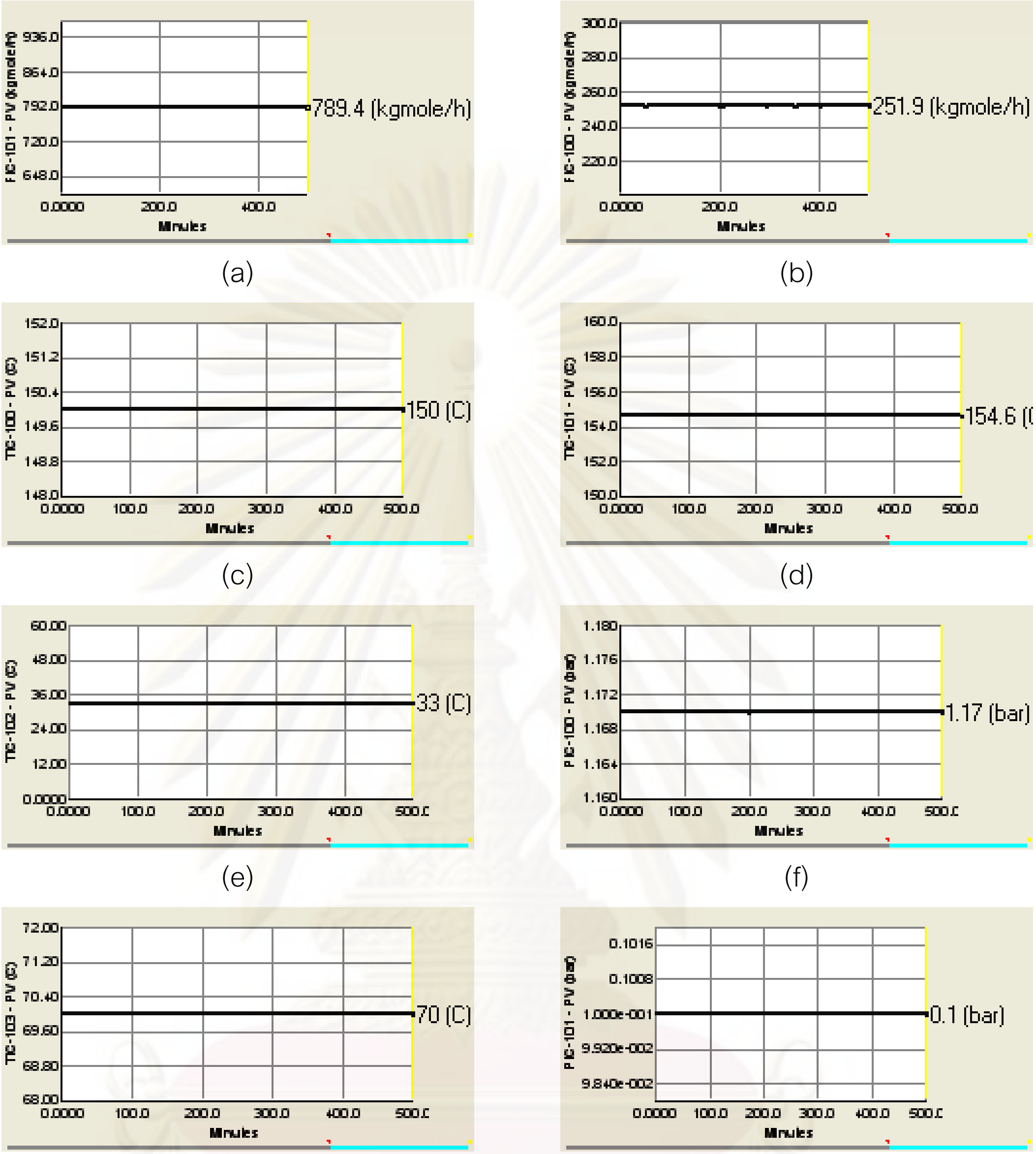
(y) (z)

(aa) (ab)

(ac) (ad)

(ae)

Figure 5.17 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



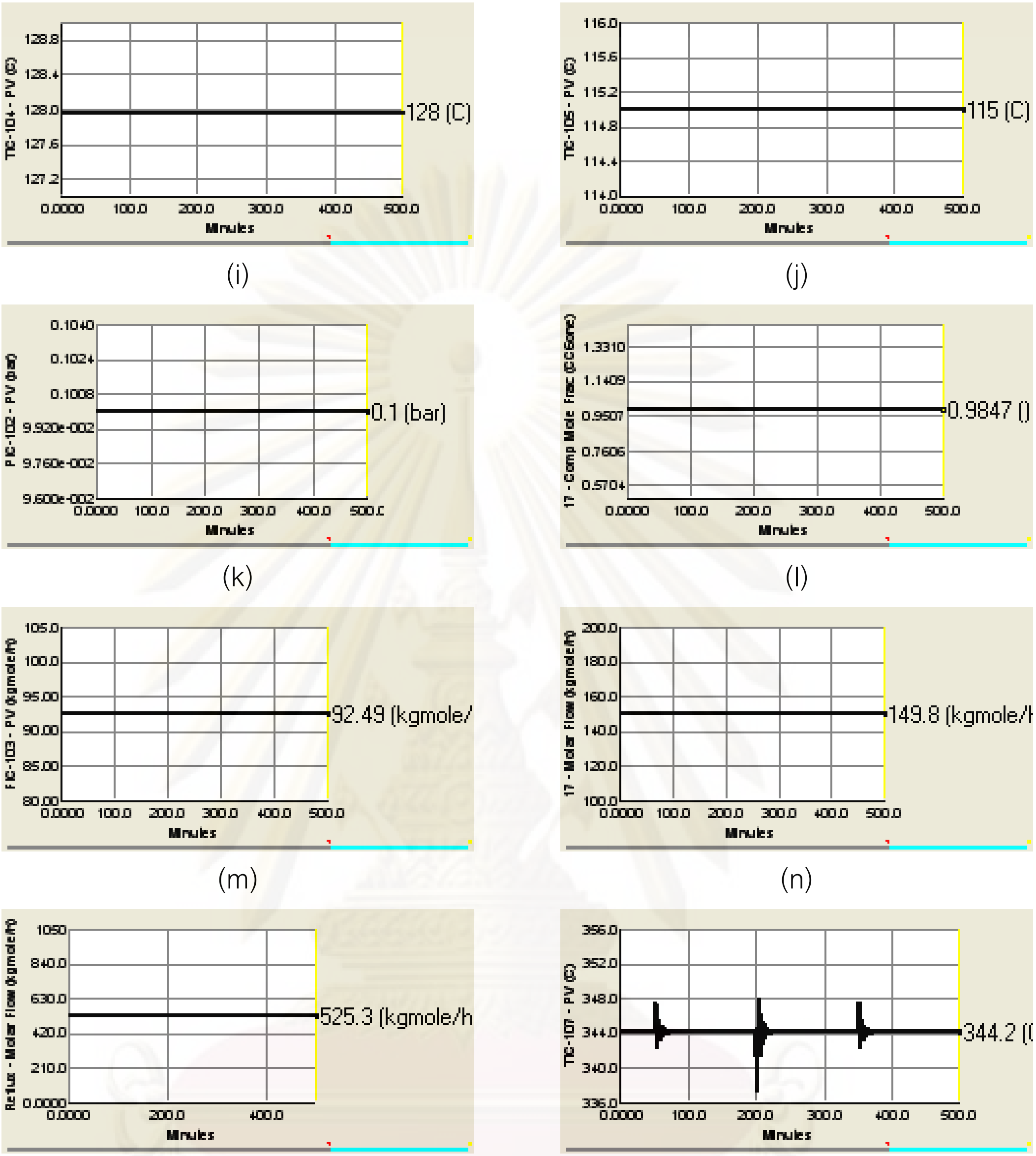
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.18 Dynamic responses of CS2 when change in dehydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycle) flow (c) hydrogenation reactor inlet temperature, (d) hydrogenation reactor temperature at 1 m length, (e) separator V-100 inlet temperature, (f) separator V-100 pressure, (g) phenol recycle column feed temperature, (h) phenol recycle column – condenser pressure



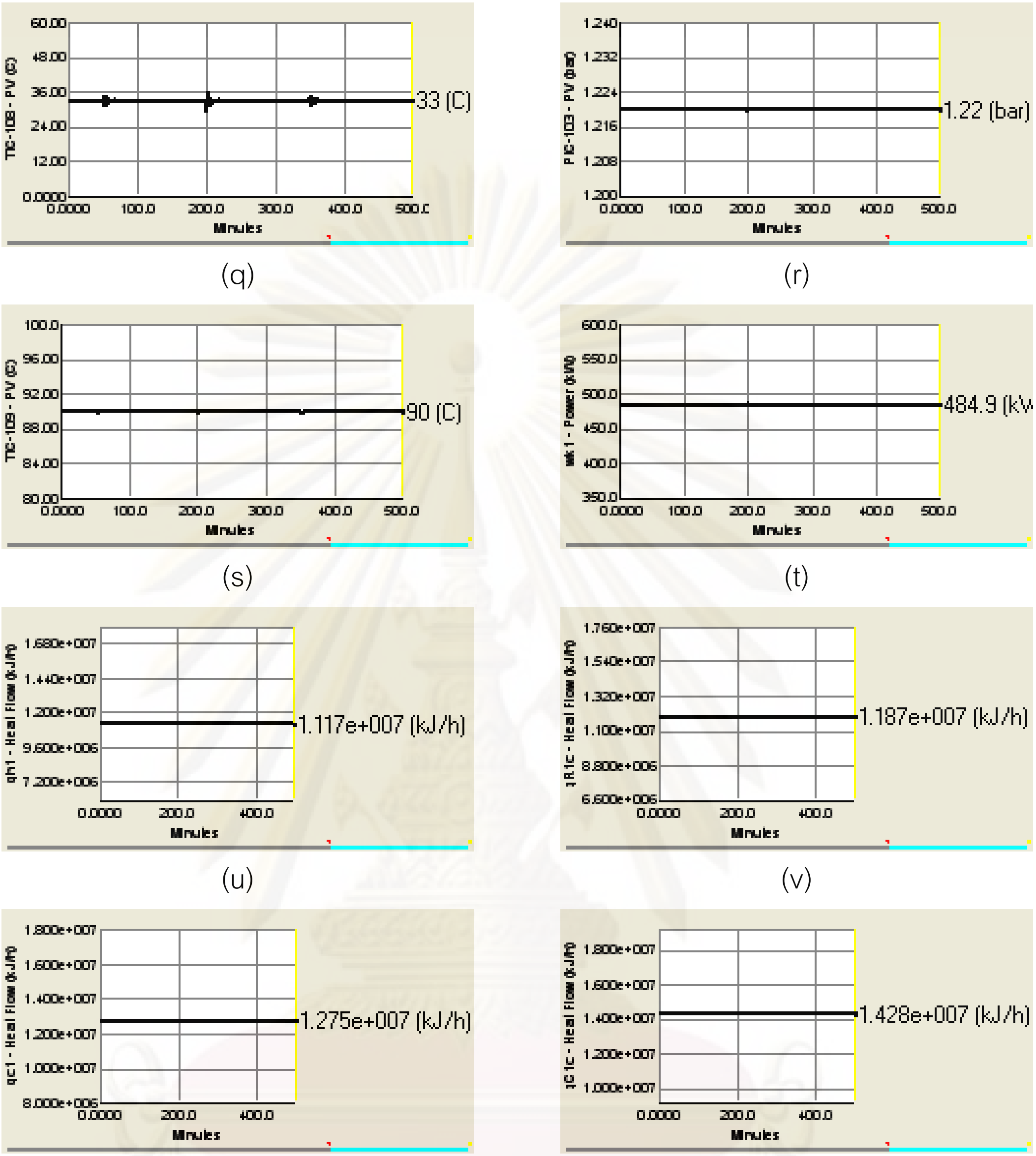
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.18 (Cont.) (i) phenol recycle column – stage 21 temperature, (j) cyclohexanone column feed temperature, (k) cyclohexanone column – condenser pressure, (l) cyclohexanol product composition, (m) cyclohexanone column – bottom flow, (n) cyclohexanone production flowrate, (o) cyclohexanone column – reflux flow, (p) dehydrogenation reactor outlet temperature



