การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ของกระบวนการไฮโดรดีอัคคิเลชันที่มี แบบแผนบูรณาการของพลังงาน

นายยูเลียส เด็ดดี้ เหอมะวัน

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DESIGN OF PLANTWIDE CONTROL STRUCTURE OF HDA PROCESS
WITH ENERGY INTEGRATION SCHEMES

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A Dissertation Submitted in Partial Fulfillment of the Requirements
for the Degree of Doctor of Engineering in Chemical Engineering
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ยูเลียส เด็ดดี้ เหอมะวัน: การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ของกระบวนการไฮโดรดีอัคคิเลชันที่มี แบบแผนบูรณาการของพลังงาน. (DESIGN OF PLANTWIDE CONTROL STRUCTURE OF HDA PROCESS WITH ENERGY INTEGRATION SCHEMES) อ.ที่ปรึกษา: อาจารย์ ดร. มนตรี วงศ์ศรี , 216 หน้า. ISBN 974-53-1194-4

แม้ว่าจะมีการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์อย่างแพร่หลาย แต่ไม่มีรายงานการศึกษาการจัดการด้านพลังงานสำหรับกระบวนการที่พลังงานเบ็ดเสร็จ (heat integration) โดยเฉพาะอย่างยิ่ง การจัดการกับเส้นทางเดินความร้อน (heat pathways) เพื่อที่จะนำพลังงานกลับคืนสูงสุดทางพลวัต (dynamic maximum energy recovery, DMER) โดยงานวิจัยนี้ได้ทำการพัฒนาฮิวริสติกสำหรับการคัดเลือก และการจัดการกับเส้นทางเดินความร้อนสำหรับควบคุมกระบวนการแบบแพลนท์ไวด์

การจัดการกับเส้นทางการเชื่อมต่อความร้อนแบบฮิวริสติก (heat pathways heuristics, HPH) ของงานวิจัยนี้ได้ถูกนำมาใช้ร่วมกับวิธีการการควบคุมแบบแพลนท์ไวด์ของ Luyben เพื่อหารูปแบบระบบการจัดการเส้นทางเดินความร้อน และรูปแบบการควบคุมของกระบวนการไฮโดรดีอัลคิเลชั่นของโทลูอีน (HDA) ที่พลังงานเบ็ดเสร็จ (รูปแบบที่ 1,4 และ 6) เส้นทางเดินความร้อนในระบบถูกสืบค้นอย่างเป็นระบบ สำหรับจุดประสงค์ในการจัดการด้านพลังงานของระบบ เส้นทางเดินความร้อนที่เหมาะสมจะถูกเลือกโดยตัวควบคุมแบบซีเล็คทีฟ ซึ่งมีตัวสลับแบบโลว์ซีเล็คเตอร์ (Low Selector Switch, LSS) เพื่อกำหนดเส้นทางเดินของตัวรบกวนไปยังหน่วยทำความร้อนหรือหน่วยหล่อเย็น เพื่อให้เข้าสู่สภาวะ DMER ระบบการควบคุมนี้ได้ถูกทดสอบอย่างเข้มงวดภายใต้ภาวะแวดล้อมจำลองโดยใช้โปรแกรมจำลองกระบวนการ HYSYS

งานวิจัยนี้แสดงให้เห็นว่า LSS มีความสำคัญต่อการเลือกเส้นทางเดินความร้อนที่เหมาะสมในกระบวนการที่มีพลังงานเบ็ดเสร็จโดยการกำหนดและจัดการตัวรบกวนให้อยู่ในเส้นทางที่เข้าสู่สภาวะ DMER โครงสร้างการควบคุมแบบแพลนท์ไวด์ที่ออกแบบใหม่นี้ได้ถูกนำมาเปรียบเทียบกับงานวิจัยที่นำเสนอโดย Luyben ในปี 1999 พบว่า ผลตอบสนองของการใช้พลังงานในเตาเผาและหน่วยหล่อเย็นดีกว่างานที่นำมาเปรียบเทียบ เนื่องจากภาระของทั้งเตาเผาและหน่วยหล่อเย็นลดลง โดยภาระนี้ขึ้นอยู่กับตัวรบกวนทางความร้อนที่เข้าสู่ระบบ จากผลการจำลองทางพลวัต HPH เป็นส่วนสำคัญเพื่อให้ได้ DMER สูงสุดที่เป็นไปได้ จากการศึกษายังแสดงให้เห็นว่ารูปแบบพลังงานเบ็ดเสร็จที่ซับซ้อนทำให้สมรรถนะทางพลวัตแย่ลง

ภาควิชา	วิศวกรรมเคมี	ลายมือชื่อนิสิต......................................	
สาขาวิชา	วิศวกรรมเคมี	ลายมือชื่ออาจารย์ที่ปรึกษา...............................	
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KEY WORD: HDA PROCESS/ PLANTWIDE CONTROL/ SELECTIVE CONTROL/ HEAT PATHWAY HEURISTICS (HPH)/ DYNAMIC MER/ DYNAMIC SIMULATION

YULIUS DEDDY HERMAWAN: DESIGN OF PLANTWIDE CONTROL STRUCTURE OF HDA PROCESS WITH ENERGY INTEGRATION SCHEMES. DISSERTATION ADVISOR: MONTREE WONGSRI, D.Sc, 216 pp. ISBN 974-53-1194-4

Although several general designs of plantwide control have been developed, none of them has reported the energy management for energy-integrated plants, particularly in manipulating heat pathways in order to achieve dynamic maximum energy recovery (DMER). In this dissertation, the new heuristic of selection and manipulation of heat pathways for plantwide process control has been developed.

The proposed heat pathway heuristics (HPH) is used in conjunction with Luyben's plantwide control procedure to model heat pathway management systems and the control configurations of the hydrodealkylation of toluene (HDA) process with different energy integration schemes (i.e. alternatives 1, 4 and 6). Various heat pathways throughout the network are systematically investigated for the purpose of plantwide energy management. An appropriate heat pathway is selected by means of a selective controller with low selector switch (LSS) to direct the disturbance load to a heating or cooling utility unit in order to achieve DMER. Such control system is rigorously examined in HYSYS' dynamic simulation environment.

This study reveals that the LSS plays a significant role in selecting proper heat pathway through a complex energy-integrated plant in order to direct and manage the disturbance load in such a way that DMER can be achieved. The new designed plantwide control structure is compared with the earlier work given by Luyben et al. (1999). Better responses of the furnace and cooler utility consumptions are achieved here compared to the Luyben's control structure, since the duties for both furnace and cooler utilities could be reduced according to the input heat load disturbance. As shown in dynamic simulation study, the HPH is therefore considered useful to achieve the highest possible DMER. This study also confirms that the complex energy integration deteriorates the dynamic performances of the process.

Department	Chemical Engineering	Student's signature ……....………….
Field of study	Chemical Engineering	Advisor's signature …………..………
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CONTENTS

CHAPTER

Page

CHAPTER

Page

CHAPTER

Page

LIST OF FIGURES

Figure		**Page**

LIST OF TABLES

NOMENCLATURES

C_i	=	cold stream i
D^+	=	positive disturbance load
D^-	=	negative disturbance load
H_i	=	hot stream i
IAE	=	integral absolute error
P_B	=	the partial pressure of benzene, psia
P_D	=	the partial pressure of diphenyl, psia
P_H	=	the partial pressure of hydrogen, psia
P_T	=	the partial pressure of toluene, psia
r_1	=	reaction rate of main reaction to produce benzene (main product)
r_2	=	reaction rate of said reaction to produce diphenyl (by-product)
sp	=	set point
t	=	time, minute
T	=	temperature, Kelvin
y	=	output response
ε	=	error

CHAPTER I

INTRODUCTION

An important problem in process control is to develop effective control structures for complex whole plants. Over the last few decades, control analysis and control system design for chemical and petroleum processes have traditionally followed the unit operation approach (Stephanopoulos, 1983). First, all of the control loops were established individually for each unit or piece of the equipment in the plant. Then the pieces were combined together into an entire plant. This method works well when the processes are in cascade form (i.e. without material and energy recycles) or large surge tanks are installed for processes with recycle streams to isolate the individual units.

Nowadays, there is growing pressure to reduce capital investment, working capital and operating cost, and to improve safety and environmental concerns. Therefore, design engineers have to achieve these tasks by, for example, eliminating many surge tanks, increasing the number of recycle streams or introducing energy integration for both existing and new plants. Somehow, recycle streams and energy integrations 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, a plantwide process control strategy is required to operate an entire plant in order to achieve its objectives.

1.1 Background

Designing control system for complete plants is the ultimate goal of a control designer. The problem is quite large and complex. It involves a large number of theoretical and practical considerations such as the quality of controlled response, stability, the safety of the operating plant, the reliability of control system, the ease of operation and the cost of control system. Essentially, the plantwide control problem is how to develop the control loops in order to operate an entire process to meet its design objectives. The problem is extremely complex and is very much open-ended. There are a combinatorial number of possible choices and alternative strategies.

Most industrial processes contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. Furthermore, for the purpose of energy management, the various heat pathways through the network need to be identified, since these have a great effect on the utility requirements. Therefore, it is essential to device a control strategy to manage the disturbance load entering the process in such a way that the maximum energy recovery (MER) can always be achieved. Actually, MER should not be taken as a static value, i.e. its value varies according to the operating conditions, e.g. the input heat load disturbances.

In this dissertation, we present a control strategy for energy management, particularly in manipulating heat pathways in order to achieve the highest possible dynamic maximum energy recovery (DMER). There is no unified and widely acceptable theory for the design of control systems for complex energy integrated plants. Therefore, instead of presenting an abstract exposition of the various factors that affect control system design, we will use a particular plant as reference. The plant chosen for our research is the plant to produce benzene from the hydrodealkylation of toluene (HDA) process, since it consists of recycle streams and energy integrations. In this case, we chose the HDA process with energy integration schemes alternatives 1, 4, and 6 that given by Terril and Douglas (1987). The commercial software HYSYS is utilized to carry out both the steady state and dynamic simulations.

1.2 Objectives of the Research

The objectives of this study are listed below:

1. Identify heat pathways through the heat exchanger networks of HDA process.
2. Design the new plantwide control structures for HDA process with energy integration schemes (i.e. alternatives 1, 4, and 6) with the objective of selecting what path through the network should be used to carry the associated load to a utility unit, so that its duty will be decreased, hence MER can be achieved.

3. Propose the new heuristics for heat exchanger networks control configuration design and operation.

1.3 Scopes of the Research

Scopes of this research are listed below:

1. The HDA process with energy integration schemes (i.e. alternatives 1, 4, and 6 given by Terril and Douglas, 1987) is chosen for a case study.
2. The description of HDA process is given by Luyben et al. (1999) and Douglas (1988).
3. HYSYS software is utilized to carry out both the steady state and dynamic simulations.

1.4 Contributions of the Research

The contributions of this work are as follows:

1. Process flow diagrams of HDA process with energy integration alternatives 1, 4, and 6 have been simulated.
2. The new plantwide control structures for HDA process alternatives 1, 4 and 6 are designed and compared with the earlier work given by Luyben et al. (1999).
3. The new heat pathway heuristics (HPH) for heat exchanger networks control are proposed in order to achieve DMER.

1.5 Research Procedures

The procedures of this research are as follows:

1. Study of plantwide process control theory, HDA process and concerned information.
2. Steady state simulation of HDA process alternatives 1, 4, and 6.

2.1. Determine the operating conditions for each HEN alternative of HDA process based on the input disturbance loads.

2.2. Identify the heat pathways through the network for each HEN alternative of HDA process based on the input disturbance loads.

3. Development of the new plantwide control structures for HDA process alternatives 1, 4, and 6.
4. Dynamic simulation of HDA process alternatives 1, 4, and 6.
5. Evaluation of the dynamic performance of the designed control structures based on the input disturbance loads.
6. Correction and summarization of simulation results.

1.6 Outline of Dissertation

This dissertation has been divided into seven chapters.

In Chapter 2, a review of the previous work on the conceptual design of chemical processes, heat exchanger networks design, plantwide control design are given. Several previous works on the design and control of HDA process are also presented.

In Chapter 3, some background information of plantwide control fundamentals, plantwide control design procedure, and plantwide energy management are presented.

In Chapter 4, the steady state simulation of HDA process with different energy integration schemes (i.e. alternatives 1, 4, and 6) using HYSYS simulator are presented. Initially, the heat pathways through the networks of HDA process are systematically investigated for the purpose of plantwide energy management. Next, the heuristics of selection and manipulation of heat pathways for energy-integrated process is proposed. The control considerations are then developed for the energy-integrated process system.

In Chapter 5, the design of plantwide control structures and dynamic simulation are presented for HDA process with different energy integration schemes (i.e. alternatives 1, 4, and 6). The new plantwide control structures with heat pathways manipulator are implemented in HDA process and compared with the previous work given by Luyben et al. (1999).

In Chapter 6, the extended heuristic design procedure for heat exchanger networks control configuration and operation to achieve the dynamic MER is proposed. Several typical heat exchanger network examples are taken to describe the proposed design procedure for HEN control configuration.

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

CHAPTER II
LITERATURE REVIEW

The purpose of engineering is to create new material wealth. The chemical engineers attempt to accomplish this goal via the chemical (or biological) transformation and separation of materials. Therefore, design and control for the process is necessary to achieve the goal. Our purpose of this chapter is to present a review of the previous work on the conceptual design of chemical processes, heat exchanger networks design, and plantwide control design.

2.1 A Hierarchical Approach to Conceptual Design

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

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

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

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

Beside controllability analysis, Fisher et al. (1988b) also focused on operability analysis. The goal of operability analysis is to ensure that there is an adequate amount of equipment over-design so that they could satisfy the process constraints and minimize a combination of the operating costs and over-design costs over the entire range of anticipated process disturbances. They also followed the same hierarchical procedure to develop operability analysis. For HDA process, the operability decisions were encountered at each level. Fisher et al. (1988c) proposed steady-state control structure for HDA process using an optimum steady-state control analysis. They found the values of manipulated variables (that minimize the total operating costs for various values of the disturbances) and used them to define the controlled variables.

2.2 Heat Exchanger Networks (HENs)

Energy conservation has always been important in process design. Thus it was common practice to install feed-effluent heat exchangers (FEHEs) in paralel with reactors and distillation columns. The starting point for an energy integration analysis is the calculation of the minimum heating and cooling requirements for heat exchanger network (HEN).

Linnhoff, 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 feature 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% energy savings, coupled with capital savings, can be realised in state-of-the art flowsheets by improving 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.

Generally, minimum cost networks feature the correct degree of energy recovery and the correct number of units. This is achieved in two stages. First, the method aims for a minimum energy solution, corresponding to a specified ΔT_{min}, with no more units that is compatible with minimum energy. This task is achieved through understanding of the pinch phenomenon, hence the method is called the pinch design method. Second, the method involves a controlled reduction in number of units. This may require "backing-off" from minimum utility usage.

The pinch design method also identifies situations where stream splitting is inevitable for a minimum utility design. The pinch design method incorporates five important stages. These are:

1. The HEN problem is divided at the pinch into separate problems.
2. The design for this separate problems is started at the pinch and developed moving away from the pinch. At the pinch essential matches, match options and stream splitting requirements are identified by applying the feasibility criteria.
3. When options exist at the pinch, the engineer is free to base his selection to suit the process requirements.
4. The heat loads of exchangers at the pinch are determined using the stream tick-off heuristic. In case of difficulty (increased utility usage) a different exchanger topology at the pinch can be chosen or the load on the offending match can be reduced.
5. Away from the pinch there is generally a free choice of matches. The procedure does not insist on particular matches but allows the designers to discriminate between matches based on his judgment and process knowledge.

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 pinch 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.