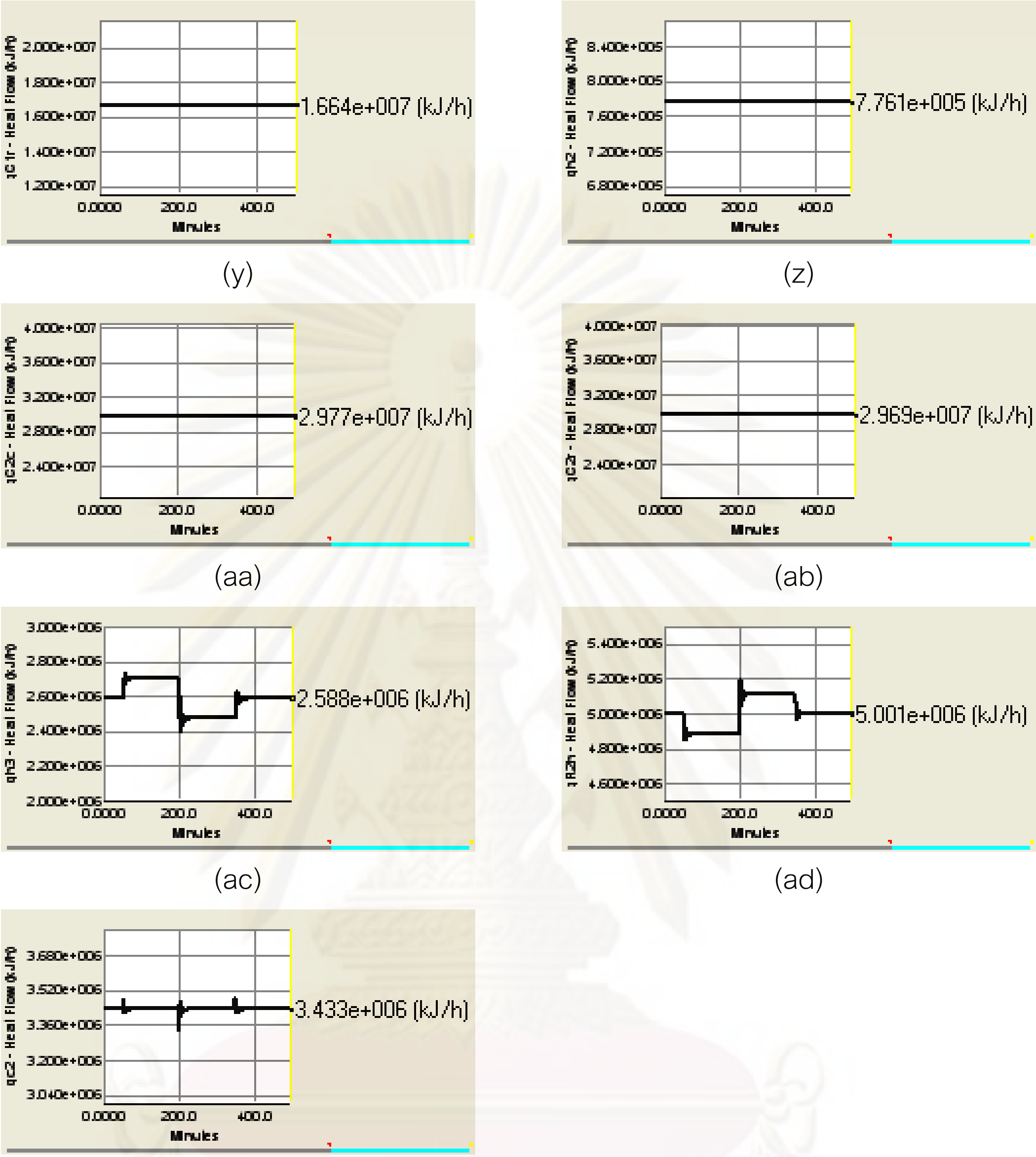
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.18 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



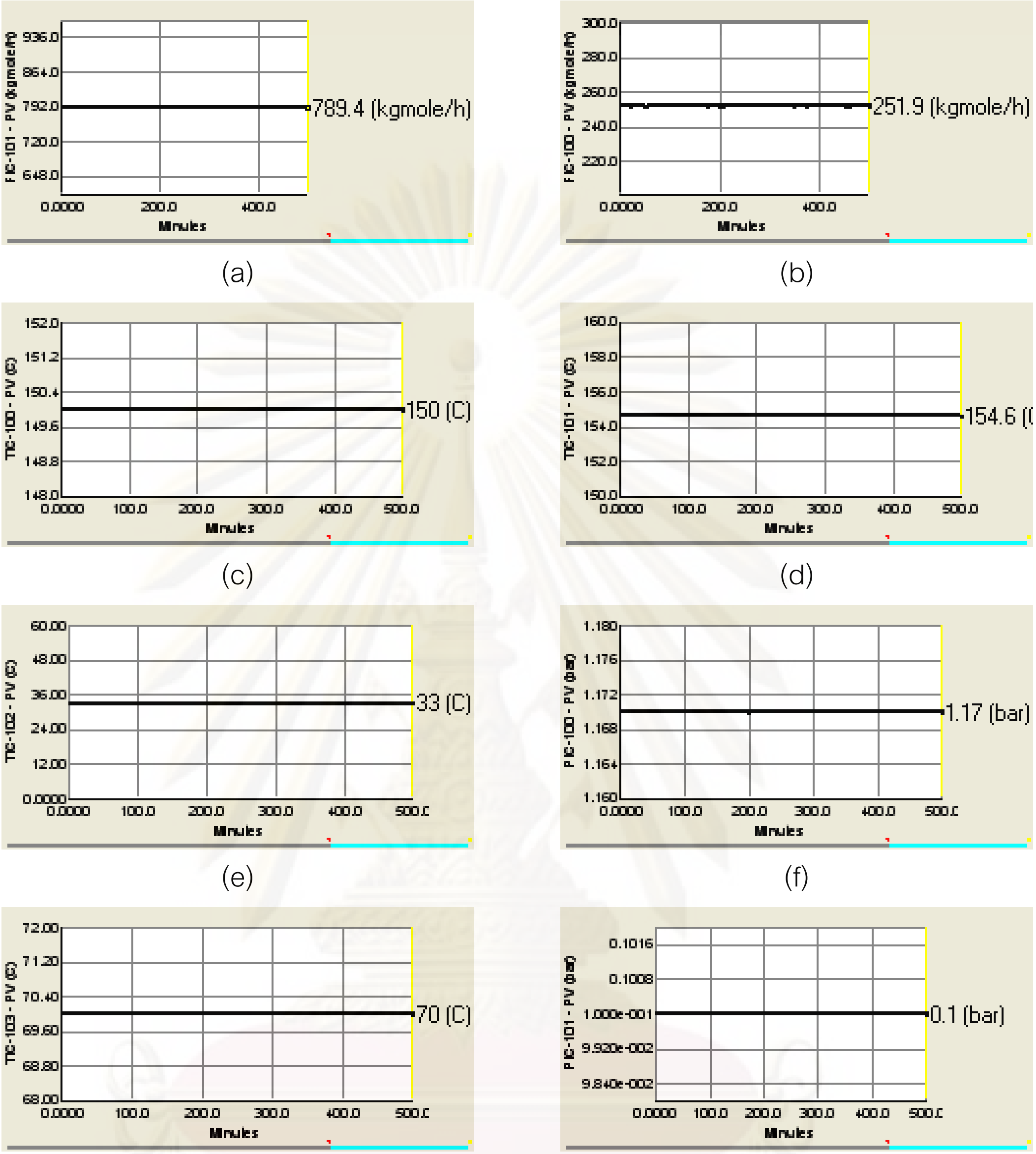
(y) (z)

(aa) (ab)

(ac) (ad)

(ae)

Figures 5.18 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2



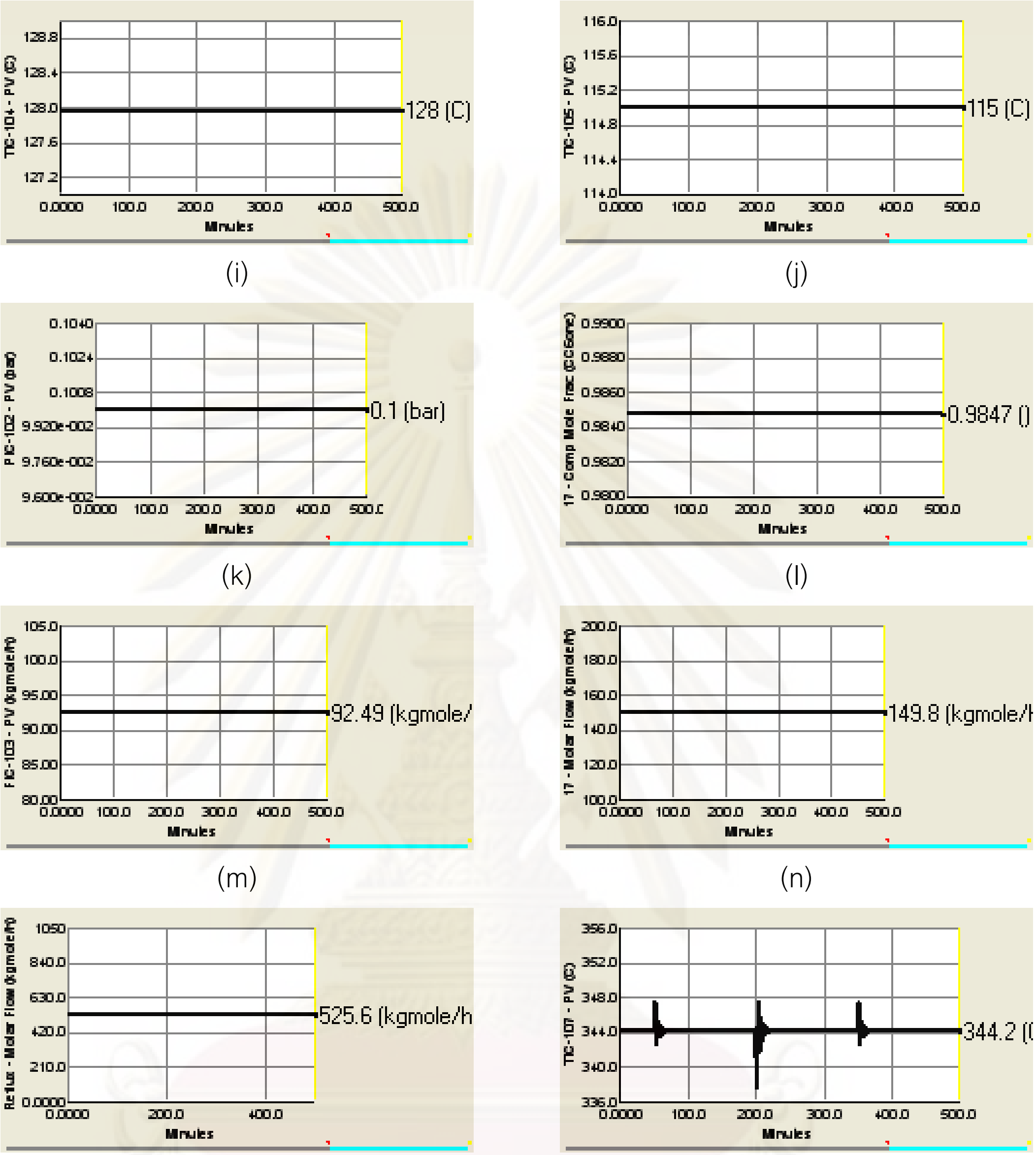
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.19 Dynamic responses of CS3 when change in dehydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycle) flow (c) hydrogenation reactor inlet temperature, (d) hydrogenation reactor temperature at 1 m length, (e) separator V-100 inlet temperature, (f) separator V-100 pressure, (g) phenol recycle column feed temperature, (h) phenol recycle column – condenser pressure



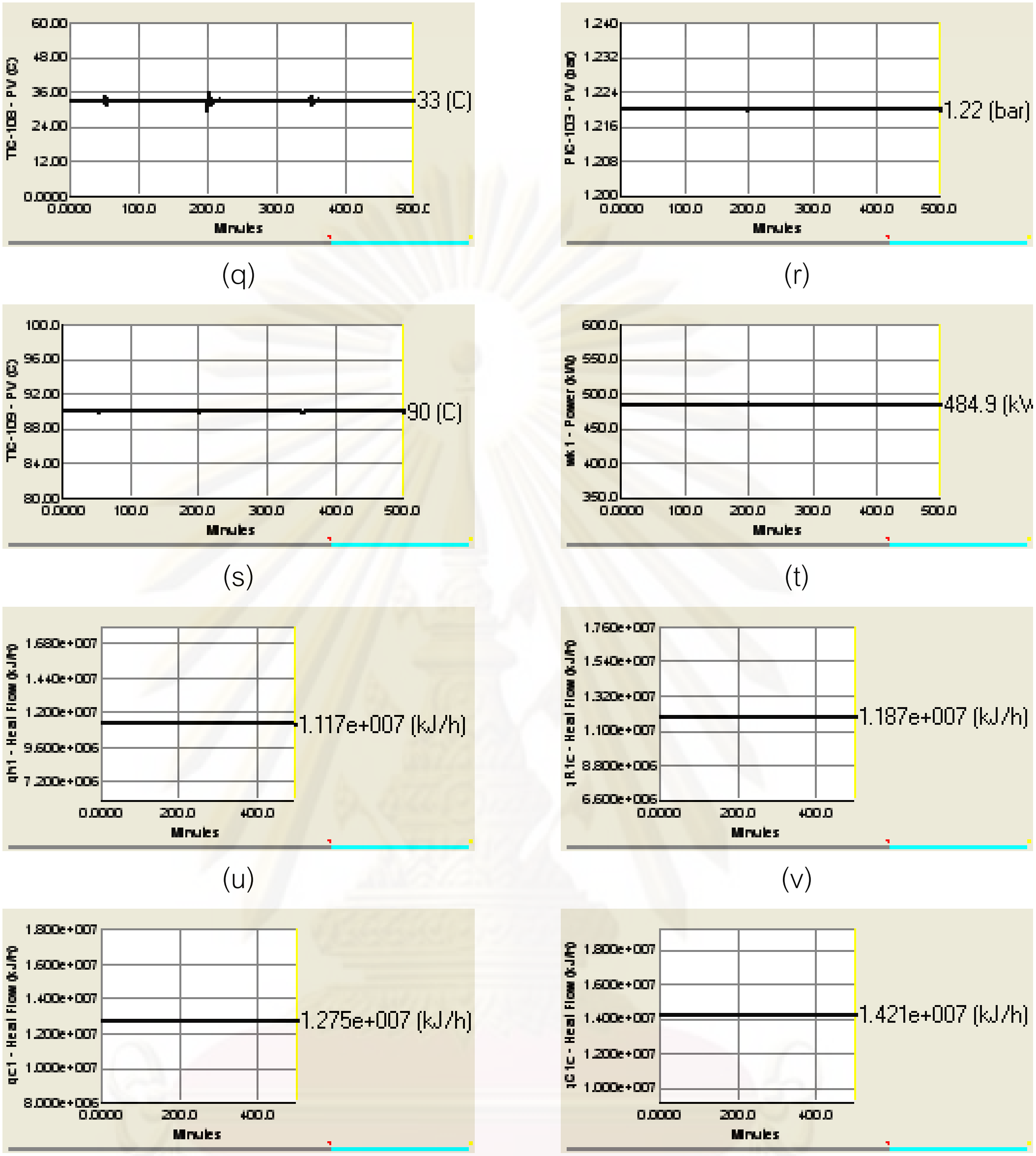
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.19 (Cont.) (i) phenol recycle column – stage 21 temperature, (j) cyclohexanone column feed temperature, (k) cyclohexanone column – condenser pressure, (l) cyclohexanol product composition, (m) cyclohexanone column – bottom flow, (n) cyclohexanone production flowrate, (o) cyclohexanone column – reflux flow, (p) dehydrogenation reactor outlet temperature