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 (the DESIGN problem), and sequence the control action of the loops, to accommodate set-point changes and reject load disturbances (the OPERATIONAL problem). The approach proposed exploits the structure characteristics of a HEN by identifying routes through the HEN structure that can allocate loads (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 existance of a process pinch. An online, real-time planning of control actions is the essence of implementational 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. Although this study provided the comprehensive summary of work on the design of control loop configuration in HENs, it did not report the control strategy, particularly in selecting and manipulating proper heat pathway. In this current study, we present the control strategy; how to select proper heat pathway to carry the associated load to a utility unit, so its duty will be decreased.

In a series of papers, Terrill and Douglas (1987a,b,c) studied the sensitivity of the total processing cost to heat exchanger network alternatives and steady state operability evaluation. They considered the temperature-enthalpy (T-H) diagram and developed six HEN alternatives for a base case design for HDA process, in which their energy saving ranges between 29 and 43%. The simplest of these designs is alternative 1, recovers an additional 29 percent of the base case heat consumption by making the reactor preheater larger and the furnace smaller. The most complex of the designs is alternative 6, recovers 43 percent of the base case net energy consumption. However, those alternatives have not been developed under dynamic simulation to study their dynamic aspects. In this dissertation, we present both the steady state and dynamic simulations for energy-integrated HDA plant (i.e. alternatives 1, 4, and 6), as presented in Chapter 4 and 5.

Wongsri, M. (1990) studied a resilient HEN 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 changes 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 temperature of hot streams are at the lowest and those of cold streams are at the highest. Thus, only the positive disturbance loads of process streams were cosidered. In this dissertation, we will consider both positive and negative disturbance loads that are coming from the process streams.

2.3 Design and Control of Energy-Integrated Plants

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

Silverstein and Shinnar (1982) discussed the linear and nonlinear stability analysis of a fixed bed catalytic reactor with heat exchange between the feed and product streams, with special emphasis on cases which are open loop unstable. They used classical frequency response techniques, contains the implicit assumption that the designer should evaluate the effect of the overall design on stability. Tyerus, B.D. and Luyben, W.L., (1993) presented a mathematical analysis of the unusual dynamic in coupled reactor/preheater process. The outlet temperature of the reactor exhibits inverse response (wrong-way behavior) for a change in the inlet reactor temperature and a large dead time.

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

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

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 units. The nine steps 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; make-up 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.

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

Although several workers have studied the general design and control of energy-integrated plants, there is no report on study of the energy management, particularly in manipulating heat pathways in order to achieve the highest posible dynamic MER. Actually, MER is not constant, its value varies according to the operating conditions, e.g. the input heat load disturbance. Therefore, for the process associated with energy integration, the study of heat pathways management is very important to manage the disturbance load in such a way that MER can always be achieved. In this dissertation, study of heat pathway management for plantwide control of energy-integrated HDA plant based on steady sate and dynamic simulations are presented in Chapters 4 and 5. The new heuristic design procedure for heat exchanger networks control configuration and operation is presented in Chapter 6.

CHAPTER III
PLANTWIDE CONTROL FUNDAMENTALS

Plantwide process control is very important to control an entire chemical plant with many interconnected unit operations. Given a complex, integrated process and a diverse assortment of equipment, we must devise the necessary logic and strategies to operate the plant safely and to achieve its design objectives. Our purpose of this chapter is to present plantwide control fundamentals.

3.1 Incentives for Chemical Process Control

A chemical plant is an arrangement of processing units (reactors, heat exchangers, pumps, distillation columns, absorbers, evaporators, tanks, etc.), integrated with one another in a systematic and rational manner. The plant's overall objective is to convert certain raw materials into desired products using available sources of energy, in the most economical way.

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

3.1.1 Suppressing the Influence of External Disturbances

Suppressing the influence of external disturbances on a process is the most common objective of a controller in a chemical plant. Such disturbances, which denote the effect that the surroundings (external world) have on a reactor, separator, heat exchanger, compressor and so on, are usually out of the reach of human operator. Consequently, we need to introduce a control mechanism that will make the proper change on the process to cancel the negative impact that such disturbances may have on the desired operation of a chemical plant. In other words, in order to face all disturbances entering the process, the strategies for control are very important.

3.1.2 Ensuring the Stability of a Chemical Process

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

3.1.3 Optimizing the Performance of a Chemical Process

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

3.2 Integrated Processes

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

3.2.1 Material Recycle

Material is recycled for six basic and important reasons

a. *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.

b. *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.

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

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

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

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

3.2.2 Energy Integration

The fundamental reason for the use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost. For energy-intensive processes, the savings can be quite significant.

3.2.3 Chemical Component Inventories

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

3.3 Basic Concepts of Plantwide Control

3.3.1 Buckley Basics:

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

3.3.2 Douglas Doctrines:

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

a. Minimize losses of reactants and products
b. Maximize flowrates through gas recycle systems.

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

3.3.3 Down Drill

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

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

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

3.3.4 Luyben Laws

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

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

b. A fresh reactant feed stream cannot be flow controlled unless there is essentially complete one pass conversion of one of reactants. This law applies to systems with reaction types such as A + B → products. In system with consecutive reactions such as A + B → M + C and M + B → D + C, the fresh feed can be flow controlled into the system, because any imbalance in the ratios of reactants is accommodated by a shift in the amounts of the two products (M and D) that are generated. An excess of A will result in the production of more M and less D. And vice versa, an excess of B results in the production of more D and less M.

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

3.3.5 Richardson Rule

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

3.3.6 Tyreus Tuning

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

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

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

$K_{TL} = K_u/3.2 \qquad \tau_{TL} = 2.2\ P_u$

The use of PID controllers should be restricted to those loops were two criteria are both satisfied: the controlled variable should have a very large signal-to-noise ratio and tight dynamic control is really essential.

3.4 Plantwide Control Design Procedure

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

3.4.1 Establish Control Objectives

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

3.4.2 Determine Control Degrees of Freedom

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

3.4.3 Establish Energy Management System

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

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

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

3.4.4 Set Production Rate

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

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

3.4.5 Control Product Quality and Handle Safety, Operational and Environmental Constraints

Select the best valves to control each of the product-quality, safety, and environmental variables. We want tight control of these quantities for economic and operational reasons. Hence we should select manipulated variables such that the dynamic relationships between controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants, and the latter prevents problems with the range-ability of the manipulated variable (control-valve saturation)

3.4.6 Control Inventories (Pressure and Liquid Level) and Fix a Flow in Every Recycle Loop

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

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

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

3.4.7 Check Component Balances

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

Light, intermediate, and heavy inert components must have an exit path from the system. Reactant must be consumed in the reaction section or leaves as impurities in the product streams. Fresh reactant makeup feed stream can be manipulated to control reactor feed composition or a recycle stream composition (or to hold pressure or level as noted in previous step). Purge stream can also be used to control the amount of high- or low-boiling impurities in a recycle stream.

3.4.8 Control Individual Unit Operations

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

3.4.9 Optimize Economic and Improve Dynamic Controllability

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

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

3.5 Plantwide Energy Management

Energy conservation has always been important in process design. Thus, it is common practice to install feed-effluent heat exchangers (FEHEs) around rectors and distillation columns. In any process flowsheet, a number of streams must be heated, and other streams must be cooled. For example, in HDA process, the toluene fresh feed, the makeup hydrogen, the recycle toluene, and the recycle gas stream must be heated up to the reaction temperature 621.1 ^oC. And, the reactor effluent stream must also be cooled to the cooling water temperature to accomplish a phase split. Therefore, the energy integration is required to reduce the utility cost and also to improve thermodynamic efficiency of the process.

3.5.1 Heat Exchanger Dynamics

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

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

3.5.2 Heat Pathways

A path is a connection between a heater and a cooler in a network. In plantwide energy management, various pathways for heat need to be identified. Furthermore, a control strategy that allows effective delivery and removal of energy is needed to minimize propagation of thermal disturbances. It is important to realize that there are no thermodynamic restrictions on the energy requirement to transition streams between unit operations. In other words, the heating and cooling of streams are done for practical reasons and not to satisfy the laws of thermodynamics. This energy would not be an issue if all the processing steps operated at the same constant temperature. Furthermore, since raw materials and products are stored at roughly the same temperature, the net energy requirement for heating and cooling equal the heat losses from the process.

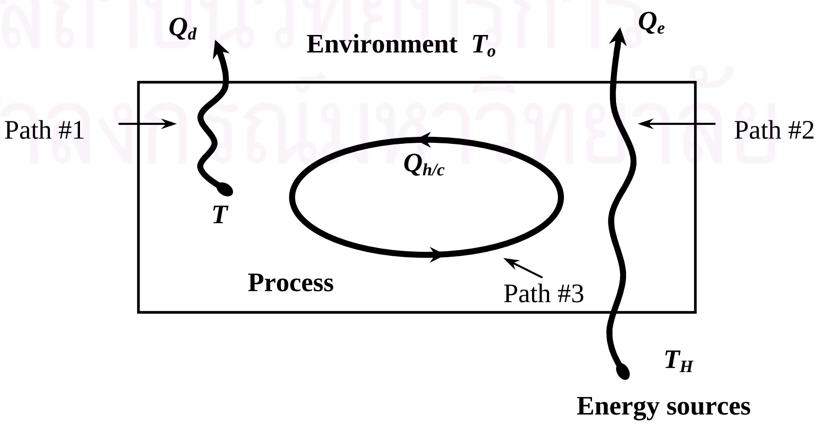


Figure 3.1 Heat pathways

From plantwide perspective we can now discern three different "heat pathways" in the process as illustrated in Figure 3.1. The first pathway, heat from the process is dissipated to the environment, e.g. heat generated by exothermic reactions and by degradation of mechanical work (e.g., compression, pressure drop and friction). This pathway is from inside the process and flows out. It is of course possible to convert some of the heat to work as it is removed from high temperature in the process.

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

The third pathway is internal to the process. Here heat flows back and forth between different unit operations. The magnitude of this energy path depends upon the heating and cooling needs and the amount of heat integration implemented. Whenever the internal path is missing, and there is a heating requirement, the heat has to be supplied from utilities. The same amount of heat must eventually be rejected to the environment elsewhere in the process.

3.5.3 Heat Recovery

Usually, chemical processes are thermally inefficient. First, the chemical work available in the reactants is dissipated as heat. Second, the work required for separation is usually supplied as heat to distillation column, which have internal inefficiencies. Finally, energy is needed for heating and cooling functions that are independent of thermodynamic constraints. This all adds up to a low thermal efficiency.

Fortunately, we can make great improvements in plant's thermal efficiency by recycling much of the energy needed for heating and cooling process streams. It is also possible to introduce heat integration schemes for distillation columns to reduce the separation heat. And finally the reaction heat can be recovered in waste heat boilers and use the steam for power generation. There is of course a capital expense associated with improved efficiency but it can usually be justified when the energy savings are accounted for during the lifetime of the project. Of more interest to us in the current context is how heat integration affects the dynamics and control of a plant and how we can manage energy in plants with a high degree of heat recovery.

3.6 Control of Process-to-Process Exchangers

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

3.6.1 Use of Auxiliary Exchangers

When the P/P exchanger is combined with a utility exchanger, we also have a few design decisions to make. The utility exchanger can be installed to P/P exchanger either in series or paralel. Figure 3.2 shows the combination of P/P exchanger with a utility exchanger. Generally, the utility system of a complex energy-integrated plant

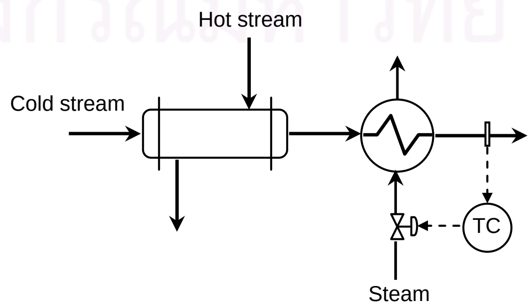


Figure 3.2 Control of process-to-process heat exchanger using the auxiliary utility.

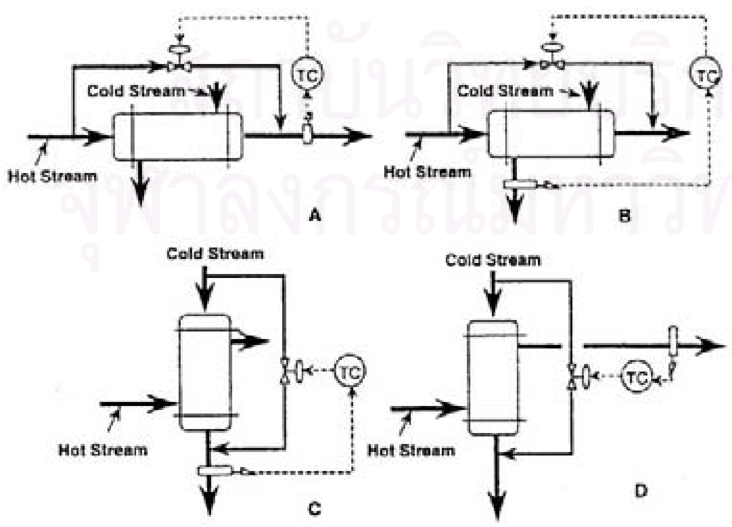
is designed to absorb large disturbances in the process, and making process-to-utility exchangers relatively easy to control.

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

3.6.2 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 3.3 shows the most common alternatives. For choosing the best option, it depends on how we define the best. Design consideration might suggest, we measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high-temperature service. Cost consideration would also suggest a small bypass flow to minimize the exchanger and control valve sizes.

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 Fig 3.3.a and c). This minimizes the effects of exchanger dynamics in the loop. We should also want to bypass a large fraction of the controlled stream since it improves



Notes:

(a) controlling and bypassing hot stream;
(b) controlling cold stream and bypassing hot stream;
(c) controlling and bypassing cold stream;
(d) controlling hot stream and bypassing cold stream.

Figure 3.3 Bypass controls of process-to-process heat exchangers the control range. This requires a large heat exchanger. There are several general heuristic guidelines for heat exchanger bypass streams. We typically want to bypass the flow of the stream whose temperature we want to control. The bypass should be about 5 to 10 percent of the flow to be able to handle disturbances. Finally, we must carefully consider the fluid mechanics of the bypass design for the pressure drops through the control valves and heat exchanger.

3.7 Dynamic Simulation in HYSYS

Dynamic simulation can help us to better design, optimize, and operate our chemical process or refining plant. Chemical plants are never truly at steady state. Feed and environmental disturbances, heat exchanger fouling and catalytic degradation continuously upset the condition of a smooth running process. The transient behavior of the process is best studied using a dynamic simulation tool like HYSYS.

The design and optimization of a chemical process involves the study of both steady state and dynamic behavior. Steady state models can perform steady state energy and material balances and evaluate different plant scenarios. The design engineer can use steady state simulation to optimize the process by reducing capital and equipment cost while maximizing production.

With dynamic simulation, we can confirm that the plant can produce the desired product in a manner that is safe and easy to operate. By defining detailed equipment specifications in dynamic simulation, we can verify that the equipment will function as expected in an actual plant situation. Off-line dynamic simulation can optimize controller design without adversely affecting the profitability or safety of the plant. We can design and test a variety of control strategies before choosing one that may be suitable for implementation. We can also examine and the dynamic response to system disturbance and optimize the tuning of controllers. Dynamic analysis provides feedback and improves the steady state model by identifying specific areas in a plant that may have difficulty achieving the steady state objectives.

In HYSYS, the dynamic analysis of a process system can provide insight into understanding it that is not possible with steady state modeling. The dynamic simulations in HYSYS are involving process optimization, controller optimization, safety evaluation, transitions between operating conditions, and startup/shutdown conditions. The HYSYS dynamic model simulates the thermal, equilibrium and reactive behavior of the chemical system in similar way to the steady state model.

On the other hand, the dynamic model uses different set of conservation equations, which account for changes occurring over time. The equations for material, energy, and composition balances include an additional accumulation term, which is differentiated with respect to time. Non-linear equations can be formulated to approximate the conservation principles. However, an analytical solution method does not exist.

Therefore, numerical integration is used to determine the process behavior at distinct time steps. The smaller the time step, the more closely the calculated solution will match with the analytic solution. However, this gain in rigor is offset by the additional calculation time required to simulate the same amount of elapsed real time. A reasonable compromise may be achieved by using the largest possible step size, while maintaining an acceptable degree of accuracy without becoming unstable.

CHAPTER IV
DESIGN OF HEAT PATHWAYS FOR DYNAMIC MER: PART 1. HEAT LOAD TRAFFIC MANAGEMENT OF HDA PROCESS

In this chapter, design of heat pathways for dynamic maximum energy recovery (DMER) is introduced and applied to the hydrodealkylation of toluene (HDA) process with different energy integration schemes (i.e. alternatives 1, 4, and 6) based on steady state considerations. Our purpose of this chapter is to illustrate the important phenomena of heat load traffic occurring in the process.

4.1 Introduction

Most industrial processes contain a complex flowsheet with several recycle streams and energy integrations. In an adiabatic reactor, the heat of the exothermic reactions can be recovered by preheating the reactants. A typical example is the feed-effluent-heat-exchanger (FEHE), where the hot reactor product is used to heat up the reactants prior to the furnace (see Figure 4.1.a). However, the use of FEHE can recover some of energy from the adiabatic reactor. This reduces the amount of fuel required in the furnace to heat up the reactants and the duty required to cool the reactor effluent stream. The process configurations can become even more complex as plantwide energy management is taken into consideration. For example, multiple FEHEs (see Figure 4.1.b) are required when the hot reactor product is also used to drive reboiler in the distillation column.

In view of the importance of energy integration for large industrial processes, the goals of this chapter are to identify the various heat pathways through the whole network with single FEHE and multiple FEHEs. Strategies for plantwide control can be then generated based on the heat pathway heuristics (HPH) with the objective of selecting what path through the HEN should be used to carry the associated load to the utility unit, so that the DMER will be obtained.

Heat integrated schemes can become very complex when plantwide energy management is taken into consideration (e.g. alternatives 4 and 6 of HDA process). Furthermore, the positive feedback (i.e. mass and heat recycle streams) makes the plants more difficult to control. Therefore, it is necessary to first understand the steady state heat load traffic management of the process associated with energy integration before a full dynamic study is undertaken. Consequently, the understanding of the steady state operation, specifically the manipulation of the flow of heat loads is one of the key objectives in this study.

The HDA processes with different energy integration schemes (i.e alternative 1, 4 and 6) are chosen to demonstrate the effective principles of plantwide control using the heat pathway heuristics (HPH). Kinds of disturbance loads and heat pathways are identified, and then strategies for plantwide control are considered. The commercial software HYSYS is utilized to carry out both the steady state and dynamic simulations. The dynamic behaviors of designed plantwide control in the energy-integrated HDA process will be explored in Chapter 5.

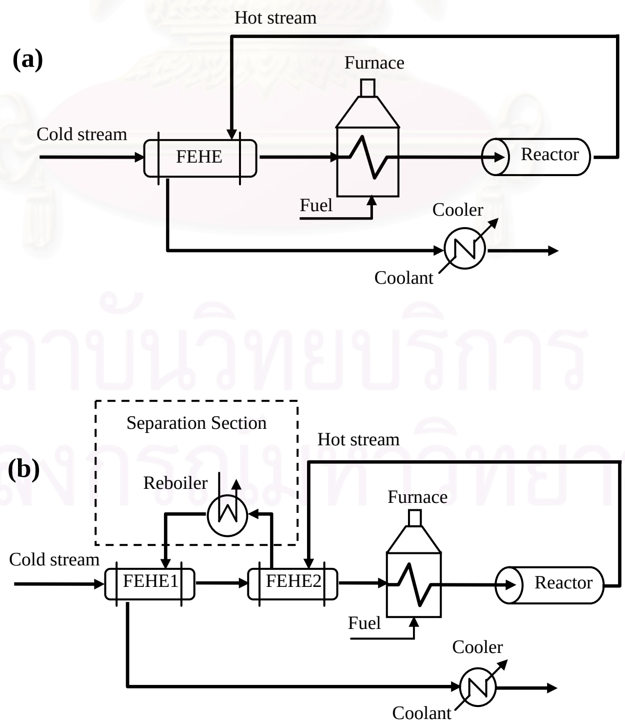


Figure 4.1 Heat-integrated reactor systems with: (a) single FEHE, (b) multiple FEHEs

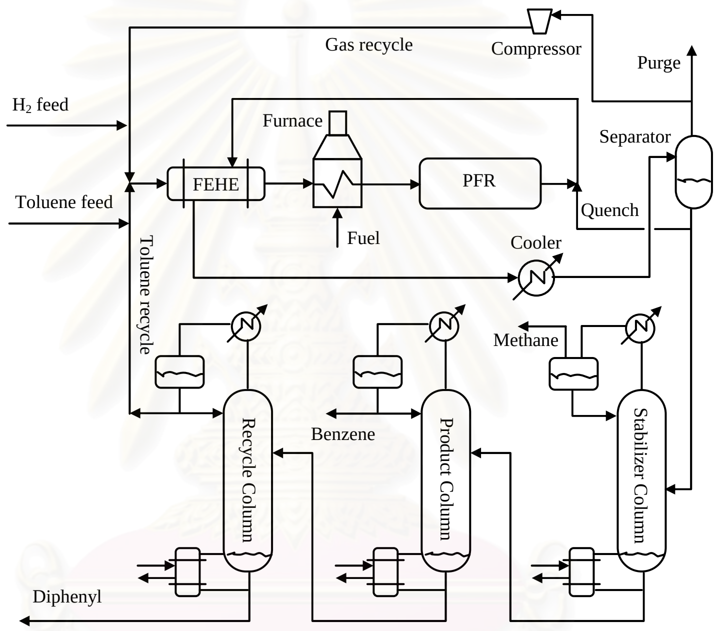


Figure 4.2 Process flow diagram of HDA process alternative 1*

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* from Terrill and Douglas (1987)

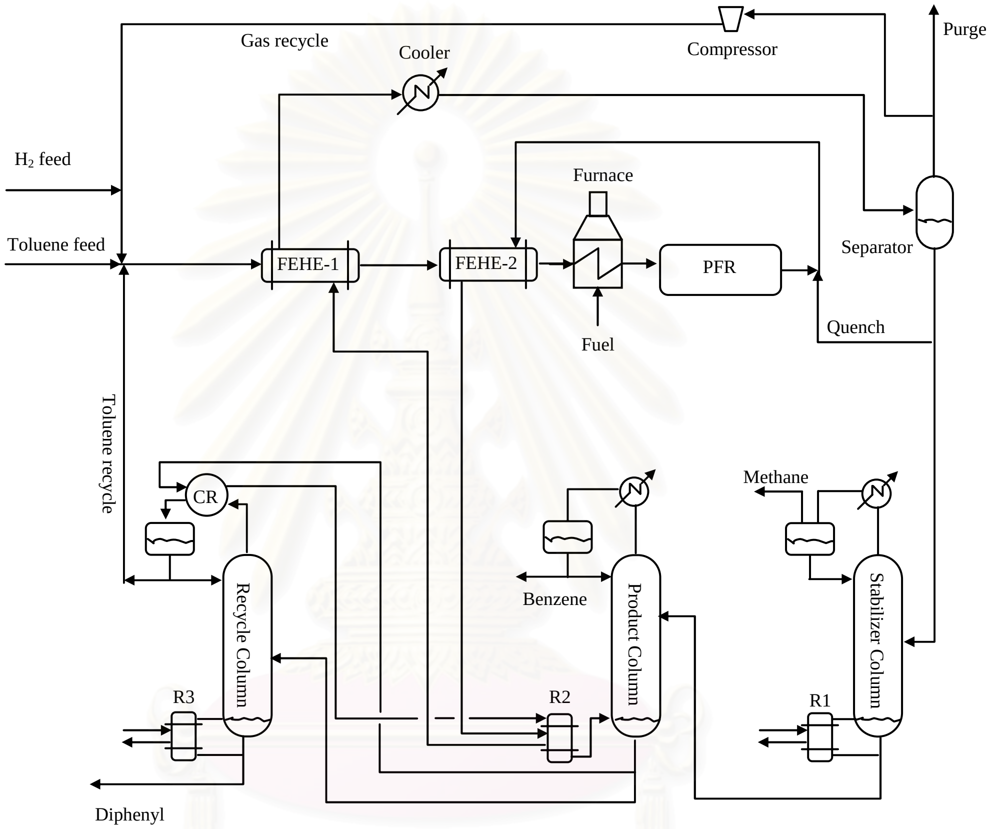


Figure 4.3 Process flow diagram of HDA process alternative 4*

* from Terrill and Douglas (1987)

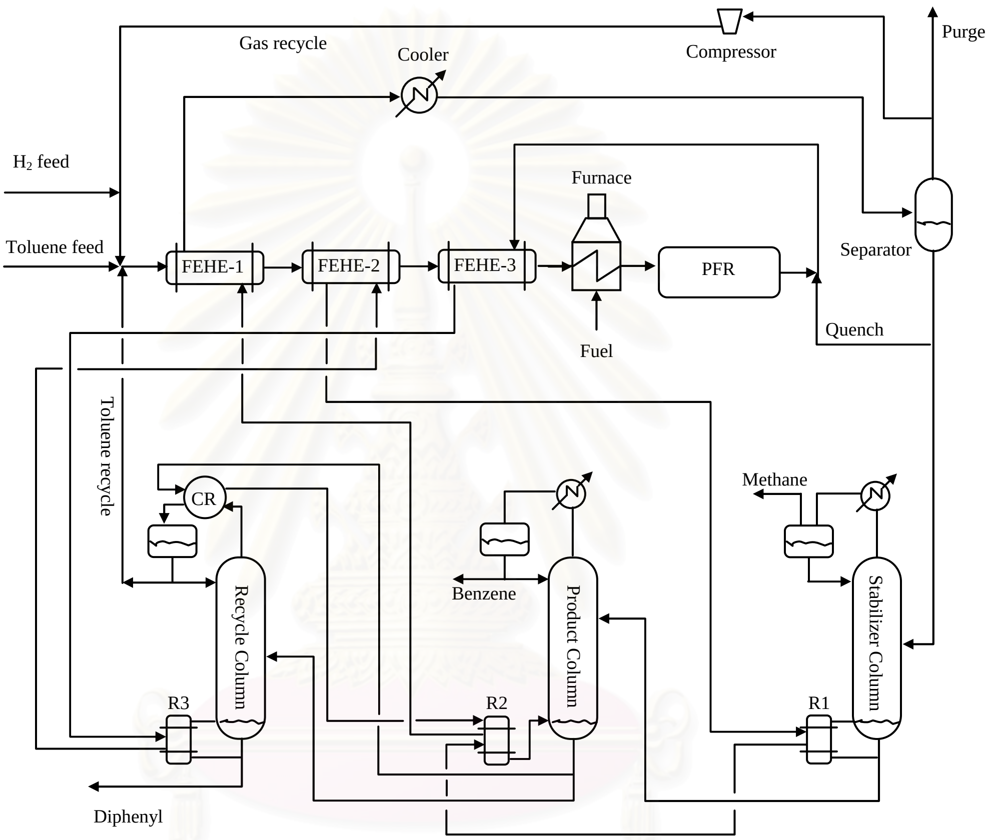


Figure 4.4 Process flow diagram of HDA process alternative 6*

* from Terril and Douglas (1987)

4.2 HDA Process Description

The HDA process (Figure 4.2) contains nine basic unit operations: reactor, furnace, cooler, separator, compressor, feed-effluent-heat-exchanger (FEHE), and three distillation columns (Douglas, 1988). Hydrogen and toluene are converted into the benzene product in the adiabatic plug flow reactor (PFR), with methane and diphenyl produced as by-products. The two vapor-phase reactions are:

$$C_7H_8\ (Toluene) + H_2\ (Hydrogen) \rightarrow C_6H_6\ (Benzene) + CH_4\ (Methane) \qquad (4.1)$$

$$2\ C_6H_6\ (Benzene) \leftrightarrow C12H10\ (Diphenyl) + H_2\ (Hydrogen) \qquad (4.2)$$

The effluent from the adiabatic reactor is quenched with liquid from the separator to prevent coking in the heat exchanger. This quenched stream is the hot-side feed to the FEHE, where the cold stream is the reactor feed stream prior to the furnace. The reactor effluent is then cooled with cooling water, and the vapor (hydrogen, methane) and liquid (benzene, toluene, diphenyl) are separated. Part of the vapor coming from the separator is purged to remove the methane by-product and the remainder is compressed and recycled back to the reactor.

The liquid stream from the separator, after a fraction of it is taken for quenching, is fed to the stabilizer column, which has a partial condenser and removes any remaining hydrogen and methane gas from the liquid components. The bottoms stream from stabilizer is fed to the product column, where the distillate is the benzene product from the process and the bottoms is toluene and diphenyl that is fed to the recycle column. The distillate from the recycle column is toluene recycled back to the reactor and the bottoms is the diphenyl by-product. Make up toluene liquid and hydrogen gas are added to both the gas and toluene recycle streams. This combined stream is the cold-side feed to the FEHE. The cold-side exit stream is then heated further up to the required reactor inlet temperature in the furnace, where heat is supplied via combustion of fuel.

Six alternative HENs for the HDA process had been generated (Terril and Douglas, 1987). Alternative 1 has simply an enlarged FEHE (Figure 4.2). Alternative 2 is the same as alternative 1, except the recycle column is pressure shifted to be above the pinch temperature, and the condenser for the recycle column is used to drive the product column reboiler. All of the other alternatives also include this pressure shifting. In alternative 3, the reactor effluent is used to drive the stabilizer column reboiler, whereas in alternative 4 the reactor effluent is used to drive the product column reboiler. For alternative 5, the reactor effluent stream is used to drive both the stabilizer column reboiler and the product column reboiler consecutively. Alternative 6 is the most complex one, since it consists of three FEHEs and all the reboilers in the three columns are driven by the reactor effluent stream. In this work, we consider only alternatives 1, 4 and 6. Figures 4.3 and 4.4 show the process flow diagram for HDA process alternatives 4 and 6, respectively.

4.3 Heat Pathway Heuristics (HPH) for Energy-Integrated Plants

The optimum steady state design must be able to tolerate the plant disturbances. Since the plant disturbances (e.g. the feed stream temperature, the feed flowrates) are not taken as static values, the heat load changes. Thus, those disturbances can propagate to the whole process. A control strategy is required to manage those disturbance loads, so that MER can always be achieved.

4.3.1 Disturbance Loads and Propagations

In the process heat integration, there are two kinds of disturbance loads (Wongsri, 1990). The first disturbance load is *Positive disturbance load* D^+ i.e. a disturbance that will increase the heat load of stream. For example, when the inlet temperature of a disturbed hot stream increases or when the inlet temperature of a disturbed cold stream decreases. The disturbance load must be dissipated as much as possible by transferring or shifting it to the streams that are serviced by utility exchangers. The positive disturbance load of a hot stream will increase heat duties of coolers and decrease heat duties of heaters. The positive disturbance load of a cold stream will increase heat duties of heaters and decrease heat duties of coolers.

The second disturbance load is *Negative disturbance load* D^- i.e. a disturbance that will decrease the heat load of stream. For example, when the inlet temperature of a disturbed hot stream decreases or when the inlet temperature of a disturbed cold stream increases. The differences in heat load must be then provided by utility exchangers so that the design objective is to construct a network that has thermal links between the disturbance source and the utility exchangers. The negative disturbance load of a hot stream will increase heat duties of heaters and decrease heat duties of coolers. The negative disturbance load of a cold stream will decrease heat duties of heaters and increase heat duties of coolers.

4.3.2 Design of Heat Pathways for HEN with single FEHE

In this work, the heuristics of selection and manipulation of heat pathways is proposed. For the purpose of plantwide energy management, various pathways for heat need to be identified. It is expected that the heat load disturbance through the heat and mass integrated network vary significantly, so does the maximum energy recovery (MER). Therefore, the plantwide control strategies to achieve the highest possible dynamic MER based on the heat pathway heuristics (HPH) i.e. selecting an appropriate heat pathway to carry associated load to a utility unit is very crucial.