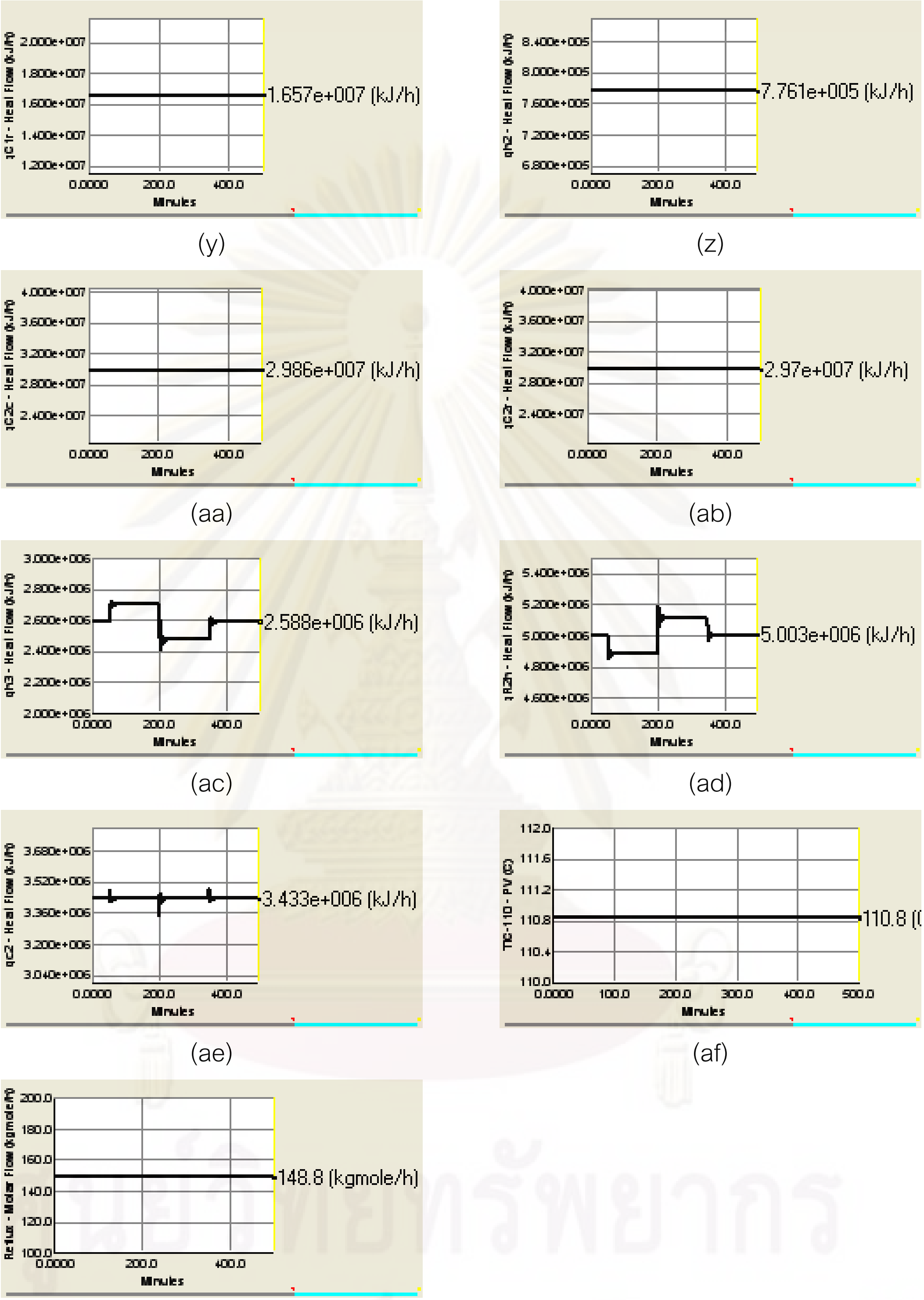
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.19 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

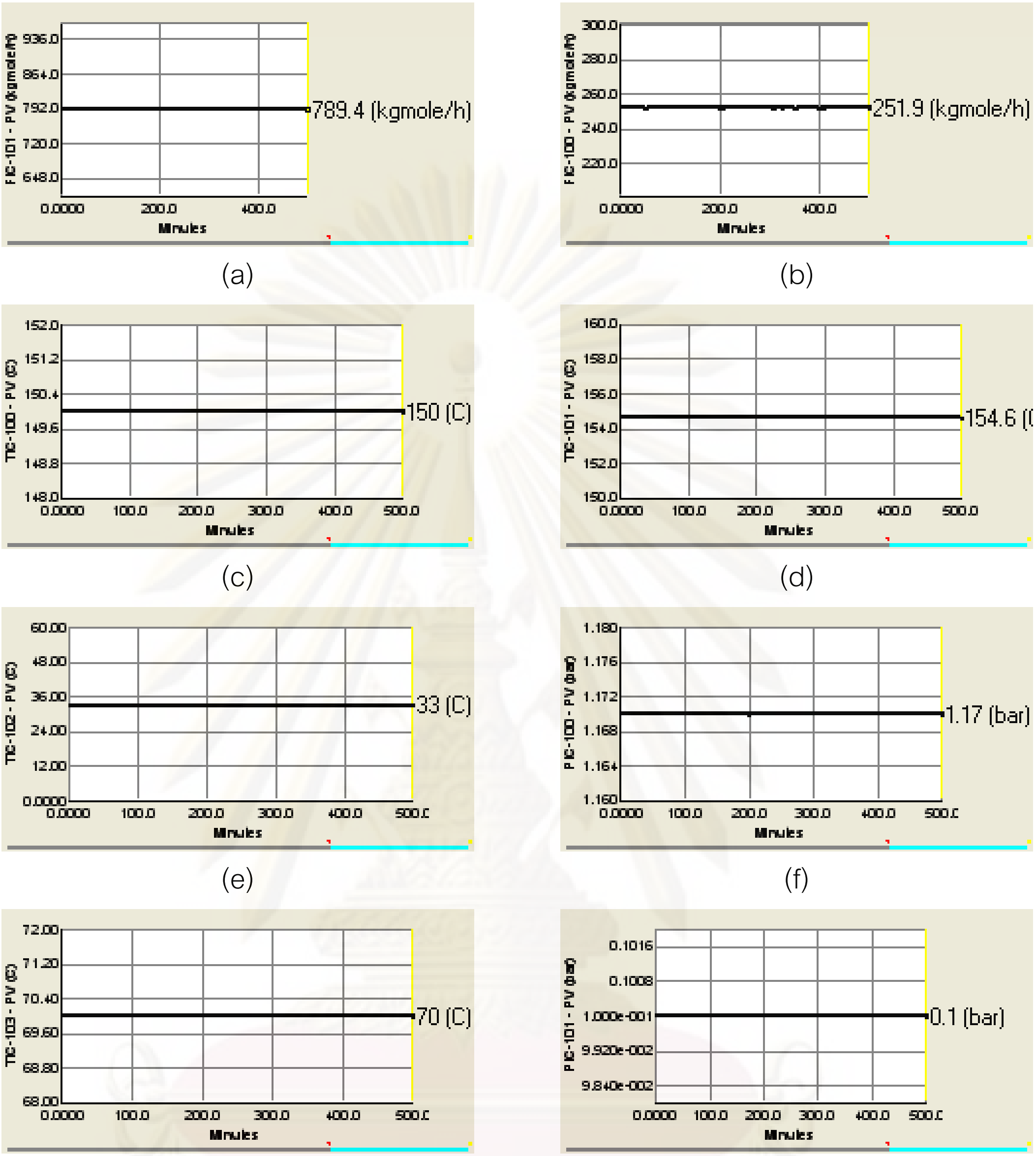
(aa) (ab)

(ac) (ad)

(ae) (af)

(ag)

Figure 5.19 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow



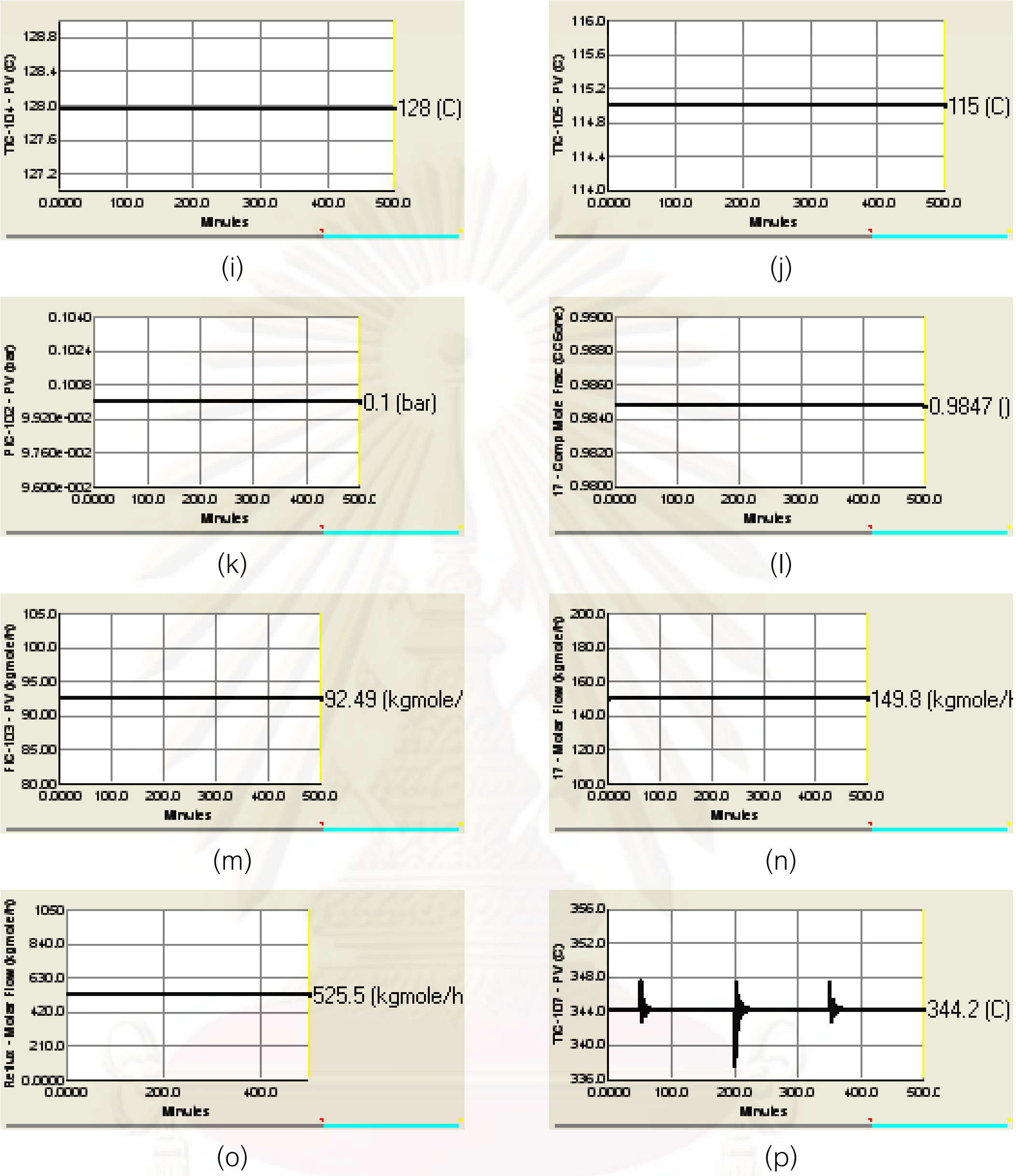
(a) (b)

(c) (d)

(e) (f)

(g) (h)

Figure 5.20 Dynamic responses of CS4 when change in dehydrogenation reactor inlet temperature: (a) hydrogen (fresh + recycle) flow, (b) phenol (fresh + recycle) flow (c) hydrogenation reactor inlet temperature, (d) hydrogenation reactor temperature at 1 m length, (e) separator V-100 inlet temperature, (f) separator V-100 pressure, (g) phenol recycle column feed temperature, (h) phenol recycle column – condenser pressure