Based on the positive effects of the disturbance loads on the utility requirements, we attempt to shift the heat load disturbances to either heater or cooler utility unit in a way that the DMER is realized. Therefore, the utility duties of these units will be decreased as the disturbance is entering the process. A simplified HEN as shown in Figure 4.5 is used to explain how an appropriate heat pathway should be activated to carry associated load to the utility unit. For instance, when the inlet temperature of a disturbed cold stream decreases, path 1 (Figure 4.5.a) should be activated by controlling the cold outlet temperature of FEHE. This will have the effect of shifting the positive disturbance load to the cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty. Consider the case when the inlet temperature of a disturbed cold stream increases, path 2 (Figure 4.5.b) should be activated by controlling the hot outlet temperature of FEHE to shift its negative disturbance load to heater. Thus, the negative disturbance load of a cold stream will result in decrease of the heater duty.

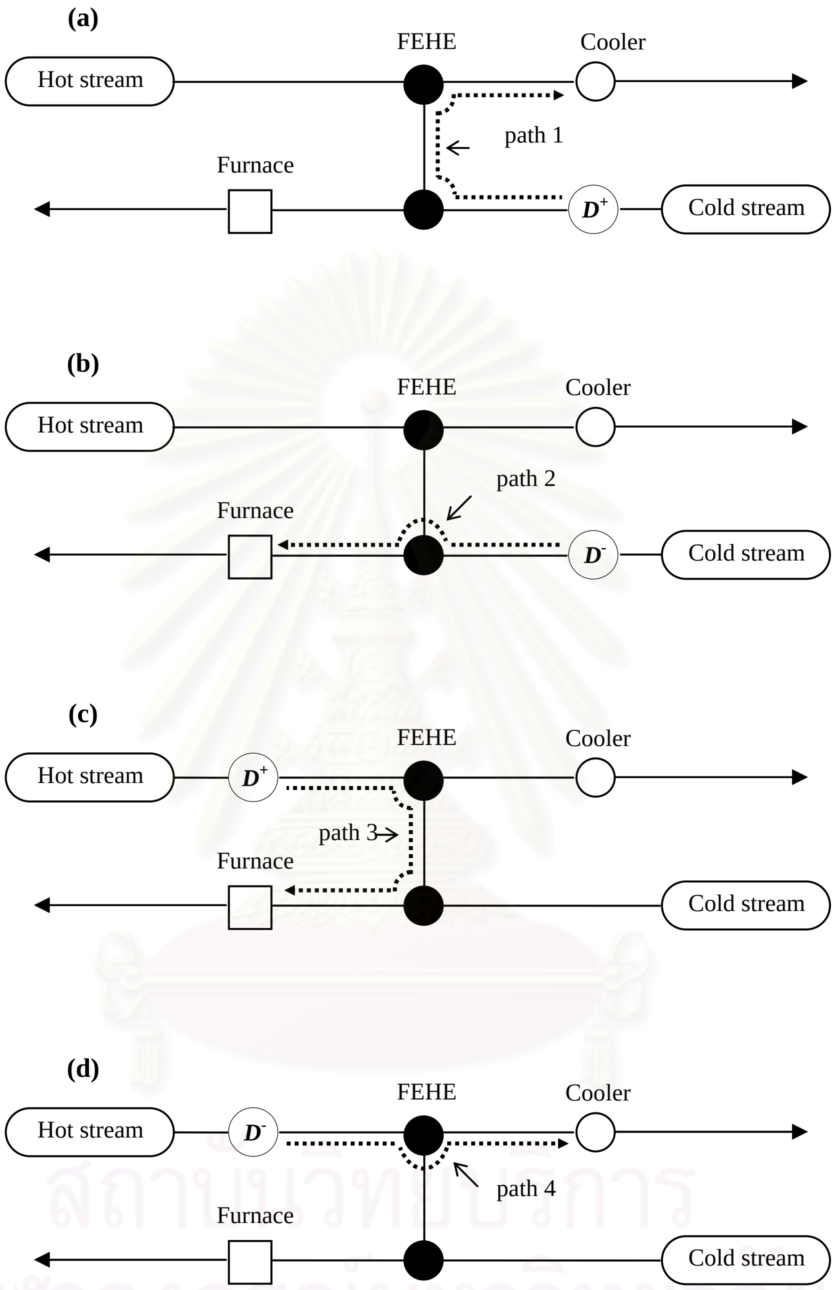


Figure 4.5 Heat pathways through HEN with single FEHE (e.g. HDA process alternative 1) to achieve DMER, where: (a) path 1 is used to shift the positive disturbance load of the cold stream to the cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream to the heater, (c) path 3 is used to shift the positive disturbance load of the hot stream to the heater, and (d) path 4 is used to shift the negative disturbance load of the hot stream to the cooler.

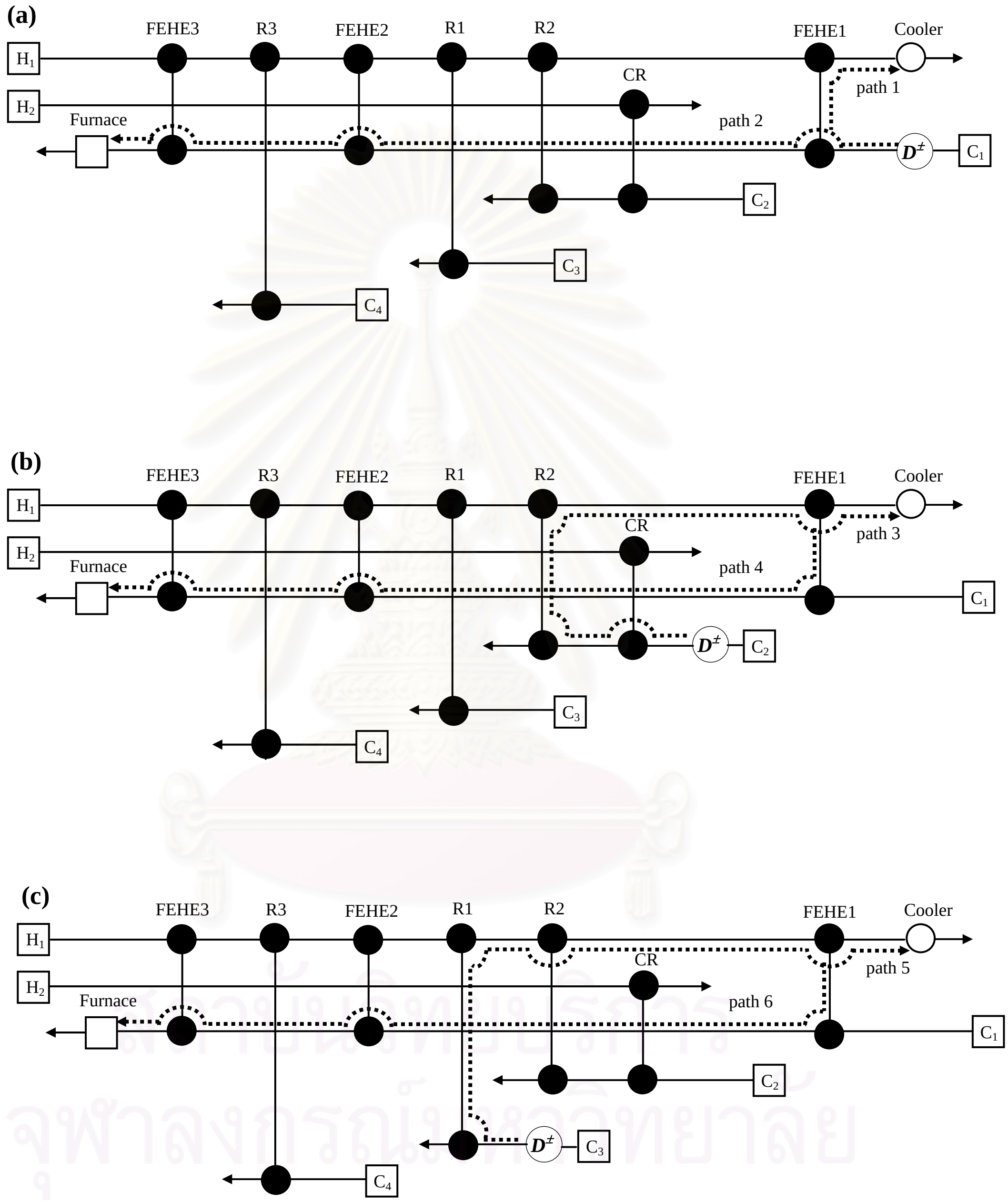


Figure 4.6 Heat Pathways through HEN with multiple FEHEs (e.g. HDA process alternative 6) that be designed to direct and manage the disturbance loads of: (a) the cold stream C_1, (b) the cold stream C_2, (c) the cold stream C_3, (d) the cold stream C_4, and (e) the hot stream H_1.

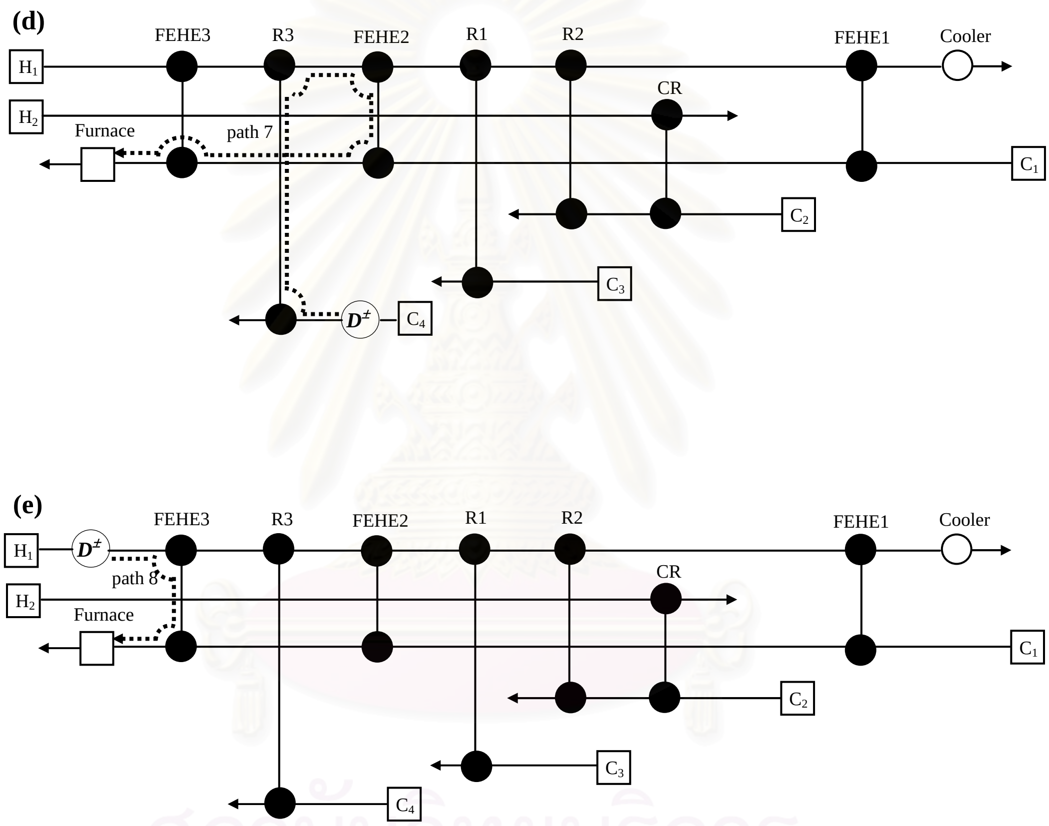


Figure 4.6 *Continued*.

On the other hand, when the inlet temperature of a disturbed hot stream increases, path 3 (Figure 4.5.c) should be activated by controlling the hot outlet temperature of FEHE to shift its positive disturbance load to heater. As a result, the heater duty will be decreased. Consider the case when the inlet temperature of a disturbed hot stream decreases, path 4 (Figure 4.5.d) should be activated by controlling the cold outlet temperature of FEHE to shift its negative disturbance load to cooler. As a result, the cooler duty will be decreased.

4.3.3 Design of Heat Pathways for HEN with Multiple FEHEs

The heat pathway management realization for multiple heat exchangers is explained by several illustrations using the heat integrated HDA plant alternative 6 (Figure 4.6) as the illustrative cases. In Figure 4.6, H_1 is the quenched reactor product stream, and H_2 is the hot-side stream from the top tray of the recycle column. C_1 is the reactor feed stream prior to the furnace. C_2, C_3, and C_4 are the cold-side streams coming from the bottoms of product, stabilizer, and recycle columns, respectively.

For FEHE units, there are two a priori specified variables and two a priori unknown variables. In order to complete the calculation of mass and energy balance for this case, one of the two unknown variables should be specified. In this case all of the target temperatures of the cold and hot streams are fixed. On the other hand, the hot reactor product temperature affects significantly the performance of the distillation column. Change in this temperature at the entrance of the reboiler will affect the boilup. Therefore, this should be treated as a disturbance to the column. In order to prevent the propagation of this thermal disturbance, the hot temperature at the entrance of the reboiler should be maintain constant.

Illustration a. In this illustration (Figure 4.6.a), we suppose that the inlet temperature of a disturbed cold stream C_1 decreases, path 1 should be activated by controlling the cold outlet temperature of FEHE1 at its set point and let the hot outlet temperature vary. This will have the effect of shifting the positive disturbance load to the cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty. When the inlet temperature of a disturbed cold stream C_1 increases, path 2 should be activated by controlling the hot outlet temperature of FEHE1 at its set point to shift its negative disturbance load to furnace. Thus, the negative disturbance load of a cold stream will result in decrease of the furnace duty.

Illustration b. Figure 4.6.b shows the two possible heat pathways when the heat load disturbances are originating from the cold stream C_2 (the bottoms of product column). Since the target temperatures of C_2 and H_2 should be kept constant, both the positive and negative disturbance loads of the cold stream C_2 must be shifted to the hot stream H_1 to be further directed to heat sink or heat source according to its effects. Consider the case when the cold inlet temperature of reboiler R2 decreases, the hot outlet temperature of reboiler R2 will decrease. The deficit heat load should be directed to the cooler to reduce its duty. Therefore, path 3 should be activated by maintaining the cold outlet temperature of FEHE1 at its set point. On the other hand, consider the case when the cold inlet temperature of reboiler R2 increases, the hot outlet temperature of reboiler R2 will increase. Thus, path 4 should be activated by maintaining the hot outlet temperature of FEHE1 at its set point. This lets the furnace inlet temperature increase as the supply temperature of cold stream C_2 increases; therefore, the furnace duty will be minimized.

Illustration c. Figure 4.6.c shows the heat pathways when the heat load disturbances are coming from the cold stream C_3 (the bottoms of stabilizer column). The heat pathways resulting from the cold stream C_3 are similar with those from the cold stream C_2. Thus, whenever the temperature of cold stream C_3 decreases, path 5 will be activated to maintain the cold outlet temperature of FEHE1 at its set point. Consequently, the cooler duty will be decreased. And vice versa, whenever the temperature of cold stream C_3 increases, path 6 will be activated to maintain the hot outlet temperature of FEHE1 at its set point. Following this action, the furnace duty will be decreased.

Illustration d. Figure 4.6.d shows the heat pathway when the heat load disturbances are originating from the cold stream C_4 (the bottoms of recycle column). In this particular case, the process has only one shortest feasible heat pathway (path 7 in Figure 4.6.d), since the thermal propagation of the down stream units is witnessed through our simulation study and we must keep the target temperature of cold stream C_4 at its designed value. When the cold inlet temperature of reboiler R3 decreases, the hot outlet temperature of R3 will decrease. Since the hot outlet temperature of FEHE2 has to be maintained at its set point, the heat load in the disturbed hot stream H_1 is then shifted to the cold stream $C_{1.}$ As a result, the furnace duty increases, since the furnace inlet temperature decreases. On the other hand, when the cold inlet temperature of reboiler R3 increases, the hot outlet temperature of reboiler R3 will increase. Therefore, the furnace duty will be reduced, since the furnace inlet temperature increases.

Illustration e. Figure 4.6.e shows when the disturbance is coming with the hot stream H_1. Both the negative and positive disturbance loads of hot stream H_1 should be shifted to the furnace via the shortest path (path 8 in Figure 4.6.e). We prefer to shift the negative disturbance load of hot stream H_1 to furnace instead of cooler, because there are four units downstream that will be affected by thermal disturbance propagation which resulting in unaccepted oscillation of the outlet temperatures of those units. Consider the case when the hot inlet temperature of FEHE3 decreases, the deficit heat load of hot stream H_1 is shifted to the furnace, the furnace duty will be increased and vice versa.

4.4 Modeling and Simulation of HDA Process

In order to illustrate the effective principles of the use of the HPH for heat load traffic management, the HDA process with energy integration schemes (i.e. alternative 1, 4 and 6) are used as a case study and discussed below.

4.4.1 Steady State Simulation Results of HDA Process Alternative 1

First, a steady-state model is built in HYSYS, using the flowsheet and equipment design information, mainly taken from Douglas (1988) and Luyben et al. (1999). For the simulation, the Peng-Robinson model is selected for the calculation of the physical properties because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions.

The kinetic rate expressions are functions of the partial pressures (in psia) of toluene p_T, hydrogen p_H, benzene p_B and diphenyl p_D, with an Arrhenius temperature dependence. The equations used in the HYSYS simulation are:

$$r_1 = P_T P_H^{0.5}\left(3.686x10^6\right)\exp\left(\frac{-90{,}800}{RT}\right) \tag{4.3}$$

$$r_2 = P_B^2\left(9x10^4\right)\exp\left(\frac{-90{,}800}{RT}\right) - P_D P_H\left(2.553x10^5\right)\exp\left(\frac{-90{,}800}{RT}\right) \tag{4.4}$$

Figure 4.7 shows the HYSYS flowsheet of HDA process alternative 1. The steady state simulation results are summarized in Tables 4.1 to 4.4. For the comparison, the steady state simulation results given by Luyben et al. (1999) are also listed in those tables. The data and specifications for the different equipments are given in Appendix B.

Since there are four material recycle streams in HDA process alternative 1, four RECYCLE modules are inserted in the streams: hot stream to FEHE, gas recycle, quench, and toluene recycle stream. Proper initial values should be chosen for these streams; otherwise the iterative calculations might converge to another steady state due to the non-linearity and unstable characteristics of the process.

All of the three columns are simulated using the "distillation column" module. When columns are modeled in steady state, besides the specification of inlet streams, pressure profiles, number of trays and feed tray, two additional variables should be additionally specified for columns with condenser or reboiler. These could be the duties, reflux rate, draw stream rates, composition fraction, etc. We chose to specify a priori overhead and bottom component mole fraction for all columns. These mole fractions are specified to meet the required purity of product given in Douglas (1988). The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on sieve trays. The column specifications of HDA process alternative 1 are given in Appendix B (see Table B.2). Although the tray diameter and spacing, weir length and height are not required for steady state modeling, they are required for dynamic simulation.

4.4.2 Comparison with the Previous Study by Luyben et al. (1999)

The steady state simulation results are found to be consistent with those in Luyben et al. (1999). These data come from their TMODS, DuPont's in-house simulator and included in Tables 4.1 to 4.4. However, there are also some differences: for example, in the current study the flowrates of the reflux streams in the product and the recycle columns are larger and the reactor effluent temperature is lower than those used in Luyben's work.

The possible reasons for these differences may be that in Luyben et al. (1999), vapor-liquid equilibrium behavior was assumed to be ideal and the stabilizer column was modeled as a component splitter and tank whereas the current study is based on the Peng-Robinson equation of state and the stabilizer column is modeled rigorously. The operating pressure for this column is chosen to be 1034 kPa according to the design information in Douglas (1988), whereas in Luyben's work is assumed to be 3310 kPa. Consequently, the pressures for the streams around the stabilizer column are different. In our simulation, the heats of reaction are directly calculated by HYSYS. The heats of reaction in the current study are –41,867 Joule/mole for the first reaction and 8,141 Joule/mole for the second reaction, whereas in Luyben et al. (1999) they are –50,008 Joule/mole and 0 Joule/mole for the first and second reaction respectively. Therefore, it is understandable that the reactor effluent temperature in the current work is lower than that obtained in Luyben's work, since the absolute value of the heat of reaction for the first reaction is small, and also, the second reaction is slightly endothermic.

4.4.3 Steady State Simulation Results of HDA Process Alternatives 4 and 6

The steady state simulation results of HDA process alternative 1 have been compared with the earlier study by Luyben et al. (1999), and the results are found consistent with those in the earlier study. Then, considering the consistency of the simulation results of the HDA process alternative 1 with respect to the previous work, the other alternatives considered in this work, i.e. alternatives 4, and 6 are also developed in the HYSYS software environment. Figures 4.8 and 4.9 show the HYSYS flowsheets of the HDA process with energy integration schemes for alternatives 4 and 6, respectively. The data for the selected streams for these alternatives are not included in this chapter but listed in Appendix A. The data and specifications for the equipments are summarized in Appendix B.

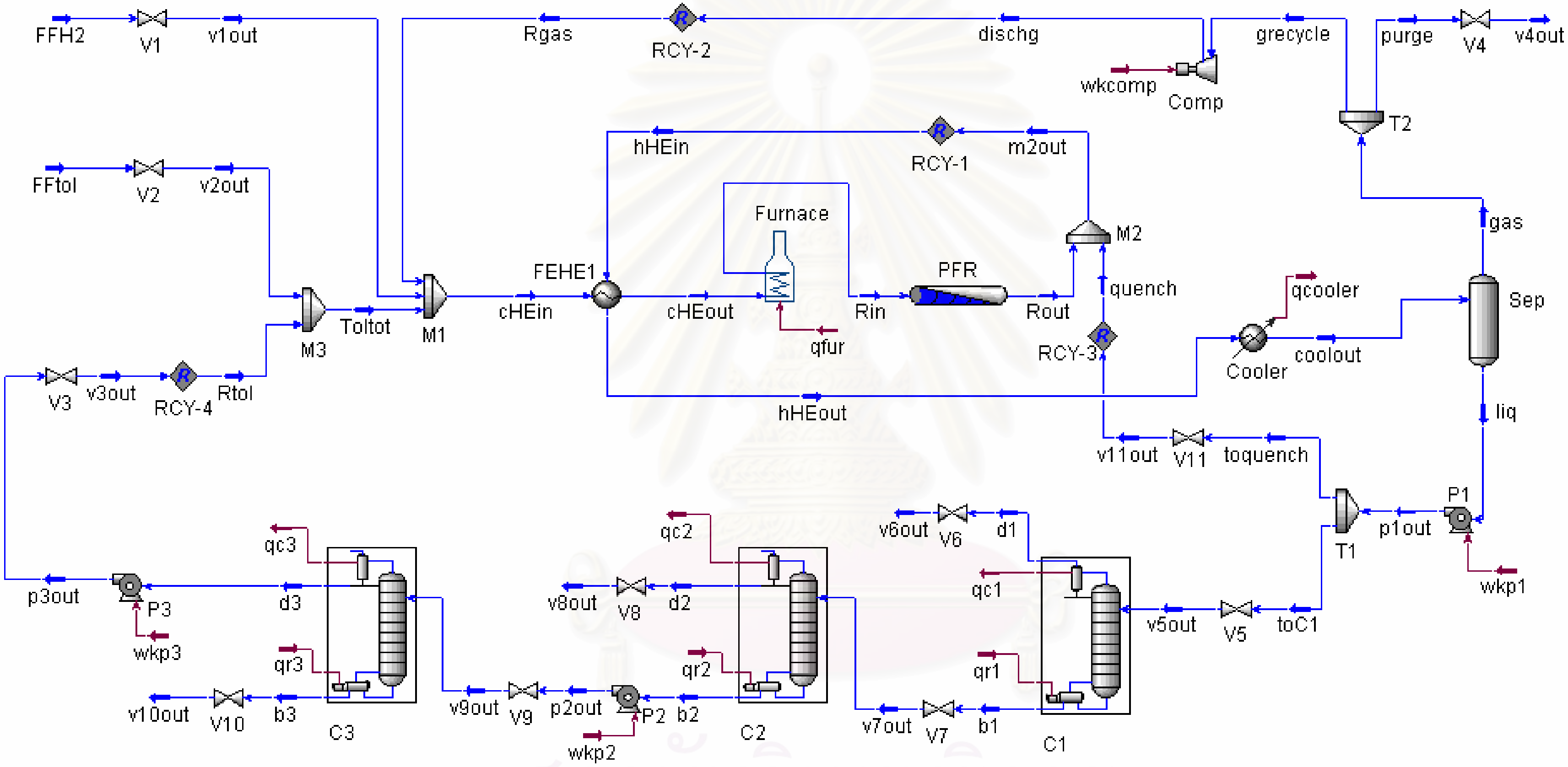


Figure 4.7 HYSYS flowsheet of the steady state modeling of HDA process alternative 1

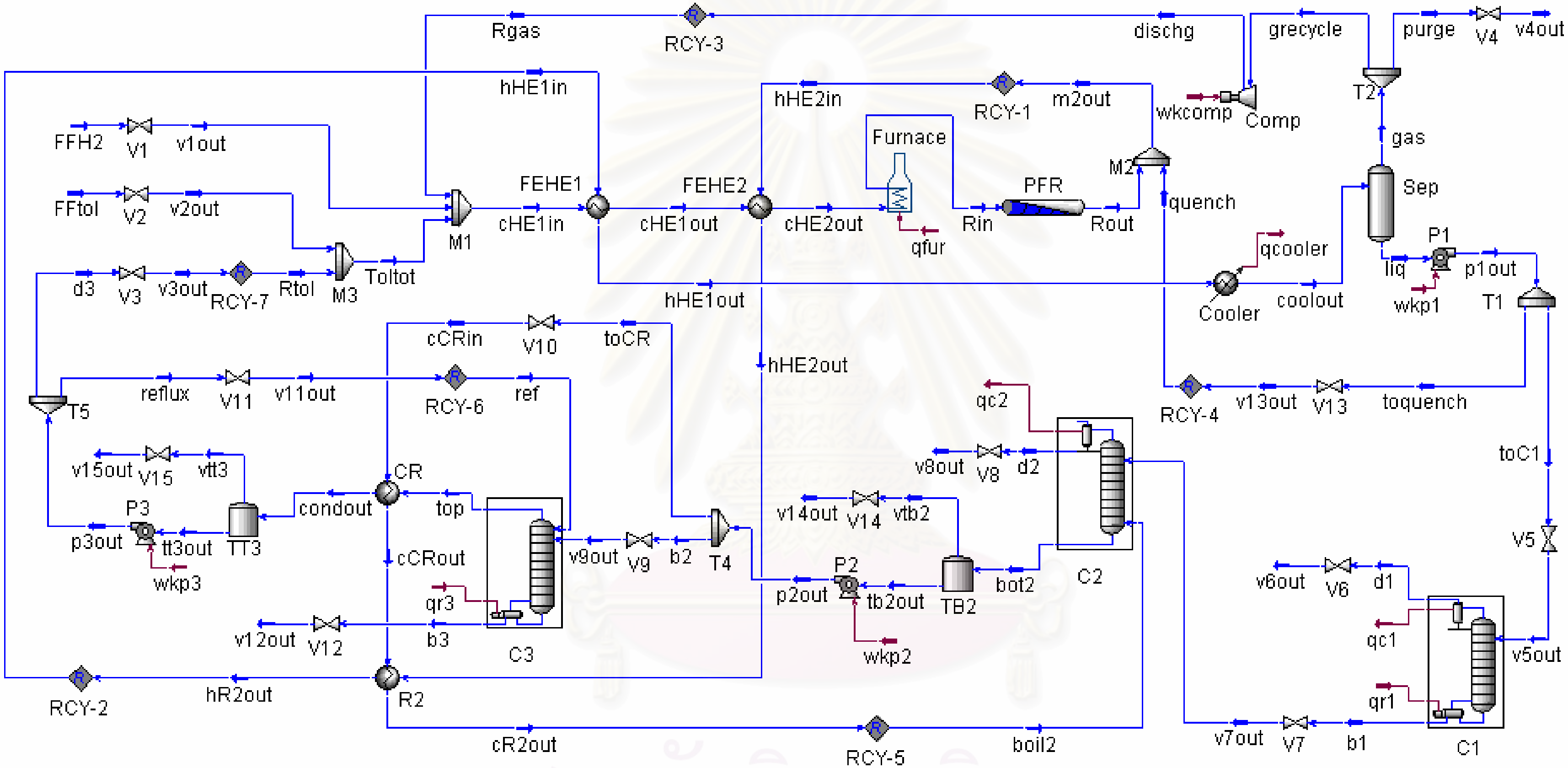


Figure 4.8 HYSYS flowsheet of the steady state modeling of HDA process alternative 4

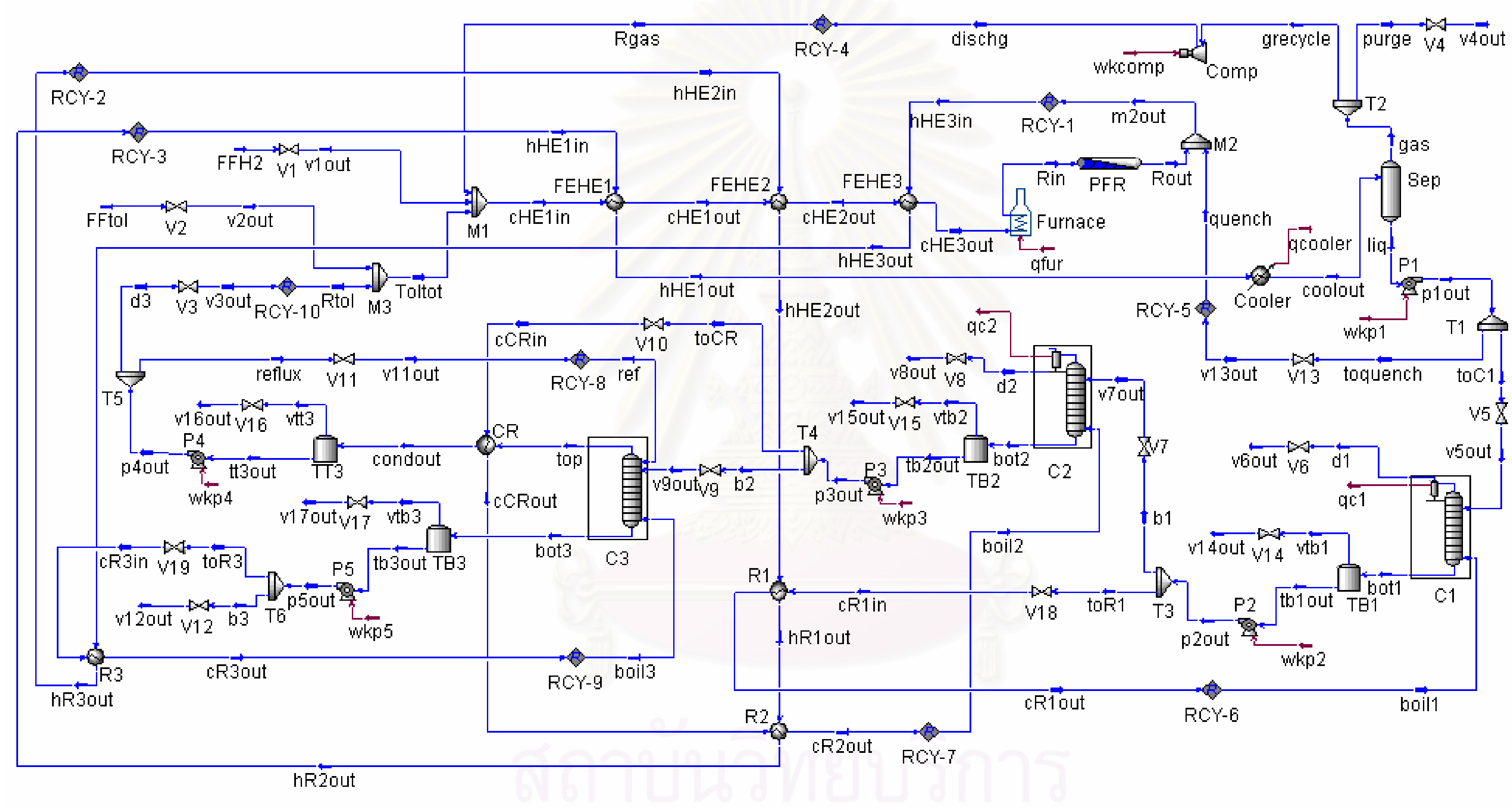


Figure 4.9 HYSYS flowsheet of the steady state modeling of HDA process alternative 6