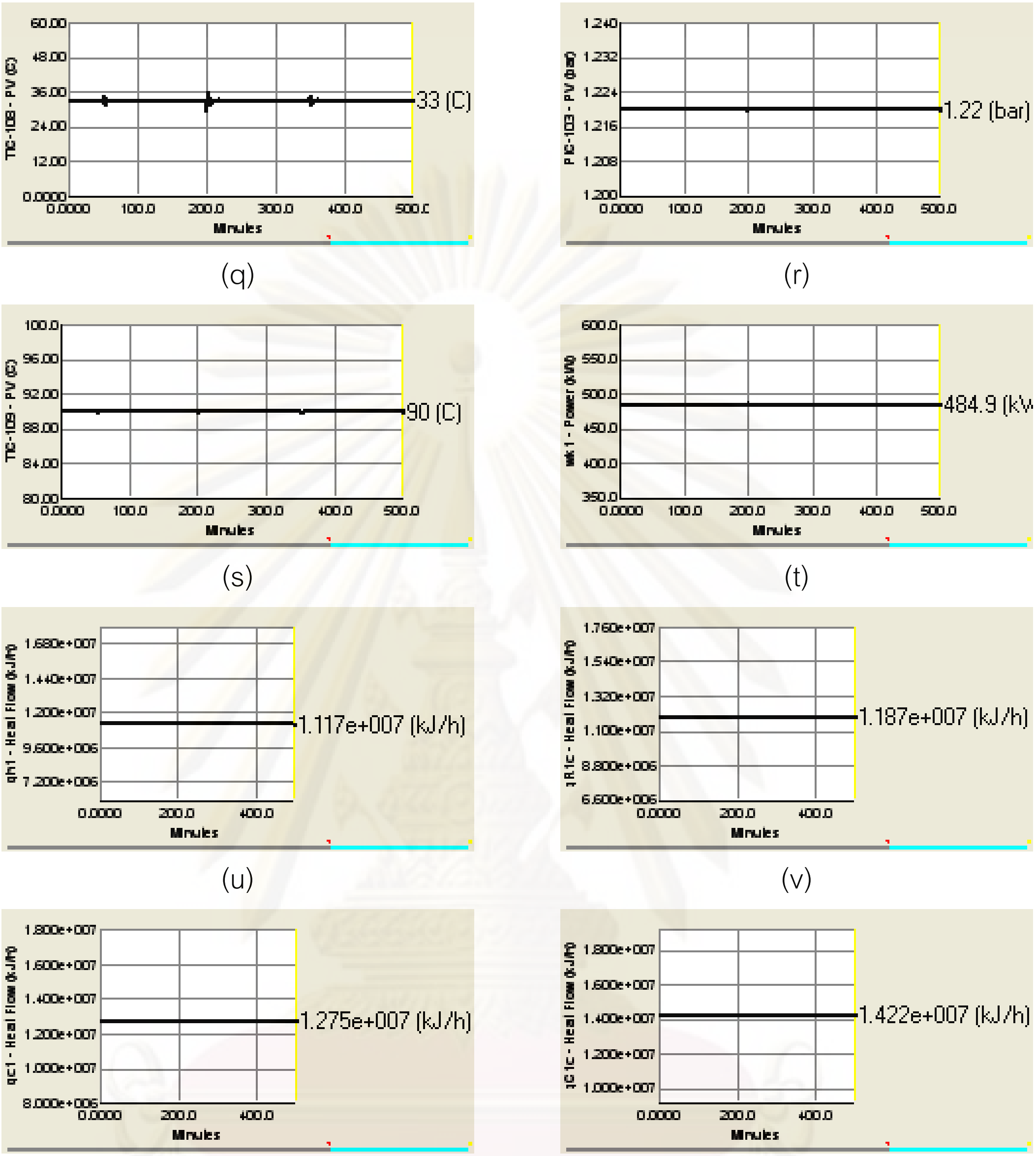
(i) (j)

(k) (l)

(m) (n)

(o) (p)

Figure 5.20 (Cont.) (i) phenol recycle column – stage 21 temperature, (j) cyclohexanone column feed temperature, (k) cyclohexanone column – condenser pressure, (l) cyclohexanol product composition, (m) cyclohexanone column – bottom flow, (n) cyclohexanone production flowrate, (o) cyclohexanone column – reflux flow, (p) dehydrogenation reactor outlet temperature



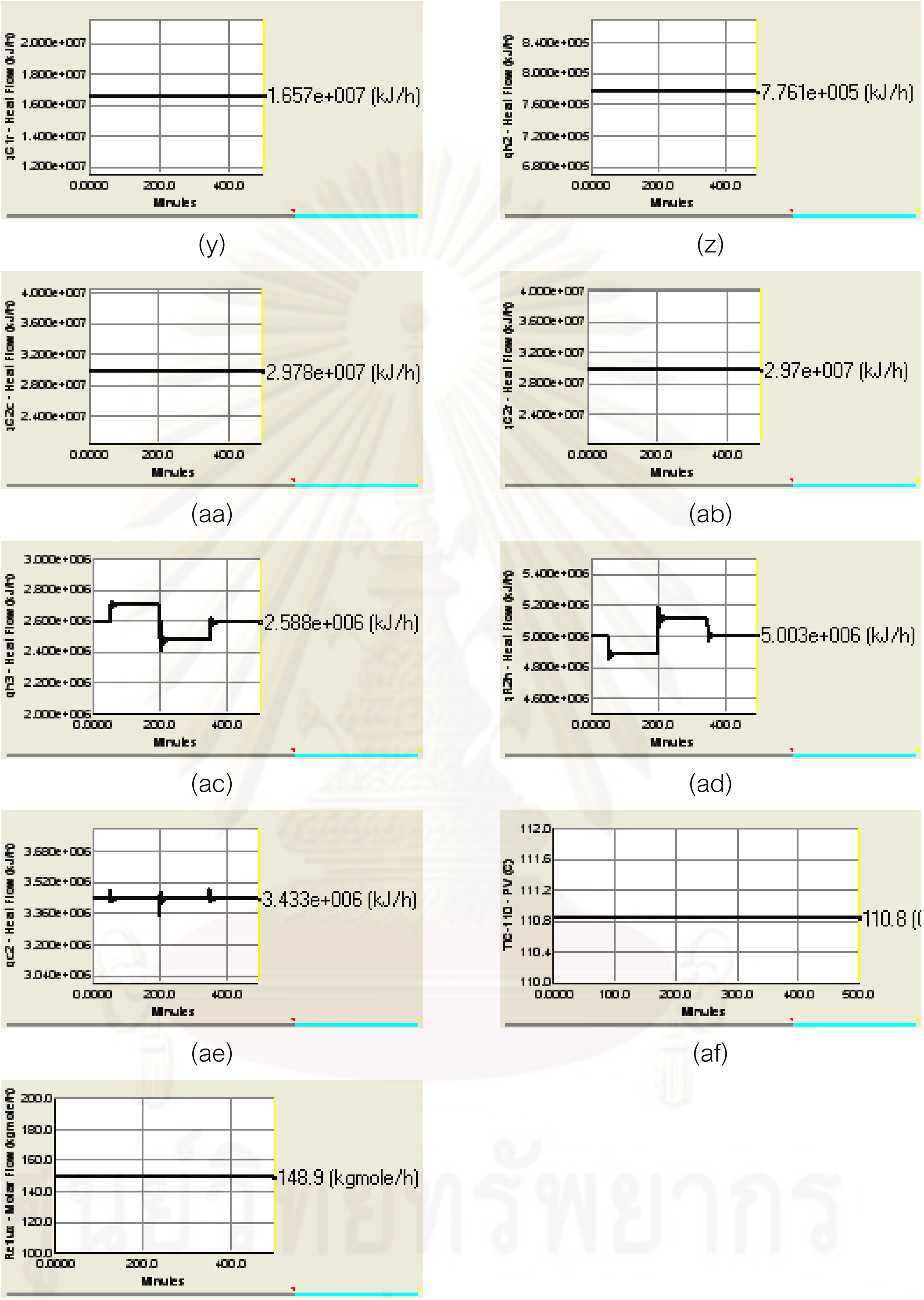
(q) (r)

(s) (t)

(u) (v)

(w) (x)

Figure 5.20 (Cont.) (q) separator V-101 inlet temperature, (r) separator V-101 pressure, (s) cyclohexanone column recycle temperature, (t) work input to compressor, (u) qh1, (v) hydrogenation reactor cooling duty, (w) qc1, (x) condenser duty of phenol recycle column



(y) (z)

(aa) (ab)

(ac) (ad)

(ae) (af)

(ag)

Figure 5.20 (Cont.) (y) reboiler duty of phenol recycle column, (z) qh2, (aa) condenser duty of cyclohexanone column, (ab) reboiler duty of cyclohexanone column, (ac) qh3, (ad) dehydrogenation reactor heating duty, (ae) qc2, (af) phenol recycle column – stage 16 temperature, (ag) phenol recycle column – reflux flow

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:

$$\mathrm{IAE} = \int \left| \varepsilon(t) \right| dt$$

Note that $\varepsilon(t) = y_{sp}(t) - y(t)$ 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 structures. Table 5.8 show the summation of IAE value result for the change in material disturbance of phenol (fresh + recycle) stream, Table 5.9 show the summation of IAE value result for the change in thermal disturbance of inlet temperature of hydrogenation reactor and Table 5.10 show the summation of IAE value result for the change in thermal disturbance of inlet temperature of dehydrogenation reactor.

For performance in used energy, the summation value of all energy that used in management disturbance is evaluated to find the designed control structure which is the most minimize energy use. From Table 5.11 to Table 5.13 show the summation value of all energy use.

Table 5.8 The IAE result for handle disturbance to the change in phenol (fresh + recycle) flow

Controller	Integral Absolute Error				Controller	Integral Absolute Error			
	CS1	CS2	CS3	CS4		CS1	CS2	CS3	CS4
FIC-102	0.0410	0.0516	0.0344	0.0335	**TIC-103**	19.5418	19.5389	19.4719	19.4612
PIC-100	0.0086	0.0086	0.0086	0.0086	**TIC-104**	4.4379	4.4374	6.5758	6.5768
PIC-101	0.0042	0.0042	0.0046	0.0046	**TIC-105**	3.0000	3.0039	2.5161	2.4963
PIC-102	0.0008	0.0008	0.0006	0.0006	**TIC-106**	0.3910	0.4034	0.2840	0.3521
PIC-103	0.0016	0.0015	0.0014	0.0015	**TIC-107**	0.7002	0.8117	0.6511	0.6938
TIC-100	2.0562	2.0583	2.0881	2.0907	**TIC-108**	1.0270	1.0950	0.8133	0.9016
TIC-101	11.9916	11.9863	12.1307	12.1257	**TIC-109**	0.0936	0.1146	0.0666	0.0811
TIC-102	64.0428	64.0475	63.9805	63.9551	**XIC-100**	0.0124	0.0138	0.0090	0.0106
					SUM	107.3507	107.5775	108.6366	108.7937

Table 5.9 The IAE result for handle disturbance to the change in inlet temperature of hydrogenation reactor

Controller	Integral Absolute Error				Controller	Integral Absolute Error			
	CS1	CS2	CS3	CS4		CS1	CS2	CS3	CS4
FIC-100	5.9680	5.9348	5.9495	6.1715	TIC-103	3.7932	3.7715	3.8142	3.8649
FIC-102	0.0227	0.0237	0.0260	0.0187	TIC-104	0.8218	0.8052	0.6742	0.6785
PIC-100	0.0071	0.0076	0.0077	0.0071	TIC-105	0.6292	0.6832	0.6571	0.6453
PIC-101	0.0006	0.0006	0.0004	0.0004	TIC-106	0.2741	0.2966	0.3638	0.2047
PIC-102	0.0001	0.0001	0.0002	0.0001	TIC-107	0.5222	0.5734	0.7395	0.4922
PIC-103	0.0053	0.0059	0.0059	0.0049	TIC-108	0.5448	0.6455	0.6890	0.5519
TIC-101	10.4397	10.4373	10.4472	10.4523	TIC-109	0.0237	0.0261	0.0348	0.0257
TIC-102	25.6639	25.4846	26.0090	26.7970	XIC-100	0.0010	0.0017	0.0014	0.0020
					SUM	48.7174	48.6978	49.4198	49.9174

Table 5.10 The IAE result for handle disturbance to the change in inlet temperature of dehydrogenation reactor

Controller	Integral Absolute Error				Controller	Integral Absolute Error			
	CS1	CS2	CS3	CS4		CS1	CS2	CS3	CS4
FIC-100	0.2378	0.1933	0.1917	0.2202	TIC-102	0.7997	0.7762	0.7098	0.7304
FIC-102	1.0689	1.0672	0.9452	0.9463	TIC-103	0.0313	0.0306	0.0282	0.0290
PIC-100	0.0004	0.0004	0.0003	0.0003	TIC-104	0.0000	0.0000	0.0000	0.0000
PIC-101	0.0002	0.0002	0.0002	0.0002	TIC-105	0.0000	0.0000	0.0000	0.0000
PIC-102	0.0002	0.0001	0.0001	0.0001	TIC-107	55.2653	55.3003	54.4138	54.4434
PIC-103	0.0008	0.0008	0.0008	0.0008	TIC-108	30.8812	30.8888	30.6845	30.7438
TIC-100	0.0375	0.0383	0.0292	0.0314	TIC-109	1.9345	1.9333	1.7244	1.7271
TIC-101	0.0051	0.0050	0.0053	0.0048	XIC-100	0.0011	0.0012	0.0010	0.0017
					SUM	90.2638	90.2357	88.7345	88.8794

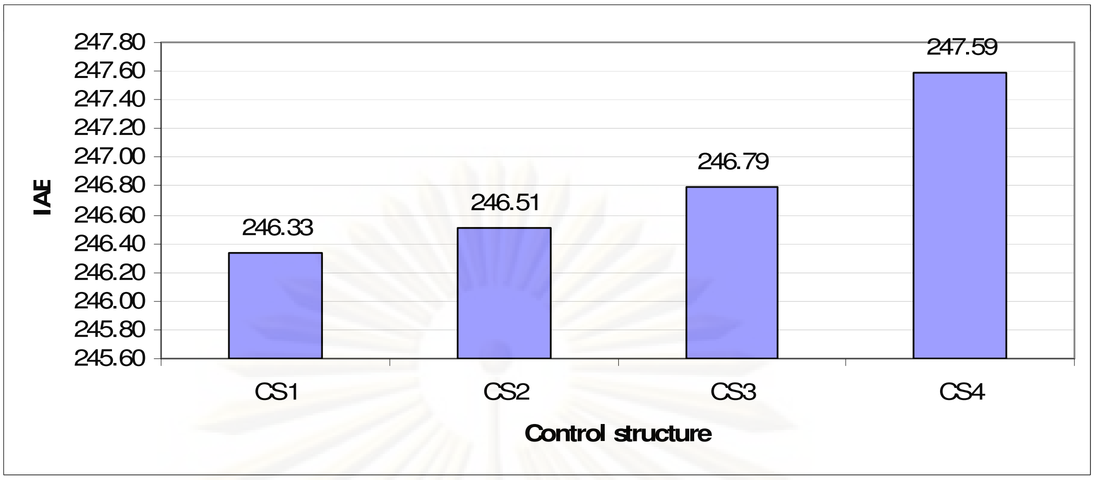


Figure 5.21 The IAE summations for handle disturbances to the change in all disturbances testing

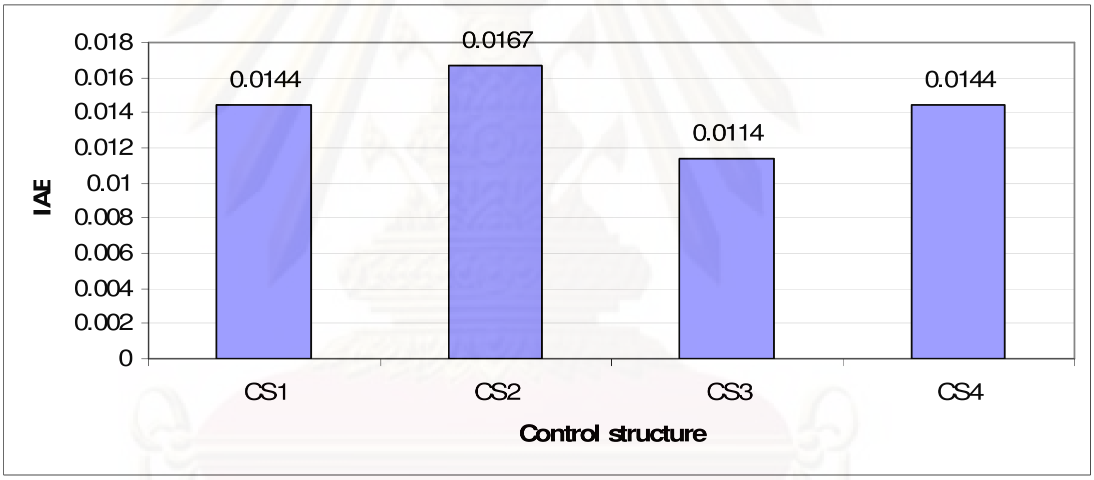


Figure 5.22 The IAE summations of product variation to the change in all disturbances testing

From Figure 5.21, designed control structure 1 (CS1) has the least IAE value so CS1 is the best control structure in handling disturbances entering the process.