Table 4.1 Process stream data of HDA process alternative 1, part 1

(a) Current Study

	Fresh toluene	Fresh hydrogen	Purge gas	Stabilizer gas	Benzene product	Diphenyl product
Stream name	FFtol	FFH2	purge	d1	d2	b3
Temperature [C]	30.00	30.00	45.00	51.05	105.55	292.68
Pressure [kPa]	4378.17	4378.17	3287.42	1034.21	206.84	213.74
Molar Flow [kgmole/hr]	130.00	222.72	219.34	8.93	121.70	2.78
$H_{2,}$ mole fraction	0	0.97	0.3993	0.0897	0	0
CH_4	0	0.03	0.5894	0.8680	0	0
C_6H_6	0	0	0.0100	0.0420	0.9997	0
C_7H_8	1	0	0.0012	0.0003	0.0003	0.00026
$C_{12}H_{10}$	0	0	0	0	0	0.99974

(b) Luyben et al. (1999)

	Fresh toluene	Fresh hydrogen	Purge gas	Stabilizer gas	Benzene product	Diphenyl product
Stream name	1	2	3	4	5	6
Temperature [C]	30	30	46.11	45	99.44	292.77
Pressure [kPa]	3964	3964	3309.12	3309.12	206.84	213.74
Molar Flow [kgmole/hr]	131.93	222.43	218.12	9.55	123.60	3.06
$H_{2,}$ mole fraction	0	0.97	0.3992	0	0	0
CH_4	0	0.03	0.5937	0.9349	0	0
C_6H_6	0	0	0.0065	0.0651	0.9997	0
C_7H_8	1	0	0.0006	0	0.0003	0.00026
$C_{12}H_{10}$	0	0	0	0	0	0.99974

Table 4.2 Process stream data of HDA process alternative 1, part 2

(a) Current Study

	Gas recycle	Toluene recycle	Furnace inlet	Reactor inlet	Reactor effluent	Quench
Stream name	dischg	d3	cHEout	Rin	Rout	quench
Temperature [C]	70.31	137.64	596.67	621.11	665.67	45.46
Pressure [kPa]	4171.33	206.84	3743.85	3468.06	3350.85	3350.85
Molar Flow [kgmole/hr]	1596.30	38.58	1987.63	1987.63	1987.63	49.00
$H_{2,}$ mole fraction	0.3993	0	0.4290	0.4290	0.3652	0.0047
CH_4	0.5894	0	0.4771	0.4771	0.5423	0.0450
C_6H_6	0.0100	0.00064	0.0081	0.0081	0.0706	0.7097
C_7H_8	0.0012	0.99934	0.0857	0.0857	0.0205	0.2244
$C_{12}H_{10}$	0	0.00002	0	0	0.0014	0.0162

(b) Luyben et al. (1999)

	Gas recycle	Toluene recycle	Furnace inlet	Reactor inlet	Reactor effluent	Quench
Stream name	7	8	9	10	11	12
Temperature [C]	46.11	133.33	596.67	621.11	684.0	45
Pressure [kPa]	3536.62	206.84	3537.01	3468.06	3350.85	3350.85
Molar Flow [kgmole/hr]	1596.30	37.26	1987.86	1987.86	1987.86	70.77
$H_{2,}$ mole fraction	0.3992	0	0.4291	0.4291	0.3644	0
CH_4	0.5937	0	0.4800	0.4800	0.5463	0.0515
C_6H_6	0.0065	0.00064	0.0053	0.0053	0.0685	0.7159
C_7H_8	0.0006	0.99934	0.0856	0.0856	0.0193	0.2149
$C_{12}H_{10}$	0	0.00002	0	0	0.0015	0.0177

Table 4.3 Process stream data of HDA process alternative 1, part 3

(a) Current Study

	FEHE hot in	FEHE hot out	Separator gas out	Stabilizer feed	Stabilizer bottoms	Product bottoms
Stream name	hHEin	hHEout	gas	toC1	b1	b2
Temperature [C]	621.07	110.64	45.00	45.25	190.51	144.67
Pressure [kPa]	3350.85	3309.48	3287.42	3803.15	1054.90	227.53
Molar Flow [kgmole/hr]	2036.63	2036.63	1815.64	171.99	163.07	41.37
H_2, mole fraction	0.3565	0.3565	0.3993	0.0047	0	0
CH_4	0.5304	0.5304	0.5894	0.0450	0	0
C_6H_6	0.0860	0.0860	0.0100	0.7097	0.7462	0.0006
C_7H_8	0.0254	0.0254	0.0012	0.2244	0.2367	0.9321
$C_{12}H_{10}$	0.0018	0.0018	0	0.0162	0.0171	0.0673

(b) Luyben et al. (1999)

	FEHE hot in	FEHE hot out	Separator gas out	Stabilizer feed	Stabilizer bottoms	Product bottoms
Stream name	13	14	15	16	17	18
Temperature [C]	621.1	169.44	45	45	93.33	139.44
Pressure [kPa]	3350.85	3309.5	3350.85	3309.5	3309.5	227.53
Molar Flow [kgmole/hr]	2058.62	2058.62	1885.12	173.5	163.93	40.33
H_2, mole fraction	0.3518	0.3518	0.3992	0	0	0
CH_4	0.5294	0.5294	0.5937	0.0515	0	0
C_6H_6	0.0907	0.0907	0.0065	0.7159	0.7538	0.0006
C_7H_8	0.0260	0.0260	0.0006	0.2149	0.2275	0.9234
$C_{12}H_{10}$	0.0021	0.0021	0	0.0177	0.0187	0.0760

Table 4.4 Process stream data of HDA process alternative 1, part 4

(a) Current Study

	Column reflux			Column boilup		
	C1	C2	C3	C1	C2	C3
Temperature [C]	51.05	105.55	137.64	190.51	144.67	292.68
Pressure [kPa]	1034.21	206.84	206.84	1054.90	227.53	213.74
Molar Flow [kgmole/hr]	15.84	371.15	9.94	182.99	384.99	36.15
H_2, mole fraction	0.0003	0	0	0	0	0
CH_4	0.0214	0	0	0.00004	0	0
C_6H_6	0.9575	0.9997	0.00064	0.84132	0.0013	0
C_7H_8	0.0208	0.0003	0.99934	0.15796	0.9969	0.003
$C_{12}H_{10}$	0	0	0.00002	0.00068	0.0018	0.997

(b) Luyben et al. (1999)

	Product column reflux (C2)	Recycle column reflux (C3)
Stream name	19	20
Temperature [C]	99.44	133.33
Pressure [kPa]	206.85	206.85
Molar Flow [kgmole/hr]	136.08	5.44
H_2, mole fraction	0	0
CH_4	0	0
C_6H_6	0.9997	0.00061
C_7H_8	0.0003	0.99937
$C_{12}H_{10}$	0	0.00002

In alternative 4, there are two FEHEs, and additionally the reboiler in the product column is driven by hot reactor product. Clearly, alternative 6 is the most complex one, since it includes three FEHEs, and all reboilers of the three columns are driven by the hot reactor product. Several RECYCLE modules should be inserted in the streams for these alternatives in the simulations. The numbers of RECYCLE modules are 7 and 10 for alternative 4 and 6, respectively. As the earlier explanation, proper initial values should be chosen for these streams; otherwise the iterative calculations might converge to another steady state due to the non-linearity and unstable characteristics of the process.

All process-to-process heat exchangers are simulated using a heat exchanger with a hot stream on the shell side and a cold stream on the tube side. In general HEN design, the minimum temperature difference in the heat exchangers, ΔT_{min} is set to 10 ^oC. Heat-integrated distillation system is used for both the product and recycle columns. The basic idea is to use the overhead vapor from one column as the heat source the other column. The pressures in the two columns should be adjusted so that there is a reasonable differential temperature driving force for heat transfer in the heat exchangers, so they can act as the condenser for the high-temperature column and as the reboiler for the low-temperature column, respectively. In this case, the pressure required in the recycle column is 540 kPa to provide a reasonable temperature differential in the condenser/reboiler (CR).

The stabilizer column (C1) for alternative 4 is simulated using a ‘distillation column’ module, and for alternative 6, it is simulated using a ‘refluxed absorber’ that it does not include a reboiler. Product column (C2) is simulated using a ‘refluxed absorber’ with no reboiler for both alternative 4 and 6. The recycle column (C3) in alternative 4 is simulated using a ‘reboiled absorber’ module that does not include a condenser. Finally, for alternative 6, column C3 is simulated using an ‘absorber’ with neither reboiler nor condenser. Since a ‘refluxed absorber’ and‘reboiled absorber’ modules are used, only one variable needs to be specified for the columns with condenser or reboiler. The overhead mole fraction is chosen to be specified for a ‘refluxed absorber’ module and the bottom mole fraction for a ‘reboiled absorber’ module. On the other hand, the ‘absorber’ module used to simulate column C3 in alternative 6 does not require any a priori specified variables.

In alternative 4, two tanks are needed to accommodate liquid from the bottoms of product column (TB2) and condensed vapor from the top of recycle column (TT3). Four additional tanks are needed for alternative 6 to accommodate liquid streams from the bottoms of the three columns C1, C2 and C3 (TB1, TB2, and TB3), and condensed vapor from the top of column C3 (TT3). In a dynamic sense, these intermediate tanks have positive effect on the process control since any variability in composition, temperature, or flow is damped out in these tanks. In reality, all tanks have only liquid streams. Unfortunately, HYSYS requires that a tank must have both vapor and liquid exit streams. Therefore, a vapor line must be artificially introduced with a control valve in this line to keep the flowrate of the gas at zero. Hence, this valve is specified to be shut, i.e. the valve opening is set to be 0% with an arbitrary size coefficient C_V value.

4.5 Heat Load Traffic Management Illustration for HDA Process

Study of heat load traffic management of HDA process can be done by using steady state considerations. The heat pathways are systematically identified to generate plantwide control strategies. In this work, the HENs to be used to study heat load traffic management are based on the steady state flowsheet of HDA process with energy integration schemes. The operating conditions of HENs are determined based on the disturbances entering the plant. In order to design the heat pathways to obtain the highest possible DMER, several disturbances were made and the results are as follows:

4.5.1 Change in the Disturbance Load of Cold Stream for HDA Process Alternative 1

Figure 4.10.a shows the operating conditions and heat pathways for HDA process alternative 1, when the cold inlet temperature of FEHE1 varies, so that the heat load changes. In Figure 4.10, stream C_1 is the cold-side feed to FEHE1 (i.e. reactor feed stream prior to the furnace), and stream H_1 is the hot-side feed to FEHE1 (i.e. quenched reactor products). Furthermore, for all HENs described here, the

nominal conditions are given in *italic font style*, whereas regular font style and **bold font style** are used to represent the conditions corresponding to a decrease and an increase from the nominal value, respectively.

When the inlet temperature of a disturbed cold stream decreases from *63.5* to 61.8 ^oC, the resulting positive disturbance load (D^+ = 53 kW) causes the activation of path-1 by maintaining the cold outlet temperature of FEHE1 at its nominal value (*596.7* ^oC). Consequently, the FEHE1 duty increases from *17964* to 18017 kW. Following this, path-1 will decrease the cooler duty from *2719* to 2666 kW while the furnace duty remains at the same nominal value of *918.4 kW*. This positive disturbance load is shifted to the cooler to decrease its duty. Hence, the DMER can be achieved.

When the inlet temperature of a disturbed cold stream increases from *63.5* to **65.3** ^oC because of the negative disturbance load (D^- = 53 kW), **path-2** is activated to maintain the hot outlet temperature of FEHE1 at its nominal value (*110.6* ^oC). As a result, **path-2** will cause a decrease in the furnace duty from *918.4* to **865.4** kW while the cooler duty remains at its nominal value of *2719 kW*. Thus, this negative disturbance load is shifted to the furnace to decrease its duty. Again, by selecting an appropriate heat pathway to carry the associated load to a utility unit, so its duty will be decreased according to the input heat load disturbance, hence the dynamic MER can be achieved.

4.5.2 Change in the Disturbance Load of Hot Stream for HDA Process Alternative 1

Figure 4.10.b shows the operating conditions and heat pathways for HDA process alternative 1, when the hot inlet temperature of FEHE1 varies, so that the heat load changes. When the inlet temperature of a disturbed hot stream decreases from *621.1* to 616.1 ^oC, the resulting negative disturbance load (D^- = 200 kW) causes the activation of path-1 by maintaining the cold outlet temperature of FEHE1 at its nominal value (*596.7* ^oC). Consequently, the FEHE1 duty decreases from *17964* to 11764 kW. Following this, path-1 will decrease the cooler duty from *2719* to 2519

kW while the furnace duty remains at the same nominal value of *918.4 kW*. This negative disturbance load is shifted to the cooler to decrease its duty.

When the inlet temperature of a disturbed hot stream increases from *621.1* to **626.1** °C because of the positive disturbance load (D^+ = 200 kW), **path-2** is activated to maintain the hot outlet temperature of FEHE1 at its nominal value (*110.6 °C*). As a result, **path-2** will cause a decrease in the furnace duty from *918.4* to **718.4** kW while the cooler duty remains at its nominal value (*2719 kW*). Thus, this negative disturbance load is shifted to the furnace to decrease its duty.

4.5.3 Change in the Disturbance Load of Cold Stream from the Bottoms of Product Column for HDA Process Alternative 4

Figure 4.11.a shows the operating conditions and heat pathways for HDA process alternative 4, when the disturbance loads are originating from the bottoms of product column. In Figure 4.11, stream H_1 is the quenched reactor products, and stream H_2 is the hot-side stream from the top tray of recycle column. Stream C_1 is the reactor feed stream prior to the furnace. Stream C_2 is the cold-side streams from the bottoms tray of product column. The pinch temperature is found to be 150 °C.

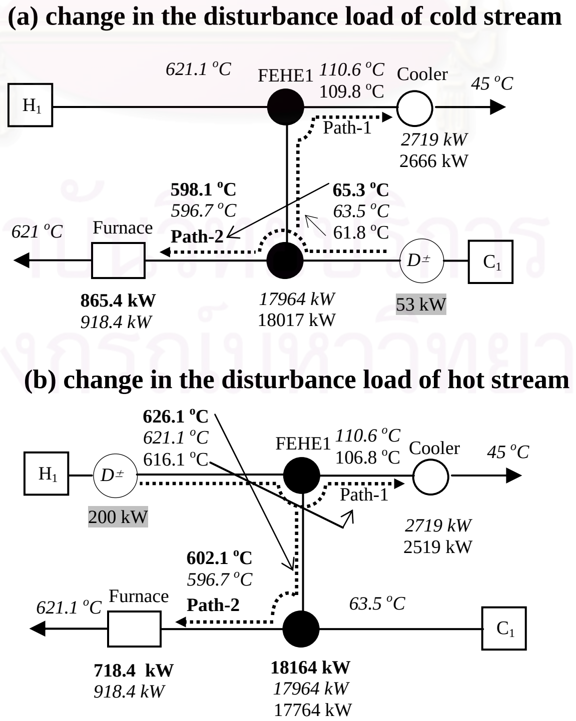


Figure 4.10 Operating conditions and heat pathways for HDA process alternative 1

As stated before, the hot reactor product temperature affects significantly the performance of the three columns. Change in this temperature at the entrance of the reboilers will affect the boilup. Therefore, this should be treated as a disturbance to the column. In order to prevent the propagation of this thermal disturbance, the hot temperature at the entrance of the reboiler should be maintained constant. This control strategy will be applied for alternative 4 and 6.

As shown in Figure 4.11.a, when the cold inlet temperature of reboiler R2 decreases from *162.5* to 160.6 ^{o}C because of the positive disturbance load (D^{+} = 50 kW), the R2 duty increases, so the hot outlet temperature of R2 decreases from *176.1* to 174.4 ^{o}C, i.e this becomes the negative disturbance for stream H_1. Since the temperature of a disturbed hot stream decreases, path-1 is activated to maintain the cold outlet temperature of FEHE1 at its nominal value. Consequently, the cooler duty will be decreased (from *1912* to 1862 kW). In this case, the new negative disturbance load of stream H_1 is transferred across the pinch in order that it can be dissipated to the cooler utility. If we don't transfer this disturbance across the pinch, we don't get the true MER, i.e. resulting in increase of the utility duty.

When the cold inlet temperature of reboiler R2 increases from *162.5* to **164.4** ^{o}C, the R2 duty decreases, so the hot outlet temperature of R2 increases from *176.1* to **177.6** ^{o}C. Since the temperature of a disturbed hot stream increases, **path-2** will be activated to maintain the hot outlet temperature of FEHE1 at its nominal value. Following this action, the furnace duty will be decreased (from *3964* to **3914** kW). Hence the dynamic MER will also be achieved.

4.5.4 Change in the Disturbance Load of Hot Stream for HDA Process Alternative 4

In this particular case, the process has one heat pathway, since the hot inlet temperatures of the reboilers have to be kept constant. Figure 4.11.b shows the operating conditions and heat pathway for HDA alternative 4, when the disturbance loads are coming with the hot stream (the hot reactor product).

When the hot inlet temperature of FEHE2 decreases from *621.1* to 616.1 ^{o}C because of the negative disturbance load (D^{-} = 200 kW), the FEHE2 duty decreases from *11502* to 11302 kW. Since the hot outlet temperature of FEHE2 has to be maintained constant, the heat load in the hot stream is shifted to the cold stream, so the cold outlet temperature of FEHE2 decreases from *513.1* to 507.6 °C. Hence, the furnace duty increases from *3964* to 4164 kW, since the cold inlet temperature of furnace decreases.

When the hot inlet temperature of FEHE2 increases from *621.1* to **626.1** °C because of the positive disturbance load (D^+ = 200 kW), the FEHE2 duty increases from *11502* to **11702** kW. This is a desired condition since whenever the temperature of a disturbed hot stream increases it is desirable, as stated before to shift the disturbance load to the cold stream. Therefore, the furnace duty will be decreased (from *3964* to **3764** kW).

(a) change in the disturbance load of cold stream from the bottoms of product column

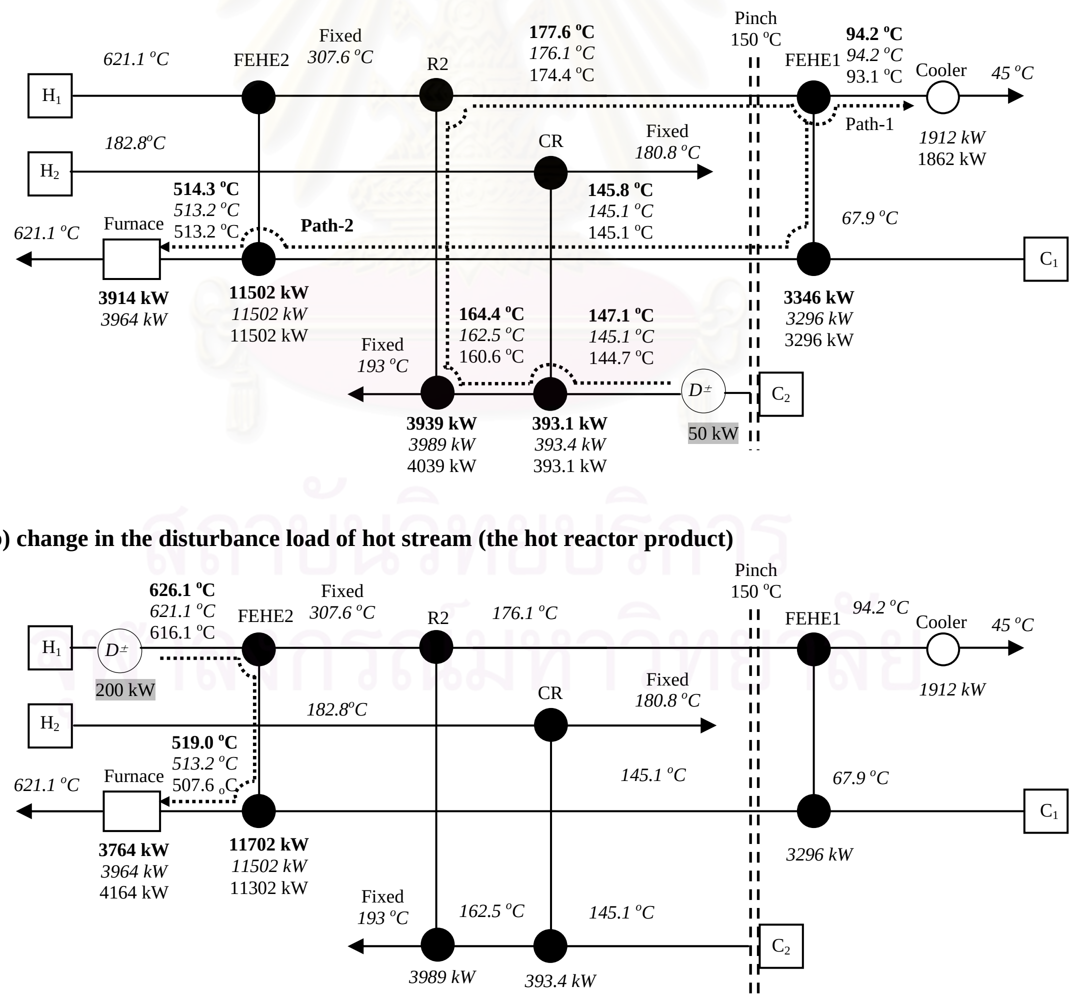


Figure 4.11 Operating conditions and heat pathways for HDA process alternative 4

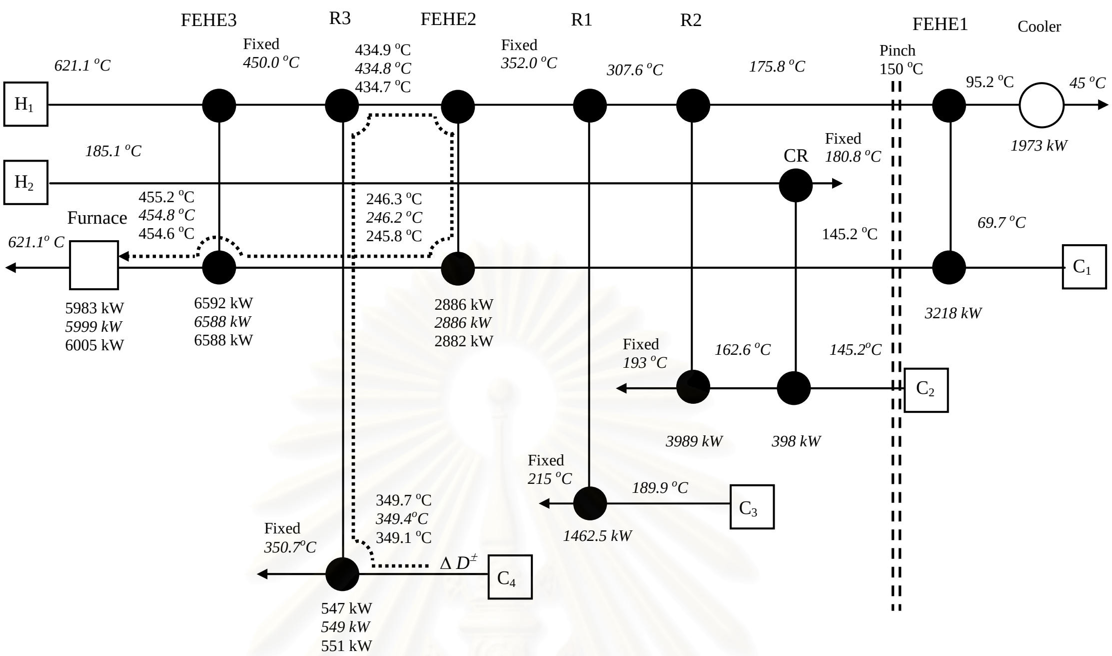


Figure 4.12 Operating conditions and heat pathways for HDA process alternative 6, when the disturbance loads are originating from the bottoms of recycle column

4.5.5 Change in the Disturbance Load of Cold Stream from the Bottoms of Recycle Column for HDA Process Alternative 6

The heat pathways resulting from the bottoms of product column in HDA process alternative 6 are similar with those in HDA process alternative 4. Now, we discuss the phenomena of heat traffic resulting from the bottoms of recycle column in HDA process alternative 6. Again, the process has only one heat pathway, since the hot inlet temperatures of the reboilers have to be kept constant. Figure 4.12 shows the operating conditions and heat pathway for HDA alternative 6, when the disturbance loads are originating from the bottoms of the recycle column.

When the cold inlet temperature of reboiler R3 decreases, the R3 duty increases, so the hot outlet temperature of R3 decreases. Since the hot outlet temperature of FEHE2 has to be maintained constant, the heat load in the hot stream is shifted to the cold stream, so the cold outlet temperature of FEHE2 decreases. Hence, the furnace duty increases, since the cold inlet temperature of furnace decreases. When the cold inlet temperature of reboiler R3 increases, the R3 duty decreases, so the hot outlet temperature of R3 increases. This is a desired condition since whenever the temperature of a disturbed hot stream increases it is desirable, as stated before to shift the disturbance load to the cold stream. Therefore, the furnace duty will be decreased.

4.6 Control Strategy Considerations Using HPH

Figures 4.13.a and 4.13.b show the control strategy to obtain the highest possible DMER for energy-integrated plant with single FEHE and multiple FEHEs, respectively. Based on the HPH to achieve DMER, the control strategy for this process should be strongly related to energy integration objectives. For this study, we assume that:

- The utility exchangers can handle all variations of heat load.
- Any heat exchangers will have enough heat transfer area to accommodate increases in heat loads of disturbed process stream.
- The bypass lines are provided to all heat exchangers as a standard feature to adjust heat load.

4.6.1 Control Strategy for Energy-Integrated Plant with Single FEHE

For energy-integrated plant with single FEHE, all the target temperatures of the cold and hot streams (i.e. T_3 and T_6 in Figure 4.13.a) are controlled at its nominal value by manipulating the furnace and cooler utility duties, respectively. In this work, to obtain the highest possible DMER, the disturbance loads are eventually shifted to either cooler or furnace utility according to the HPH, so its utility duties will be decreased based upon the input disturbance load. A control strategy for the FEHE is required such as an appropriate heat pathway will be selected at any given time.

During the normal operation of the FEHE in a plant, it is possible that unwanted-conditions may arise which may lead to move the heat load to other utility units. For examples, when the cold outlet temperature (T_2 in Figure 4.13.a) of FEHE decreases to values smaller than its nominal temperature the furnace duty will increase. Alternatively, when the hot outlet temperature (T_5 in Figure 4.13.a) of

FEHE increases to values larger than its nominal temperature the cooler duty will consequently increase. In such cases it is necessary to switch from the normal control strategy and attempt to prevent a process variable from exceeding an allowable upper or lower limit. This can be achieved through the use of special types of switches. The high selector switch (HSS) is used whenever a variable should not exceed an upper limit, and the low selector switch (LSS) is employed to prevent a process variable from exceeding a lower limit. This is known as an override control.

Thus, a selective controller with low selector switch (LSS) for FEHE is employed as shown in Figure 4.13.a. This is a control system that involves one manipulated variable and two controlled variables. This control system works as follows: The temperature T_5 is controlled at its normal set point by manipulating the valve on the bypass line i.e. loop 1 in Figure 4.13.a. At the same time, the temperature T_2 should not be allowed to drop below a lower limit value, which is necessary to keep the furnace duty at a good level.

Whenever the temperature T_2 drops below the allowable limit due to, for example, a disturbance load entering the process, the LSS switches the control action from the hot temperature control (TC101) to the cold temperature control (TC102), i.e. switches the control action from loop 1 to loop 2, and closes the valve on the bypass line. As a result, the temperature T_2 will rise to its nominal temperature and the temperature T_5 will be further decreased, so the cooler duty will also be decreased. Whenever the temperature T_2 increases above a lower limit, a desired-condition during operation, due to the disturbance load entering the process, the LSS switches the control action from loop 2 to loop 1, and closes the valve on the bypass line. Consequently, T_5 will drop to its nominal temperature and T_2 will be further increased, so the furnace duty will also be decreased.

4.6.2 Control Strategy for Energy-Integrated Plant with Multiple FEHEs

Figure 4.13.b shows control strategy for energy-integrated plant with multiple FEHEs. The major loops in energy-integrated plant with multiple FEHE are the same as those used in HEN with single FEHE. In this heat integration system (Figure 4.13.b), in order to prevent the propagation of thermal disturbance to the separation

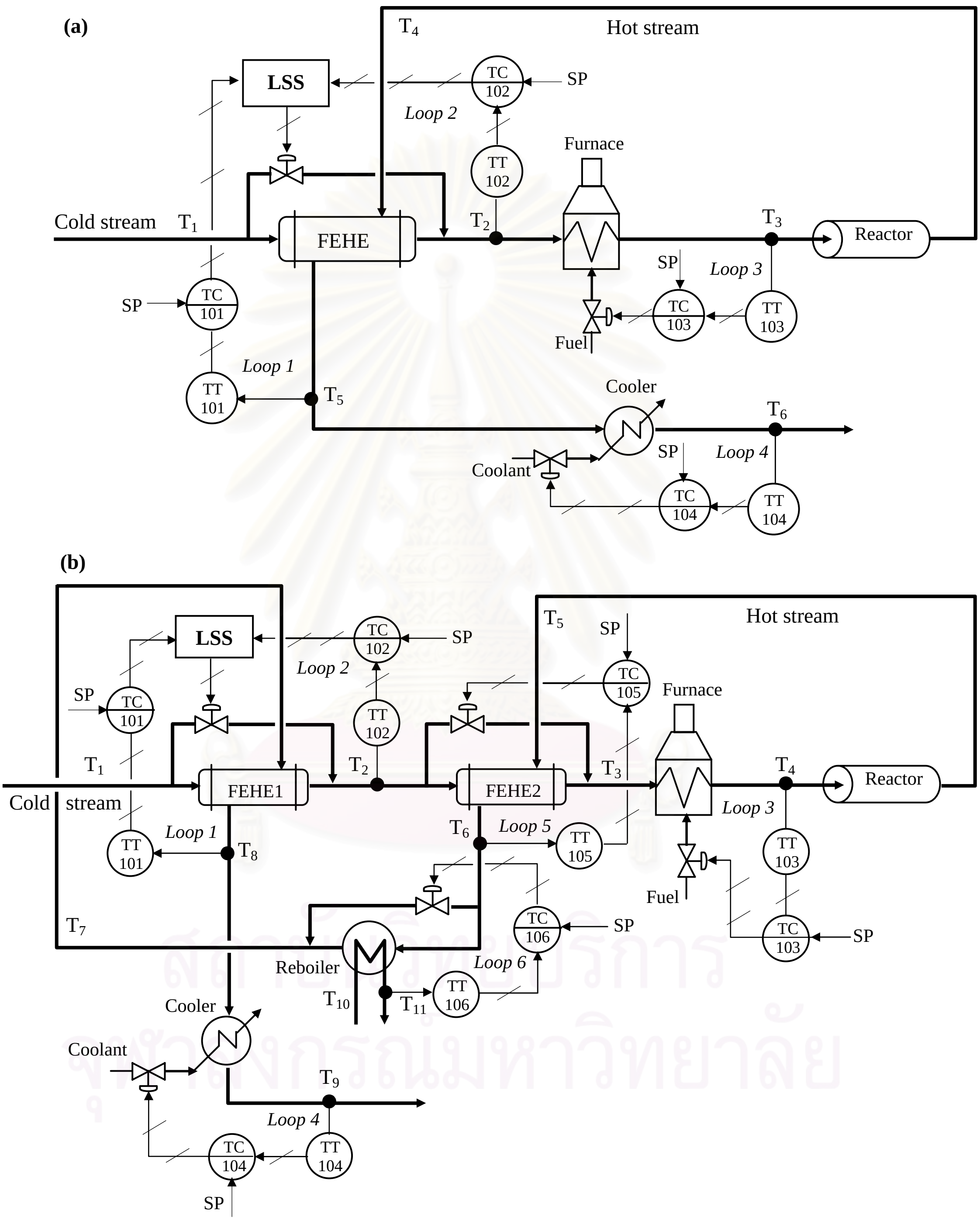


Figure 4.13 Control strategy using the HPH for energy-integrated plants with: (a) single FEHE, (b) multiple FEHEs

section, the hot inlet temperatures of reboilers (T_6 in Figure 4.13.b) should be controlled, i.e. loop 5 as shown in Figure 4.13.b. Thus all disturbance loads of the hot stream are shifted to the furnace utility. The furnace and cooler utility duties are manipulated to control the target temperatures of cold stream (T_4 in Figure 4.13.b) and hot stream (T_9 in Figure 4.13.b), respectively. The cold outlet temperature of reboiler (T_{11} in Fig. 4.13.b) is controlled by manipulating the valve on the bypass line.