From Figure 5.22, designed control structure 3 (CS3) has the least IAE value so CS3 is the best control structure in maintain product quality aspect.

From Figure 5.23, designed control structure 2 (CS2) has the least IAE value so CS3 is the best control structure in minimize used energy for handling disturbance entering the process.

Table 5.11 The summation value of all energy use to the change in phenol (fresh + recycle) flow

Energy	Summation value (kW *10^7)			
	CS1	CS2	CS3	CS4
qc1	2.1243	2.1243	2.1248	2.1249
qc2	0.5724	0.5724	0.5720	0.5720
qC1c	2.3921	2.3920	2.4583	2.4593
qC1r	2.7738	2.7739	2.8474	2.8484
qC2c	5.0070	4.9842	4.9955	4.9664
qC2r	4.9640	4.9615	4.9521	4.9504
qh1	1.8601	1.8601	1.8605	1.8606
qh2	0.1294	0.1294	0.1293	0.1293
qh3	0.4315	0.4315	0.4311	0.4311
qR1c	1.9788	1.9788	1.9798	1.9798
qR2h	0.8339	0.8339	0.8329	0.8329
wk1	0.0001	0.0001	0.0001	0.0001
SUM	23.0673	23.0419	23.1840	23.1552

Table 5.12 The summation value of all energy use to the change in inlet temperature of hydrogenation reactor

Energy	Summation value (kW *10^7)			
	CS1	CS2	CS3	CS4
qc1	1.4810	1.4810	1.4808	1.4808
qc2	0.4006	0.4006	0.4007	0.4007
qC1c	1.6740	1.6740	1.6560	1.6563
qC1r	1.9433	1.9433	1.9238	1.9241
qC2c	3.4886	3.4838	3.5026	3.4910
qC2r	3.4705	3.4709	3.4745	3.4756

Table 5.12 (Continued)

Energy	Summation value (kW *10^7)			
	CS1	CS2	CS3	CS4
qh1	1.1968	1.1968	1.1967	1.1967
qh2	0.0907	0.0907	0.0907	0.0907
qh3	0.3020	0.3020	0.3021	0.3021
qR1c	1.2919	1.2919	1.2917	1.2917
qR2h	0.5836	0.5836	0.5838	0.5838
wk1	0.0001	0.0001	0.0001	0.0001
SUM	**15.9230**	**15.9185**	**15.9034**	**15.8935**

Table 5.13 The summation value of all energy use to the change in inlet temperature of dehydrogenation reactor

Energy	Summation value (kW *10^7)			
	CS1	CS2	CS3	CS4
qc1	2.1248	2.1248	2.1246	2.1247
qc2	0.5721	0.5721	0.5722	0.5722
qC1c	2.3809	2.3809	2.3696	2.3703
qC1r	2.7737	2.7737	2.7622	2.7630
qC2c	4.9675	4.9619	4.9789	4.9651
qC2r	4.9486	4.9486	4.9497	4.9505
qh1	1.8617	1.8617	1.8616	1.8616
qh2	0.1294	0.1294	0.1293	0.1293
qh3	0.4313	0.4313	0.4314	0.4314
qR1c	1.9788	1.9788	1.9786	1.9786
qR2h	0.8335	0.8335	0.8338	0.8337
wk1	0.0001	0.0001	0.0001	0.0001
SUM	**23.0024**	**22.9968**	**22.9922**	**22.9804**

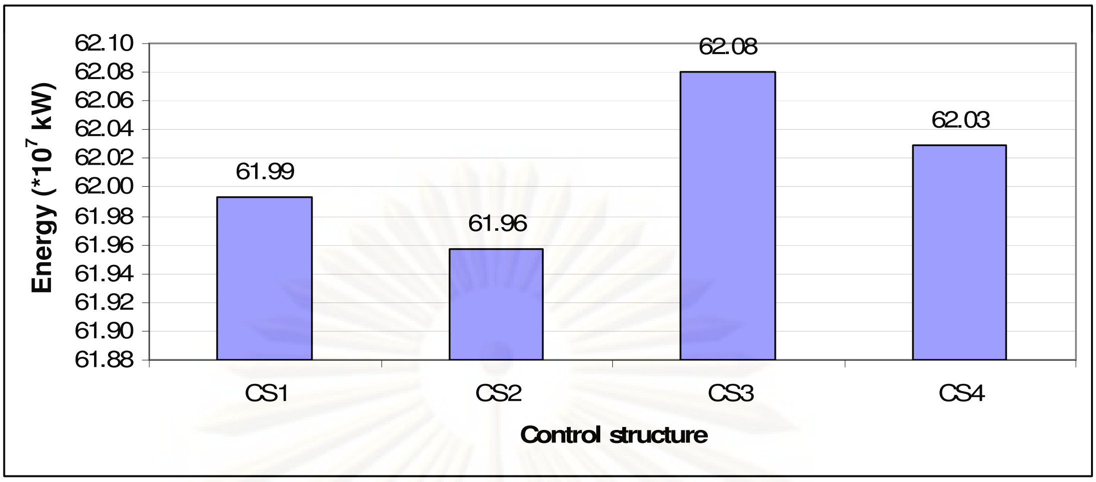


Figure 5.23 The summation value of all energy use to the change in all disturbances testing

CHAPTER VI

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

In this research has discussed control structure design for phenol hydrogenation to cyclohexanone process, using the design procedure of Luyben (1998) and new design procedure of Wongsri (2009). Wongsri (2009) procedure is based on heuristics and mathematical analysis. The precedence of control variables is established. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

The best control structure should handle disturbances entering the process, maintain product quality, minimize energy use and achieve all process constraints. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the material disturbances and thermal disturbances.

In material disturbance, designed control structure 1 (CS1) can handle disturbance the best, designed control structure 3 (CS3) can maintain product quality the best and designed control structure 2 (CS2) is the most minimize energy use.

In thermal disturbance based on hydrogenation section, designed control structure 2 (CS2) can handle disturbance the best, designed control structure 1 (CS1) can maintain product quality the best and designed control structure 4 (CS4) is the most minimize energy use.

In thermal disturbance based on dehydrogenation section, designed control structure 3 (CS3) can handle disturbance the best, designed control structure 3 (CS3) can maintain product quality the best and designed control structure 4 (CS4) is the most minimize energy use.

For all disturbance testing, designed control structure 1 (CS1) can handle disturbance the best, designed control structure 3 (CS3) can maintain product quality the best and designed control structure 2 (CS2) is the most minimize energy use.

In sum, using new design procedure of Wongsri (2009) and using Luyben's heuristics can also design the same control structures depending on designer's judgment in matching the CVs and MVs. However, the new design procedure gives the priority of CVs, so in principle the new design procedure will give designer the important information of what CV to be considered first if there are conflicts of matching two or more CVs with appropriate MVs. New design procedure of Wongsri (2009) can design control structures to find the good performance control structures and can apply this procedure of Wongsri (2009) to design control structures of the complex process.

6.2 Recommendation

Apply new design procedure of Wongsri (2009) in other process.

REFFERENCES

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

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

Chakkraphong Thaicharoen. Design of Control Structure for Energy-Integrated Hydrodealkylation Process. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2004.

Dimian, A.C., and Bildea, C.S. Chemical Process Design: Computer –Aided Case Studied. New York: Wiley, 2008.

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

Jatuporn Kunlawaniteewat. Heat Exchanger Network Control Structure Design. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2001.

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

Linnhoff, B., Dunford, H., and Smith, R. Heat Integration of Distillation Columns into Overall Processes. Chem. Eng. Sci. 38 (1983): 1175.

Linnhoff, B., and Hindmarsh, E. The Pinch Design Method for Heat Exchanger Networks. Chem. Eng. Sci. 38 (1983): 1175-1188.

Linnhoff, B., and Kotjabasakis, E. Design of Operable Heat Exchanger Networks. First U.K. National Heat Transfer Conference I. Chem. E. Symp. Ser. 86 (1984): 599.

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 (1995): 3885-3898.

Luyben, M.L., Tyreus, B.D., and Luyben, W.L. Plantwide Process Control. New York: McGraw-Hill, 1999.

Luyben, M.L., Tyreus, B.D., and Luyben, W.L. Design Plantwide Control Procedure. AIChE Journal 43 (1997): 3161-3174.

Luyben, W.L. Control of Outlet Temperature in Adiabatic Tubular Reactor. Ind. Eng. Chem. Res. 39 (2000): 1271-1278.

Luyben, W.L. Design and Control of Gas-Phase Reactor/Recycle Process with Reversible Exothermic Reactions. Ind. Eng. Chem. Res. 39 (2000)

Luyben, W.L. Plantwide Dynamic Simulations in Chemical Processing and Control. New York: Marcel Dekker, 2002.

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.

Richard Dale Colberg. Area, Cost and Resilience Targets for Heat Exchanger Networks. Doctoral dissertation, Cal Tech, Pasadena, 1989.

Saboo, A. K., and Morari, M. Design of Resilient Processing Plants-IV: Some New Result on Heat Exchanger Network Synthesis. Chem. Eng. Sci. 3 (1984): 579-592.

Sayfon Kietawarin. Control Structure Design Applied to Hydrodealkylation Process Plantwide Control Problem. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2002.

Wongsri, M., and Gayapan, U. Design of Heat Exchanger Networks and Control Structures for Natural Gas Expander Plant. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2008.

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.

Wongsri, M., and Sae-Leaw, B. Design of Control Structures of Energy-integrated HDA Plant with Minimum Auxiliary Reboilers. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2006.

Wongsri, M., and Sapsawaipol, B. The Design and Control of Resilient Heat Exchanger Network, Target Temperature Variation Case. Master's Thesis, Department of Chemical Engineering, Engineering, Chulalongkorn University, 2007.

APPENDICES

APPENDIX A

PROCESS STREAM DATA AND EQUIPMENT DATA

Table A.1 Process streams data

Stream Name	1	2	3	4	4A	5
Vapour fraction	0.00	1.00	1.00	0.00	0.00	0.78
Temperature °C	70.0	33.0	110.0	103.0	146.0	117.0
Pressure (kPa)	341	299	299	341	299	299
Molar Flow (kmole / hr)	150	313	789	252	252	1,041
Component mole fraction						
Hydrogen	0.000	1.000	0.999	0.000	0.000	0.757
Phenol	1.000	0.000	0.000	0.870	0.870	0.211
Cyclohexanone	0.000	0.000	0.001	0.024	0.024	0.007
Cyclohexanol	0.000	0.000	0.000	0.106	0.106	0.026

Stream Name	6	6A	7	7B	7C	8
Vapour fraction	1.00	1.00	1.00	0.86	0.82	0.62
Temperature °C	150.0	154.6	154.6	146.4	138.5	33.0
Pressure (kPa)	162	158	147	137	127	117
Molar Flow (kmole / hr)	1,041	873	669	669	669	669
Component mole fraction						
Hydrogen	0.757	0.710	0.622	0.622	0.622	0.622
Phenol	0.211	0.160	0.104	0.104	0.104	0.104
Cyclohexanone	0.007	0.089	0.126	0.126	0.126	0.126
Cyclohexanol	0.026	0.041	0.148	0.148	0.148	0.148

Table A.1 (Continued)

Stream Name	9	10	11	12	13	14
Vapour fraction	1.00	1.00	1.00	0.00	0.00	0.00
Temperature ^{o}C	33.0	33.0	159.7	33.0	70.0	145.1
Pressure (kPa)	117	117	299	117	19	28
Molar Flow (kmole / hr)	417	477	477	252	252	102
Component mole fraction						
Hydrogen	0.998	0.998	0.998	0.000	0.000	0.000
Phenol	0.000	0.000	0.000	0.275	0.275	0.680
Cyclohexanone	0.001	0.002	0.002	0.332	0.332	0.059
Cyclohexanol	0.001	0.001	0.001	0.393	0.393	0.261

Stream Name	15	16	17	18	19	20
Vapour fraction	0.00	0.00	0.00	0.00	1.00	1.00
Temperature ^{o}C	92.0	114.5	87.4	127.3	330.0	344.2
Pressure (kPa)	10	25	10	34	203	152
Molar Flow (kmole / hr)	150	150	150	92	92	163
Component mole fraction						
Hydrogen	0.000	0.000	0.000	0.000	0.000	0.431
Phenol	0.000	0.000	0.000	0.000	0.000	0.000
Cyclohexanone	0.517	0.517	0.985	0.065	0.065	0.468
Cyclohexanol	0.483	0.483	0.015	0.935	0.935	0.100

Table A.1 (Continued)

Stream Name	20B	20C	21	22	22A	22B
Vapour fraction	0.76	0.64	0.43	1.00	1.00	1.00
Temperature °C	138.9	128.0	33.0	33.0	33.0	33.0
Pressure (kPa)	142	132	122	122	122	122
Molar Flow (kmole / hr)	163	163	163	70	11	60
Component mole fraction						
Hydrogen	0.431	0.431	0.431	0.995	0.995	0.995
Phenol	0.000	0.000	0.000	0.000	0.000	0.000
Cyclohexanone	0.468	0.468	0.468	0.004	0.004	0.004
Cyclohexanol	0.100	0.100	0.100	0.000	0.000	0.000

Stream Name	23	24
Vapour fraction	0.00	0.00
Temperature °C	33.0	89.9
Pressure (kPa)	122	18
Molar Flow (kmole / hr)	92	92
Component mole fraction		
Hydrogen	0.000	0.000
Phenol	0.000	0.000
Cyclohexanone	0.823	0.823
Cyclohexanol	0.177	0.177

Note: Stream Name follows as Figure 4.9.

Table A.2 Process equipments data

	Hydrogenation reactor	Dehydrogenation reactor
Length (m)	4	4
Diameter (m)	0.045	0.05
Number of tubes	12,000	2,000
Wall thickness (m)	0.005	0.005
Reactor heat duty (kW)	7,202	1,390
	Separator (V-100)	Separator (V-101)
Diameter (m)	1.83	0.76
Height (m)	6.4	4.2
	FEHE (E-100)	FEHE (E-107)
UA (kJ / C-h)	1.04*105	1.15*105
Hot outlet temperature (C)	144	207.5
Heat duty (kW)	624	1,600

Table A.3 Column specifications

	Phenol recycle column (T-100)	Cyclohexanone column (T-101)
Theoretical trays	30	40
Feed tray	17	14,25
Diameter (m)	2.5	3.3
Condenser volume (m^3)	5.65	12.55
Reboiler volume (m^3)	7.95	14.05
Reflux ratio	1	3.5

APPENDIX B

PARAMETER TUNING OF CONTROL STRUCTURES

B.1 Tuning Flow, Level, Pressure and Temperature Loops

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 Kc = 0.5 is often used. Derivative action should not be used.

In a real plant application, filtering of the flow signal is also recommended because of the noise. So filter is put at controller output signal and a good number to use for a flow loop is τ_F = 0.1 minute.

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 Kc = 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 Kc = 2 and τ_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 $\tau_{d,}$ 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.

The 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.

The maximum amplitude of the PV signal is used to calculate the ultimate gain K_u from the equation:

$$Ku = \frac{4h}{a\pi}$$

The period of the output PV curve is the ultimate period P_u. From these two parameters, controller tuning constants can be calculated for PI or PID controllers, using a variety of tuning methods proposed in the literature that require only the ultimate gain and ultimate frequency, e.g., Ziegler-Nichols, Tyreus-Luyben, etc.

The test has many positive features that have led to its widespread use in real plants as well in simulation studies:

1. Only one parameter has to be specified (relay height).
2. The time it takes to run the test is short, particularly compared to the extended periods required for methods like PRBS.
3. The test is closed loop, so the process is not driven away from the setpoint.
4. The information obtained is very accurate in the frequency range that is important for the design of a feedback controller (the ultimate frequency).
5. The impact of load changes that occur during the test can be detected by a change to asymmetric in the manipulated variable.

All these features make relay-feedback testing a useful identification tool.

Knowing the ultimate gain K_u and ultimate period P_u permits us to calculate controller setting. There are several methods that require only these two parameters. The Ziegler-Nichols tuning equations for a PI controller are:

$$Kc = \frac{Ku}{2.2}$$

$$\tau_I = \frac{Pu}{1.2}$$

These tuning constants are frequently too aggressive for many chemical engineering applications. The Tyreus-Luyben tuning method provides more conservative setting with increased robustness. The TL equations for a PI controller are:

$$Kc = \frac{Ku}{3.2}$$

$$\tau_I = 2.2Pu$$

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.

B.3 Inclusion of Lag

These are typically temperature and composition controllers. These loops have significant dynamic lags/or deadtimes. Realistic dynamic simulations require that we explicitly include lags and/or deadtimes in all the important loops. Usually this means controllers that affect product quality (temperature or composition) or process constraint (safety, environmental, etc.).

In this plant, a 3-minute deadtime is assumed in the product composition measurement.

Table B.1 Typical measurement lags

		Number	Time constant (minutes)	Type
Temperature	Liquid	2	0.5	First-Order Lag
	Gas	3	1	First-Order Lag
Composition	Chromatograph	1	3 to 10	Dead time

Table B.2 Same parameter tuning of phenol hydrogenation to cyclohexanone process in all control structures

Controller	Controlled variable	Manipulated variable	Control action	K_c	τ_I	τ_D
FIC-100	Phenol (fresh + recycle) flowrate	VLV-100	Reverse	0.5	0.3	-
FIC-101	Hydrogen (fresh + recycle) flowrate	VLV-101	Reverse	0.5	0.3	-
TIC-100	Hydrogenation reactor inlet temperature	Heater duty (qh1)	Reverse	1.51	0.319	0.07
TIC-101	Hydrogenation reactor temperature at 1 m length	Reactor cooling duty (qR1c)	Direct	2.06	1.36	0.302
TIC-102	Separator (V-100) inlet temperature	Cooler duty (qc1)	Direct	0.117	0.408	0.09
PIC-100	Separator (V-100) pressure	Compressor work (wk1)	Direct	0.503	0.034	-
LIC-100	Separator (V-100) level	VLV-103	Direct	2	-	-
TIC-103	Phenol recycle column feed temperature	VLV-104	Direct	4.22	0.412	0.092
PIC-101	Phenol recycle column condenser pressure	Condenser duty (qC1c)	Direct	2.07	0.38	-
LIC-101	Phenol recycle column condenser level	Distillate valve (VLV-107)	Direct	2	-	-
LIC-102	Phenol recycle column reboiler level	Bottom valve (VLV-106)	Direct	2	-	-
TIC-104	Phenol recycle column stage 21 temperature	Reboiler duty (qC1r)	Reverse	8.52	4.44	0.987
TIC-105	Cyclohexanone column feed temperature	Heater duty (qh2)	Reverse	2.31	0.606	0.135
PIC-102	Cyclohexanone column condenser pressure	Condenser duty (qC2c)	Direct	3.96	0.23	-
LIC-104	Cyclohexanone column reboiler level	Reboiler duty (qC2r)	Direct	2	-	-

Table B.2 (Continued)

Controller	Controlled variable	Manipulated variable	Control action	K_c	τ_I	τ_D
FIC-102	Cyclohexanone column bottom stream flow rate	VLV-110	Reverse	0.5	0.3	-
TIC-106	Dehydrogenation reactor inlet temperature	Heater duty (qh3)	Reverse	0.3	0.392	0.087
TIC-107	Dehydrogenation reactor exit temperature	Reactor heating duty (qR2h)	Reverse	0.115	0.43	0.0955
TIC-108	Separator (V-101) inlet temperature	Cooler duty (qc2)	Direct	0.164	0.404	0.0897
PIC-103	Separator (V-101) pressure	Purge valve (VLV-111)	Direct	3.59	0.0217	-
LIC-105	Separator (V-101) level	VLV-113	Direct	2	-	-
TIC-109	Cyclohexanone column recycle temperature	VLV-114	Direct	5.15	0.242	0.0538

Table B.3 Different parameter tuning of phenol hydrogenation to cyclohexanone process for all control structures

Controller	Controlled variable	Manipulated variable	Control action	K_c	τ_I	τ_D
CS1, CS3 LIC-103	Cyclohexanone column condenser level	Distillate valve (VLV-109)	Direct	2	-	-
CS2, CS4 LIC-103	Cyclohexanone column condenser level	Reflux valve	Direct	2	-	-
CS1, CS3 XIC-100	Cyclohexanone column cyclohexanol composition of distillate stream	Reflux valve	Direct	1.71	18.3	4.06
CS2, CS4 XIC-100	Cyclohexanone column cyclohexanol composition of distillate stream	Distillate valve (VLV-109)	Reverse	6.18	28.3	6.28
CS3,CS4 TIC-110	Phenol recycle column stage 16 temperature	Reboiler duty (qC1r)	Reverse	5.47	30.7	6.82

APPENDIX C

FIXTURE POINT THEOREM DATA

Table C.1 List of Manipulated Variables of the process

Manipulated Variables	Description
VLV-100	Phenol fresh feed valve
VLV-101	Hydrogen fresh feed valve
VLV-103	Vessel V-100 liquid outlet valve
VLV-104	Heat exchanger E-103 bypass valve
VLV-106	Phenol recycle column bottom valve
VLV-107	Phenol recycle column top valve
VLV-109	Cyclohexanone column top valve
VLV-110	Cyclohexanone column bottom valve
VLV-111	Vessel V-101 hydrogen purge valve
VLV-113	Vessel V-101 liquid outlet valve
VLV-114	Heat exchanger E-108 bypass valve
qc1	Cooling duty of Vessel V-100 inlet temperature
qc2	Cooling duty of Vessel V-101 inlet temperature
qh1	Heating duty of hydrogenation reactor inlet temperature
qh2	Heating duty of cyclohexanone column inlet temperature
qh3	Heating duty of dehydrogenation reactor inlet temperature
wk1	Compressor K-100 work input
qR1c	Cooling duty of hydrogenation reactor
qR2h	Heating duty of dehydrogenation reactor
qC1c	Condenser duty of phenol recycle column
qC1r	Reboiler duty of phenol recycle column
qC2c	Condenser duty of cyclohexanone column
qC2r	Reboiler duty of cyclohexanone column
T-100 reflux	Phenol recycle column reflux valve
T-101 reflux	cyclohexanone column reflux valve

Table C.2 IAE results of the process vessel

Vessel		VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
V-100	% Level	6.4416	5.0808	5.0427	0.4414	1.6334	0.0065	0.0040	0.4820	0.1478	0.0122	0.0043	2.4807	0.2015
V-100	Pressure	1.2962	9.8824	0.0158	0.0183	0.0230	0.0042	0.0017	1.9793	0.3144	0.0569	0.0105	2.4016	0.8992
V-100	Temperature	0.2890	7.5023	0.0981	0.0510	0.3266	0.0058	0.0007	1.1053	0.2044	0.0334	0.0042	8.8094	0.4553
V-101	% Level	1.7470	13.2557	0.0200	0.0275	0.0323	0.0040	0.0238	58.4580	0.5532	17.0137	1.2239	2.7205	4.9489
V-101	Pressure	1.1657	9.0536	0.0092	0.0137	0.0208	0.0033	0.0027	7.9899	0.3732	0.0923	0.0251	2.1989	1.7271
V-101	Temperature	0.0359	0.1028	0.1496	0.0314	0.0176	0.0070	0.0413	3.3227	0.0355	0.2152	0.1031	0.6263	8.9424
T-100 Condenser	% Level	0.0378	1.0379	0.7145	0.0797	0.0393	0.0875	0.0038	0.1025	0.1052	0.0168	0.0008	4.1533	0.2281
T-100 Condenser	Pressure	0.0294	0.8951	0.0142	0.0021	0.0342	0.0213	0.0003	0.1019	0.0017	0.0010	0.0005	0.0680	0.0027
T-100 Reboiler	% Level	0.3110	6.1725	11.6851	1.1483	3.9342	0.4081	0.0224	0.7117	0.2599	0.0363	0.0208	18.1778	0.3833
T-101 Condenser	% Level	0.0064	0.0294	0.0139	0.0057	0.0091	0.0096	0.0546	0.0043	0.0062	0.0991	0.0099	0.0097	0.4814
T-101 Condenser	Pressure	0.0015	0.0122	0.0059	0.0014	0.0014	0.0018	0.0135	0.0343	0.0015	0.0036	0.0019	0.0480	0.0137
T-101 Reboiler	% Level	0.2904	0.0246	2.2473	0.3289	0.1126	0.2714	0.3701	9.0869	0.3868	1.9656	0.1220	10.7231	2.0626

Table C.2 (Continued)

Vessel		qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
V-100	% Level	0.2884	0.0192	0.0447	0.7491	0.6363	0.0397	0.0317	0.5545	0.0137	0.0680	0.0592	0.0549	24.5384
V-100	Pressure	2.7013	0.0323	0.6425	1.7691	2.4862	1.3436	0.0126	0.1461	0.0102	0.1913	0.0926	0.1555	26.4869
V-100	Temperature	4.9466	0.0301	0.3384	1.1934	5.7194	0.7559	0.0173	0.3978	0.0107	0.1073	0.0264	0.0934	32.5222
V-101	% Level	3.2977	0.0039	1.3997	2.5786	3.0042	2.5785	0.0099	0.0801	0.3705	1.4503	0.1604	0.2935	115.2558
V-101	Pressure	2.4434	0.0225	1.7842	1.5897	2.2618	4.3197	0.0133	0.1233	0.0325	0.2848	0.0432	0.0281	35.6218
V-101	Temperature	0.0567	0.1031	6.0375	0.0577	0.4652	11.424	0.0195	0.1591	0.3800	0.5149	0.5113	1.2355	34.5955
T-100 Condenser	% Level	0.6970	0.7480	0.0095	0.1766	2.9489	0.0257	5.2860	2.6665	0.0780	0.0297	0.1245	0.0470	19.4446
T-100 Condenser	Pressure	0.6019	0.1451	0.0273	0.1517	0.0477	0.0632	0.0972	2.0630	0.0145	0.0026	0.0618	0.0009	4.4492
T-100 Reboiler	% Level	0.9959	2.9421	0.2794	1.1604	11.921	0.5927	3.1516	4.7362	0.3072	0.0610	12.6465	0.0604	82.1260
T-101 Condenser	% Level	0.0093	0.0078	0.0181	0.0123	0.0072	0.0441	0.0322	0.0211	5.1693	0.4085	0.0666	0.1363	6.6722
T-101 Condenser	Pressure	0.0181	0.0434	0.0812	0.0020	0.0320	0.1626	0.0011	0.0760	0.1812	1.3105	0.0366	0.1667	2.2525
T-101 Reboiler	% Level	0.5263	2.0157	0.2326	0.5595	7.7748	0.3910	0.1510	3.4291	3.1821	6.6968	8.3584	21.0803	82.3895

Table C.3 IAE results of T-100 (Phenol Recycle Column)

Tray	VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
1	0.0366	1.0927	0.0300	0.0040	0.0448	0.0270	0.1319	0.1319	0.0036	0.0016	0.0007	0.1386	0.0061
2	0.0331	1.0149	0.0285	0.0039	0.0413	0.0250	0.1217	0.1217	0.0034	0.0016	0.0008	0.1282	0.0059
3	0.0307	0.9587	0.0271	0.0037	0.0389	0.0234	0.1145	0.1145	0.0032	0.0015	0.0007	0.1186	0.0055
4	0.0285	0.9134	0.0269	0.0036	0.0370	0.0222	0.1087	0.1087	0.0032	0.0014	0.0007	0.1145	0.0054
5	0.0266	0.8746	0.0275	0.0036	0.0354	0.0210	0.1039	0.1039	0.0032	0.0014	0.0006	0.1146	0.0055
6	0.0250	0.8407	0.0284	0.0035	0.0343	0.0197	0.0999	0.0999	0.0030	0.0011	0.0004	0.1168	0.0055
7	0.0229	0.8101	0.0300	0.0039	0.0329	0.0190	0.0959	0.0959	0.0034	0.0013	0.0006	0.1209	0.0060
8	0.0211	0.7829	0.0318	0.0042	0.0317	0.0182	0.0925	0.0925	0.0037	0.0015	0.0007	0.1257	0.0065
9	0.0194	0.7585	0.0337	0.0044	0.0307	0.0175	0.0895	0.0895	0.0040	0.0016	0.0008	0.1309	0.0070
10	0.0181	0.7371	0.0352	0.0043	0.0303	0.0164	0.0872	0.0872	0.0038	0.0013	0.0005	0.1362	0.0070
11	0.0168	0.7177	0.0370	0.0043	0.0298	0.0156	0.0851	0.0851	0.0038	0.0011	0.0003	0.1420	0.0073
12	0.0152	0.7001	0.0392	0.0045	0.0292	0.0150	0.0831	0.0831	0.0040	0.0012	0.0003	0.1485	0.0078
13	0.0138	0.6841	0.0414	0.0047	0.0288	0.0143	0.0813	0.0813	0.0042	0.0011	0.0003	0.1555	0.0082
14	0.0130	0.6682	0.0443	0.0052	0.0282	0.0140	0.0793	0.0793	0.0047	0.0014	0.0005	0.1647	0.0090

Table C.3 (Continued)

Tray	qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
1	0.7489	0.1802	0.0357	0.1948	0.0962	0.0825	0.1259	2.3682	0.0181	0.0033	0.1477	0.0016	5.6527
2	0.6935	0.1661	0.0329	0.1795	0.0887	0.0761	0.1149	2.2087	0.0166	0.0030	0.1177	0.0016	5.2294
3	0.6533	0.1562	0.0310	0.1686	0.0818	0.0716	0.1069	2.0925	0.0156	0.0028	0.0909	0.0015	4.9139
4	0.6208	0.1478	0.0294	0.1597	0.0788	0.0680	0.1008	1.9976	0.0147	0.0027	0.0732	0.0015	4.6693
5	0.5928	0.1401	0.0281	0.1520	0.0787	0.0650	0.0950	1.9150	0.0139	0.0026	0.0625	0.0015	4.4689
6	0.5683	0.1332	0.0272	0.1455	0.0799	0.0627	0.0896	1.8413	0.0135	0.0024	0.0557	0.0013	4.2986
7	0.5459	0.1263	0.0260	0.1392	0.0824	0.0602	0.0852	1.7741	0.0125	0.0024	0.0519	0.0016	4.1506
8	0.5258	0.1202	0.0251	0.1336	0.0853	0.0582	0.0816	1.7130	0.0118	0.0024	0.0493	0.0017	4.0208
9	0.5077	0.1145	0.0242	0.1285	0.0885	0.0564	0.0772	1.6572	0.0111	0.0023	0.0476	0.0019	3.9047
10	0.4918	0.1097	0.0239	0.1243	0.0914	0.0551	0.0734	1.6065	0.0109	0.0022	0.0460	0.0016	3.8013
11	0.4773	0.1051	0.0235	0.1203	0.0948	0.0540	0.0700	1.5596	0.0106	0.0022	0.0451	0.0015	3.7097
12	0.4638	0.1006	0.0229	0.1164	0.0986	0.0529	0.0672	1.5160	0.0101	0.0021	0.0448	0.0016	3.6280
13	0.4515	0.0964	0.0225	0.1128	0.1027	0.0519	0.0644	1.4756	0.0097	0.0022	0.0449	0.0016	3.5554
14	0.4398	0.0919	0.0220	0.1090	0.1083	0.0508	0.0620	1.4364	0.0090	0.0022	0.0470	0.0020	3.4922

Table C.3 (Continued)

Tray	VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
15	0.0219	0.6408	0.0483	0.0052	0.0296	0.0126	0.0765	0.0765	0.0043	0.0010	0.0001	0.1861	0.0095
16	0.0917	0.5210	0.0596	0.0067	0.0378	0.0106	0.0586	0.0586	0.0036	0.0011	0.0002	0.2746	0.0114
17	0.2135	0.3375	0.0547	0.0062	0.0535	0.0095	0.0259	0.0259	0.0010	0.0001	0.0002	0.3433	0.0082
18	0.2404	0.2661	0.0882	0.0091	0.0551	0.0060	0.0218	0.0218	0.0017	0.0009	0.0012	0.3866	0.0078
19	0.3083	0.1453	0.1714	0.0164	0.0631	0.0020	0.0121	0.0121	0.0037	0.0035	0.0039	0.5101	0.0080
20	0.4083	0.0825	0.3513	0.0314	0.0779	0.0164	0.0053	0.0053	0.0063	0.0082	0.0088	0.8012	0.0108
21	0.4249	0.2686	0.5371	0.0435	0.0845	0.0284	0.0093	0.0093	0.0079	0.0128	0.0138	1.1497	0.0140
22	0.3035	0.1861	0.5146	0.0386	0.0680	0.0227	0.0127	0.0127	0.0050	0.0110	0.0121	1.1607	0.0129
23	0.1674	0.1173	0.3385	0.0243	0.0463	0.0092	0.0360	0.0360	0.0016	0.0065	0.0075	0.8232	0.0092
24	0.0864	0.3224	0.1860	0.0137	0.0321	0.0011	0.0489	0.0489	0.0009	0.0028	0.0036	0.4848	0.0066
25	0.0487	0.4216	0.0990	0.0077	0.0252	0.0063	0.0540	0.0540	0.0016	0.0010	0.0016	0.2820	0.0054
26	0.0327	0.4595	0.0551	0.0043	0.0224	0.0083	0.0558	0.0558	0.0015	0.0005	0.0011	0.1802	0.0044
27	0.0253	0.4692	0.0340	0.0030	0.0205	0.0094	0.0554	0.0554	0.0018	0.0001	0.0004	0.1313	0.0042
28	0.0218	0.4676	0.0234	0.0024	0.0195	0.0099	0.0545	0.0545	0.0018	0.0003	0.0002	0.1069	0.0041
29	0.0199	0.4615	0.0179	0.0020	0.0187	0.0100	0.0534	0.0534	0.0019	0.0005	0.0001	0.0939	0.0040
30	0.0191	0.4539	0.0146	0.0016	0.0184	0.0098	0.0525	0.0525	0.0017	0.0004	0.0001	0.0861	0.0037

Table C.3 (Continued)

Tray	qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
15	0.4289	0.0861	0.0219	0.1046	0.1220	0.0500	0.0573	1.3902	0.0089	0.0024	0.0605	0.0016	3.4468
16	0.4177	0.0697	0.0198	0.0899	0.1808	0.0447	0.0468	1.2900	0.0068	0.0018	0.1294	0.0011	3.4338
17	0.4373	0.0653	0.0173	0.0765	0.2217	0.0375	0.0432	1.2308	0.0063	0.0014	0.1483	0.0018	3.3670
18	0.4173	0.0502	0.0160	0.0757	0.2563	0.0332	0.0257	1.1831	0.0055	0.0013	0.1907	0.0026	3.3643
19	0.4013	0.0194	0.0148	0.0794	0.3515	0.0270	0.0174	1.1434	0.0046	0.0039	0.2974	0.0050	3.6249
20	0.3875	0.0390	0.0140	0.0931	0.5657	0.0184	0.0886	1.1260	0.0031	0.0096	0.5284	0.0093	4.6963
21	0.3742	0.0856	0.0151	0.1134	0.7946	0.0148	0.1413	1.1526	0.0032	0.0157	0.7694	0.0130	6.0968
22	0.3633	0.0650	0.0163	0.1197	0.7624	0.0204	0.1105	1.2023	0.0045	0.0147	0.7311	0.0105	5.7813
23	0.3571	0.0115	0.0171	0.1120	0.5187	0.0288	0.0453	1.2318	0.0062	0.0099	0.4766	0.0059	4.4440
24	0.3516	0.0335	0.0167	0.1017	0.3028	0.0334	0.0056	1.2316	0.0069	0.0056	0.2560	0.0022	3.5856
25	0.3454	0.0551	0.0164	0.0941	0.1797	0.0353	0.0288	1.2160	0.0072	0.0033	0.1321	0.0005	3.1222
26	0.3389	0.0649	0.0164	0.0894	0.1184	0.0360	0.0394	1.1959	0.0077	0.0026	0.0717	0.0005	2.8633
27	0.3315	0.0683	0.0158	0.0856	0.0889	0.0356	0.0441	1.1746	0.0074	0.0019	0.0434	0.0004	2.7076
28	0.3242	0.0692	0.0154	0.0827	0.0740	0.0349	0.0458	1.1543	0.0073	0.0015	0.0298	0.0006	2.6063
29	0.3172	0.0688	0.0150	0.0803	0.0659	0.0342	0.0462	1.1352	0.0071	0.0014	0.0230	0.0007	2.5321
30	0.3107	0.0682	0.0148	0.0785	0.0608	0.0337	0.0457	1.1177	0.0071	0.0013	0.0193	0.0006	2.4726

Table C.4 IAE results of T-101 (Cyclohexanone Column)

Tray	VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
1	0.0021	0.0437	0.0083	0.0019	0.0020	0.0026	0.0187	0.0481	0.0021	0.0053	0.0027	0.0670	0.0203
2	0.0019	0.0409	0.0078	0.0018	0.0018	0.0024	0.0173	0.0451	0.0019	0.0054	0.0026	0.0626	0.0209
3	0.0018	0.0386	0.0074	0.0017	0.0017	0.0023	0.0161	0.0425	0.0018	0.0055	0.0025	0.0589	0.0214
4	0.0017	0.0365	0.0070	0.0015	0.0016	0.0022	0.0150	0.0405	0.0017	0.0055	0.0023	0.0557	0.0218
5	0.0017	0.0346	0.0066	0.0016	0.0016	0.0023	0.0142	0.0388	0.0017	0.0056	0.0024	0.0527	0.0222
6	0.0016	0.0330	0.0063	0.0015	0.0015	0.0022	0.0133	0.0377	0.0016	0.0057	0.0023	0.0501	0.0224
7	0.0014	0.0316	0.0061	0.0013	0.0013	0.0020	0.0125	0.0374	0.0014	0.0056	0.0021	0.0480	0.0225
8	0.0013	0.0304	0.0059	0.0013	0.0013	0.0019	0.0118	0.0376	0.0014	0.0057	0.0021	0.0460	0.0226
9	0.0013	0.0292	0.0057	0.0012	0.0012	0.0019	0.0112	0.0389	0.0013	0.0057	0.0020	0.0442	0.0228
10	0.0012	0.0281	0.0055	0.0012	0.0011	0.0018	0.0107	0.0414	0.0013	0.0059	0.0020	0.0425	0.0229
11	0.0011	0.0272	0.0054	0.0011	0.0010	0.0017	0.0102	0.0454	0.0011	0.0060	0.0019	0.0411	0.0230
12	0.0012	0.0262	0.0050	0.0012	0.0011	0.0019	0.0100	0.0511	0.0013	0.0064	0.0020	0.0396	0.0234
13	0.0010	0.0254	0.0050	0.0010	0.0010	0.0017	0.0095	0.0593	0.0010	0.0065	0.0018	0.0386	0.0235
14	0.0012	0.0246	0.0047	0.0012	0.0011	0.0019	0.0094	0.0698	0.0012	0.0071	0.0021	0.0373	0.0242
15	0.0009	0.0238	0.0047	0.0010	0.0010	0.0017	0.0088	0.0594	0.0010	0.0071	0.0019	0.0364	0.0234
16	0.0006	0.0233	0.0048	0.0008	0.0007	0.0014	0.0082	0.0509	0.0007	0.0069	0.0016	0.0357	0.0224
17	0.0007	0.0226	0.0046	0.0008	0.0008	0.0015	0.0080	0.0434	0.0008	0.0071	0.0017	0.0346	0.0219
18	0.0011	0.0218	0.0041	0.0011	0.0011	0.0019	0.0081	0.0371	0.0011	0.0076	0.0021	0.0333	0.0218
19	0.0008	0.0215	0.0041	0.0009	0.0008	0.0016	0.0076	0.0325	0.0009	0.0073	0.0018	0.0326	0.0210
20	0.0008	0.0212	0.0039	0.0010	0.0008	0.0017	0.0074	0.0286	0.0010	0.0074	0.0018	0.0314	0.0205

Table C.4 (Continued)

Tray	VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
21	0.0009	0.0210	0.0035	0.0011	0.0009	0.0018	0.0073	0.0255	0.0011	0.0073	0.0019	0.0302	0.0200
22	0.0006	0.0213	0.0035	0.0008	0.0007	0.0015	0.0068	0.0234	0.0008	0.0068	0.0016	0.0291	0.0190
23	0.0007	0.0216	0.0031	0.0009	0.0007	0.0016	0.0067	0.0216	0.0009	0.0066	0.0017	0.0273	0.0183
24	0.0007	0.0225	0.0027	0.0010	0.0006	0.0016	0.0066	0.0203	0.0009	0.0061	0.0016	0.0253	0.0173
25	0.0008	0.0238	0.0020	0.0011	0.0006	0.0016	0.0066	0.0193	0.0011	0.0055	0.0016	0.0228	0.0162
26	0.0006	0.0226	0.0031	0.0009	0.0005	0.0016	0.0063	0.0185	0.0008	0.0054	0.0015	0.0275	0.0156
27	0.0007	0.0215	0.0040	0.0008	0.0007	0.0017	0.0062	0.0177	0.0008	0.0057	0.0016	0.0319	0.0154
28	0.0005	0.0206	0.0050	0.0006	0.0006	0.0018	0.0059	0.0172	0.0005	0.0059	0.0015	0.0362	0.0152
29	0.0005	0.0199	0.0060	0.0004	0.0005	0.0018	0.0056	0.0167	0.0004	0.0062	0.0015	0.0406	0.0152
30	0.0003	0.0193	0.0071	0.0001	0.0004	0.0017	0.0052	0.0163	0.0002	0.0065	0.0014	0.0450	0.0152
31	0.0001	0.0191	0.0084	0.0004	0.0001	0.0015	0.0046	0.0162	0.0005	0.0066	0.0010	0.0495	0.0151
32	0.0005	0.0189	0.0096	0.0008	0.0003	0.0013	0.0041	0.0161	0.0009	0.0070	0.0008	0.0536	0.0152
33	0.0003	0.0180	0.0099	0.0005	0.0004	0.0018	0.0043	0.0152	0.0007	0.0079	0.0013	0.0563	0.0160
34	0.0004	0.0179	0.0107	0.0008	0.0002	0.0016	0.0039	0.0151	0.0009	0.0080	0.0010	0.0588	0.0159
35	0.0005	0.0176	0.0111	0.0010	0.0003	0.0015	0.0036	0.0149	0.0011	0.0080	0.0008	0.0596	0.0157
36	0.0005	0.0169	0.0110	0.0009	0.0003	0.0016	0.0036	0.0144	0.0010	0.0080	0.0010	0.0586	0.0155
37	0.0004	0.0163	0.0104	0.0008	0.0003	0.0016	0.0036	0.0140	0.0010	0.0076	0.0010	0.0557	0.0149
38	0.0005	0.0160	0.0098	0.0010	0.0003	0.0012	0.0034	0.0140	0.0010	0.0066	0.0006	0.0515	0.0136
39	0.0003	0.0150	0.0084	0.0006	0.0003	0.0014	0.0039	0.0134	0.0007	0.0059	0.0009	0.0455	0.0127
40	0.0003	0.0143	0.0070	0.0003	0.0003	0.0013	0.0041	0.0130	0.0005	0.0048	0.0009	0.0389	0.0113

Table C.4 (Continued)

Tray	qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
1	0.0253	0.0606	0.1129	0.0029	0.0447	0.2248	0.0017	0.1055	0.2564	1.6901	0.0511	0.2485	3.0493
2	0.0237	0.0567	0.1056	0.0027	0.0419	0.2103	0.0016	0.0987	0.2380	1.5899	0.0477	0.2333	2.8624
3	0.0223	0.0533	0.0992	0.0025	0.0394	0.1977	0.0016	0.0929	0.2216	1.5023	0.0447	0.2204	2.7003
4	0.0212	0.0504	0.0938	0.0024	0.0372	0.1869	0.0016	0.0879	0.2073	1.4251	0.0422	0.2090	2.5579
5	0.0201	0.0477	0.0888	0.0023	0.0352	0.1771	0.0017	0.0833	0.1952	1.3564	0.0398	0.1988	2.4323
6	0.0192	0.0454	0.0846	0.0022	0.0335	0.1687	0.0017	0.0794	0.1841	1.2952	0.0378	0.1893	2.3202
7	0.0184	0.0435	0.0809	0.0021	0.0322	0.1613	0.0016	0.0761	0.1741	1.2404	0.0361	0.1801	2.2201
8	0.0177	0.0416	0.0776	0.0020	0.0308	0.1547	0.0016	0.0730	0.1652	1.1908	0.0345	0.1714	2.1301
9	0.0170	0.0400	0.0746	0.0020	0.0296	0.1488	0.0016	0.0702	0.1573	1.1458	0.0330	0.1629	2.0493
10	0.0164	0.0385	0.0720	0.0019	0.0285	0.1436	0.0016	0.0677	0.1502	1.1049	0.0317	0.1545	1.9772
11	0.0159	0.0372	0.0698	0.0018	0.0276	0.1391	0.0015	0.0656	0.1437	1.0678	0.0305	0.1461	1.9128
12	0.0153	0.0358	0.0676	0.0018	0.0265	0.1350	0.0017	0.0634	0.1380	1.0337	0.0292	0.1380	1.8565
13	0.0150	0.0348	0.0661	0.0018	0.0258	0.1318	0.0016	0.0618	0.1326	1.0030	0.0283	0.1297	1.8077
14	0.0145	0.0335	0.0645	0.0017	0.0249	0.1289	0.0017	0.0600	0.1280	0.9748	0.0272	0.1220	1.7675
15	0.0141	0.0327	0.0620	0.0017	0.0244	0.1239	0.0016	0.0586	0.1228	0.9478	0.0264	0.1194	1.7068
16	0.0140	0.0321	0.0599	0.0017	0.0240	0.1194	0.0014	0.0576	0.1178	0.9227	0.0258	0.1171	1.6516
17	0.0136	0.0312	0.0575	0.0017	0.0233	0.1148	0.0016	0.0563	0.1136	0.8988	0.0247	0.1154	1.6010
18	0.0131	0.0301	0.0550	0.0017	0.0223	0.1103	0.0019	0.0549	0.1098	0.8760	0.0233	0.1140	1.5547
19	0.0131	0.0296	0.0533	0.0017	0.0219	0.1067	0.0017	0.0543	0.1058	0.8552	0.0224	0.1119	1.5109
20	0.0129	0.0289	0.0514	0.0018	0.0211	0.1030	0.0018	0.0536	0.1023	0.8352	0.0210	0.1097	1.4703

Table C.4 (Continued)

Tray	qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
21	0.0128	0.0282	0.0496	0.0018	0.0202	0.0995	0.0019	0.0533	0.0991	0.8163	0.0193	0.1071	1.4317
22	0.0131	0.0279	0.0483	0.0018	0.0195	0.0966	0.0016	0.0537	0.0958	0.7989	0.0176	0.1031	1.3941
23	0.0133	0.0273	0.0467	0.0019	0.0183	0.0935	0.0017	0.0543	0.0933	0.7821	0.0152	0.0984	1.3578
24	0.0139	0.0269	0.0452	0.0021	0.0168	0.0906	0.0017	0.0557	0.0910	0.7665	0.0122	0.0922	1.3219
25	0.0147	0.0264	0.0438	0.0022	0.0150	0.0878	0.0017	0.0579	0.0890	0.7520	0.0086	0.0842	1.2862
26	0.0140	0.0264	0.0426	0.0022	0.0184	0.0854	0.0016	0.0559	0.0860	0.7410	0.0132	0.0831	1.2746
27	0.0133	0.0263	0.0413	0.0021	0.0215	0.0830	0.0016	0.0541	0.0833	0.7305	0.0175	0.0833	1.2662
28	0.0129	0.0263	0.0403	0.0021	0.0246	0.0809	0.0014	0.0528	0.0803	0.7208	0.0218	0.0846	1.2603
29	0.0126	0.0265	0.0393	0.0021	0.0277	0.0789	0.0013	0.0518	0.0772	0.7118	0.0261	0.0871	1.2577
30	0.0123	0.0268	0.0385	0.0022	0.0310	0.0772	0.0011	0.0512	0.0739	0.7034	0.0305	0.0905	1.2574
31	0.0124	0.0274	0.0380	0.0024	0.0343	0.0757	0.0009	0.0511	0.0706	0.6956	0.0348	0.0946	1.2610
32	0.0125	0.0278	0.0374	0.0027	0.0374	0.0743	0.0008	0.0510	0.0673	0.6880	0.0388	0.0991	1.2661
33	0.0119	0.0275	0.0360	0.0025	0.0393	0.0721	0.0009	0.0501	0.0648	0.6794	0.0415	0.1041	1.2629
34	0.0119	0.0277	0.0355	0.0027	0.0412	0.0707	0.0008	0.0498	0.0620	0.6712	0.0441	0.1073	1.2601
35	0.0118	0.0276	0.0348	0.0028	0.0419	0.0692	0.0008	0.0490	0.0597	0.6622	0.0453	0.1087	1.2498
36	0.0114	0.0269	0.0339	0.0026	0.0412	0.0675	0.0008	0.0476	0.0583	0.6521	0.0449	0.1076	1.2281
37	0.0109	0.0260	0.0330	0.0025	0.0392	0.0658	0.0007	0.0457	0.0575	0.6411	0.0430	0.1032	1.1965
38	0.0107	0.0251	0.0325	0.0024	0.0363	0.0645	0.0007	0.0437	0.0570	0.6297	0.0401	0.0951	1.1573
39	0.0098	0.0234	0.0314	0.0020	0.0319	0.0626	0.0007	0.0407	0.0575	0.6172	0.0355	0.0847	1.1064
40	0.0092	0.0218	0.0305	0.0017	0.0272	0.0610	0.0007	0.0378	0.0583	0.6048	0.0305	0.0720	1.0525

Table C.5 IAE results of hydrogenation reactor and dehydrogenation reactor

Hydrogenation reactor		VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
Inlet stream	Temperature	0.0283	0.7839	0.0078	0.0042	0.0618	0.0005	0.0003	0.3088	0.0275	0.0068	0.0021	0.6799	0.1584
Reactor at 1 m length	Temperature	0.1465	1.0975	0.0118	0.0032	0.0350	0.0007	0.0004	0.4868	0.0399	0.0083	0.0014	0.6442	0.1578
Dehydrogenation reactor														
Inlet stream	Temperature	1.0634	7.5780	0.2977	0.0409	0.0444	0.0165	0.0434	68.4271	0.3856	0.1547	0.0294	3.2917	1.5192
Outlet stream	Temperature	1.1550	8.1750	0.3883	0.0578	0.0553	0.0213	0.0632	90.5791	0.4300	0.2154	0.0308	3.8416	1.5786

Table C.5 (Continued)

Hydrogenation reactor		qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
Inlet stream	Temperature	1.2586	0.0037	0.1187	0.1096	0.6545	0.2635	0.0025	0.0494	0.0027	0.0208	0.0006	0.0012	4.5564
Reactor at 1 m length	Temperature	1.1201	0.0028	0.1057	0.1912	1.4172	0.2105	0.0012	0.0447	0.0009	0.0253	0.0010	0.0134	5.7675
Dehydrogenation reactor														
Inlet stream	Temperature	1.9936	0.2958	12.323	1.4836	2.9712	17.891	0.0388	0.4238	0.2319	3.1077	1.0004	2.4856	127.1395
Outlet stream	Temperature	2.1281	0.3728	12.565	1.6147	3.4148	24.565	0.0492	0.5471	0.3689	3.3842	1.3106	3.2574	160.1696

Table C.6 IAE results of temperature of inlet columns stream

Phenol recycle column		VLV-100	VLV-101	VLV-103	VLV-104	VLV-106	VLV-107	VLV-109	VLV-110	VLV-111	VLV-113	VLV-114	qc1	qc2
Inlet stream	Temperature	0.2957	5.1532	0.3424	0.0519	0.2337	0.0041	0.0005	0.6428	0.1411	0.0234	0.0033	5.7668	0.3345
Cyclohexanone column														
Inlet stream	Temperature	0.0394	1.1501	0.1513	0.0161	0.0462	0.0450	0.0005	0.1309	0.0233	0.0038	0.0007	1.0316	0.0526
Inlet(recycle) stream	Temperature	0.0589	0.3514	0.0780	0.0157	0.0096	0.0035	0.0215	1.3068	0.0322	0.4286	0.0614	0.4143	3.8194

Table C.6 (Continued)

Phenol recycle column		qh1	qh2	qh3	wk1	qR1c	qR2h	qC1c	qC1r	qC2c	qC2r	T-100_Reflux	T-101_Reflux	SUM
Inlet stream	Temperature	3.5673	0.0233	0.2462	0.7343	4.0959	0.5427	0.0130	0.3309	0.0071	0.0756	0.0122	0.0626	22.7046
Cyclohexanone column														
Inlet stream	Temperature	0.7835	1.0036	0.0296	0.2025	0.7080	0.0703	0.1481	2.6640	0.0339	0.0109	0.6037	0.0114	8.9610
Inlet(recycle) stream	Temperature	0.0775	0.0531	3.0701	0.0839	0.3284	5.9340	0.0106	0.0788	0.1956	0.2648	0.2637	0.6432	17.6051

VITA

Mr. Kumchai Sukkongwaree was born on February 22, 1986 in Chonburi, Thailand. He graduated Bachelor Degree of Engineering in Chemical Engineering from Chulalongkorn University in 2007. After that she studied for master degree in Chemical Engineering and joined Control and Systems Engineering research group at Chulalongkorn University in 2008.