The LSS controller is employed in FEHE1. In order to apply this override control strategy in HYSYS, a selector block can be added to the process flow diagram. On the connections page tab, all input signals are specified. On the parameter tab, the mode of selector is set; in this case the minimum of all input should be selected.

4.7 Conclusions

The heat load traffic management for heat-integrated-reactor systems with single FEHE and multiple FEHEs using the HPH has been discussed by using steady state considerations. The steady state modeling of HDA process with energy integration schemes (i.e. alternatives 1, 4, and 6) have been successfully simulated using HYSYS simulator.

The operating conditions are determined based on the disturbances entering the plant. The various heat pathways necessary to shift the heat load disturbances to the utility units have been systematically identified. This steady state study reveals that by designing an appropriate heat pathway, the highest possible DMER can be obtained. A selective controller with low selector switch (LSS) for FEHE is employed to select an appropriate heat pathway through the network, so the utility requirements will be decreased, hence the DMER can be achieved.

The dynamics behaviors of plantwide control using the HPH in energy-integrated HDA plant will be explored in Chapter 5. The new plantwide control systems with the LSS will be developed and compared with the earlier control system given by Luyben et al. (1999). Both of the new and earlier control systems will be evaluated based on rigorous dynamic simulation using the commercial software HYSYS.

CHAPTER V
DESIGN OF HEAT PATHWAYS FOR DYNAMIC MER: PART 2. DYNAMIC SIMULATION AND CONTROL OF HDA PROCESS

The essential task of plantwide control in a complex plant with many recycle streams and energy integrations is to maintain the plant energy and mass balances. As the operating conditions change, the designed control system must regulate the entire process to meet the desired condition. Therefore, our purpose of this chapter is to present dynamic simulation of the designed plantwide control in HDA process in order to illustrate the effective principles of the use of HPH for plantwide control.

5.1 Introduction

As discussed in Chapter 4, the heuristics of selection and manipulation of heat pathways for the process associated with energy integration have been proposed. The steady state modeling of HDA process with energy integration schemes (i.e. alternatives 1, 4 and 6) have been successfully established using HYSYS simulator, and the various heat pathways have also been systematically identified. Although the heat pathways management has been discussed, the dynamic simulations and control of heat pathway in energy-integrated HDA process are also necessary.

Control of heat-integrated systems has been studied by several authors. Pioneering papers on the control of feed-effluent-heat-exchanger (FEHE) systems include those of Douglas et al. (1962) and Silverstein and Shinnar (1982). Tyreus and Luyben (1993) presented the unusual dynamics (i.e. wrong-way behavior) in coupled reactor/preheater process. In Luyben et al. (1999), the HDA process was used as one of the four cases to apply their nine steps plantwide control design procedure. The control system was tested on a dynamic model built with TMODS, Dupont's in-house simulator. All of these literature studies have considered reactors with a single FEHE. The purpose of this study is to explore dynamic behavior of the plantwide control structures based on the HPH for more complex heat integrated systems, i.e., reactor with multiple FEHEs as illustrated in HDA process alternatives 4 and 6.

5.2 Design of Plantwide Control Structure of HDA Process

In this work, the HDA process is designed by considering several control objectives (Luyben et al., 1999); they are: achieving a specified production rates of essential pure benzene (99.97 %-mole); achieving a ratio of hydrogen to aromatic greater than 5:1 in the reactor feed; quenching reactor effluent to a temperature of 621 ^{o}C to prevent coking and by-product formation in the heat exchanger.

The plantwide control structures in the HDA process alternatives 1, 4, and 6 are designed based on the heuristic design procedure given by Luyben et al. (1999). The major loops are the same as those used in Luyben et al. (1999), but we have designed two new loops for FEHE and three new loops for the three columns. In the literature (e.g. Luyben et al., 1999), a bypass control and an auxiliary utility exchanger are used for control in the heat integration system. Only bypass control is used in the current study; the reason is that in our case the heat load of the heating stream is greater than the required heat load of reboiler.

For all the heat integration units, the bypass streams are designed to control the outlet temperatures of FEHEs and the tray temperatures in the three columns. The bypass stream should be about 5 to 10 percent of the total flow to be able to handle disturbances (Jones and Wilson, 1997). In normal operation, a control valve should operate with an opening between 20 to 80 percent (Jones and Wilson, 1997). In our study, the bypass valves in the process-to-process-heat-exchangers are designed with the valve opening of 50%, i.e. this translates into the bypass flow rates of about 6% of the total flow. In practice we have to overdesign the process-to-process-heat-exchanger, in order to be able to handle the disturbances. In this work, it is not our intention to study the best overdesign policy. The oversize of the heat exchanger is related to the estimated maximum size of disturbance loads of both the cold and hot streams. The size of disturbance in this study is about 5 to 10% according to Luyben's recommendations.

5.2.1 Steps of Plantwide Process Control Design Procedure

The plant wide control structures in the HDA process are designed based on the heuristic design procedure given by Luyben et al. (1999) and discussed below.

Step 1: Establish control objectives. For the HDA process, we must able to achieve a specified production rate of essentially pure benzene while minimizing yield losses of hydrogen and diphenyl. The reactor effluent gas must be quenched to 621 ^{o}C to prevent coking and byproduct formation in the heat exchanger.

Step 2: Determine control degrees of freedom. There are 23 control degrees of freedom. They include: two fresh feed valves for hydrogen and toluene; purge valve; separator base and overhead valves, cooler cooling water valve; liquid quench valve; furnace fuel valve; stabilizer column steam, bottoms, reflux, cooling water, and vapor product valves; product column steam, bottoms, reflux, cooling water, and distillate valves; and recycle column steam, bottoms, reflux, cooling water, and distillate valves.

Step 3: Establish energy management system. The reactor operates adiabatically, thus the exit temperature depends upon the heat capacities of the reactor gases, reactor inlet temperature, and reactor conversion. Heat from the adiabatic reactor is carried in the effluent stream and is not removed from the process until it is dissipated to utility in the separator cooler. To ensure heat removal from the process, we are constrained by the process design to assign two control loops. We must control reactor inlet temperature with the furnace and control reactor exit temperature with the quench flow. In addition, a selective controller with low selector switch (LSS) is employed in FEHE to select an appropriate heat pathway to carry the associated load to a cooling or heating utility unit.

Step 4: Set production rate. Hydrogen feed come from a header and toluene feed is drawn from a supply tank. The benzene, methane, and diphenyl products go to headers or tanks. Hence we are not constrained to set production rate either via supply or demand. From the kinetic expressions, we see that only three variables could be potentially dominant for the reactor: temperature, pressure, and toluene concentration.

Pressure is not a viable choice for production rate control because we want to run at maximum system pressure and compressor capacity for yield purposes. This gives us two viable options: change reactor inlet temperature or inlet toluene composition. We select toluene composition. This allows us to control the total flow of toluene to reactor (recycle plus fresh). Fresh toluene feed flow is used to control toluene inventory reflected in the recycle column overhead receiver level as an indication of the need for reactant makeup. Controlling the total toluene flow sets the reactor composition indirectly.

Step 5: Control product quality and handle safety, operational, and environmental constraints. The distillate stream from the product column is salable benzene. Benzene quality can be affected primarily by two components, methane and toluene. Any methane that leaves in the bottoms of stabilizer column contaminates the benzene product. The easy separation in stabilizer column allows us to prevent this by using a temperature to set column steam rate (boilup). Toluene in the overhead of the product column also affects benzene quality. In this column the separation between benzene and toluene is also fairly easy. Thus we can control product column boilup by using a tray temperature control.

Step 6: Fix a flow in every recycle loop and control inventories. The recycle flow of toluene should be fixed. Four pressures must be controlled: in the three distillation columns and in the gas loop. The pressure in the gas loop is controlled with the fresh hydrogen feed flow since it indicates hydrogen inventory in the gas recycle loop. In the stabilizer column, vapor product flow is the most direct manipulator to control pressure. In the product and recycle columns, pressure control can be achieved by manipulating cooling water flow to regulate overhead condensation rate. In HDA process alternatives 4 and 6, since heat-integrated distillation system was used for both the product and recycle columns, the cold inlet stream of process-to-process-heat-exchanger (condenser/reboiler CR) is bypassed and manipulated to control pressure in the recycle column.

Seven liquid levels are in the process: separator and two (base and overhead receiver) in each column. The most direct way to control separator level is with the liquid flow to the stabilizer column. Then stabilizer column overhead receiver level is controlled with cooling water flow and base level is controlled with bottoms flow. In the product column, distillate flow controls overhead receiver level and bottoms flow controls base level. Contrary to the other columns, the boilup ratio in the recycle column is large since the bottoms diphenyl flow is quite small compared with the toluene recycle rate. For this case, we choose to control base level in the recycle column with the steam flow because it has a much larger effect. The fresh makeup toluene feed is used to control the overhead receiver level since it represents the toluene inventory in the process.

Step 7: Check component balance. Methane is purged from the gas recycle loop to prevent it from accumulating, and its composition can be controlled with purge flow. Diphenyl is removed in the bottoms stream from the recycle column, where steam flow control base level. Here, we control the temperature with the bottoms flow. The inventory of benzene is accounted for via temperature and overhead receiver level control in the product column. Toluene inventory is accounted for via level control in the recycle column overhead receiver. Purge flow and gas-loop pressure control account for hydrogen inventory.

Step 8: Control individual unit operations. We can now assign control loops within individual units. Cooling water flow to the cooler controls the separator temperature. Reflux to the stabilizer, product, and recycle columns can be flow controlled because there is no requirement at the unit operations level to do anything beyond this.

Step 9: Optimize economics and improve dynamic controllability. The basic regulatory strategy has now been established. For the purpose of plantwide energy management, the proper heat pathway through the process is selected by means of a selective controller with low selector switch (LSS) to direct the disturbance load to a heating or cooling utility unit. Therefore, the utility duties could be reduced according to the input disturbance load.

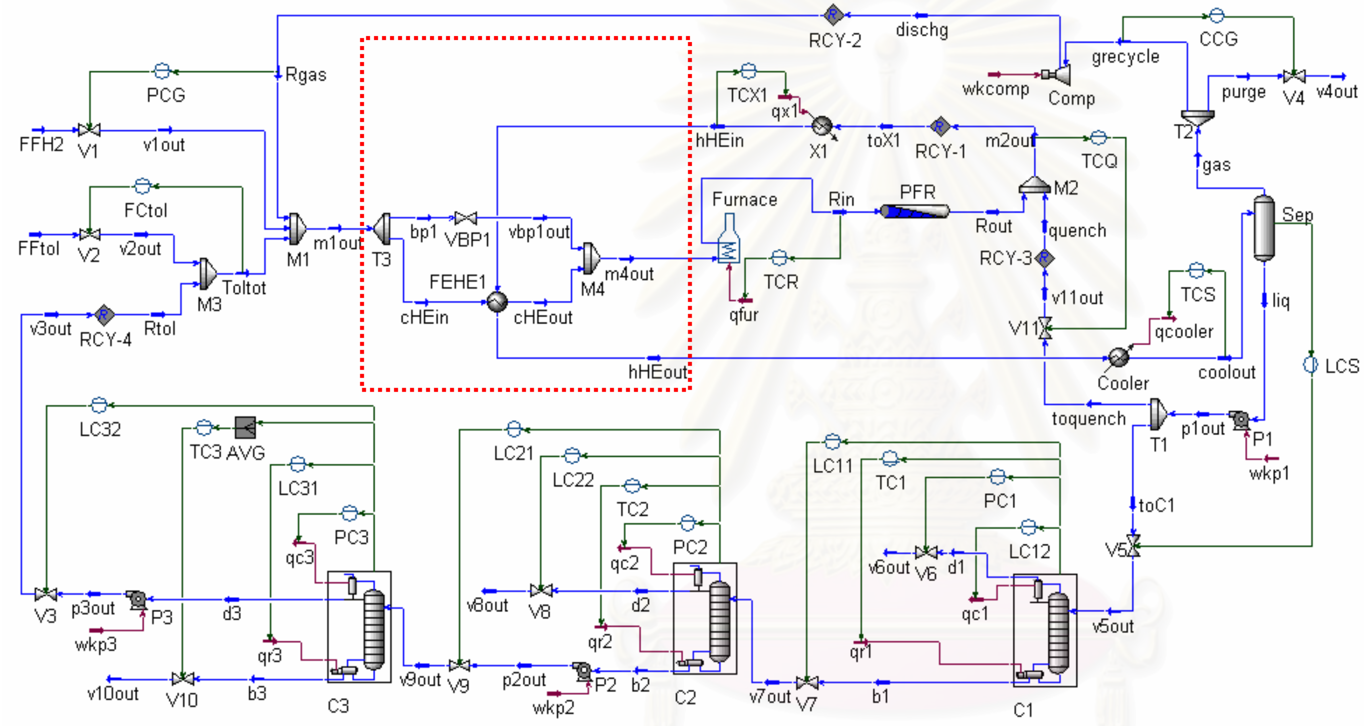
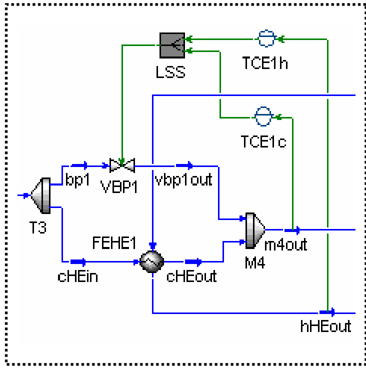
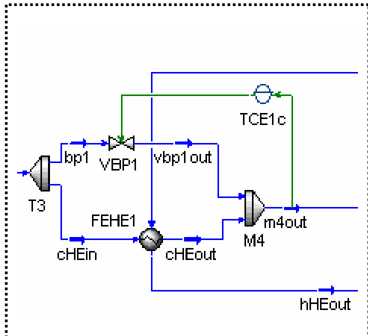


Figure 5.1 The plantwide control structure of the HDA process alternative 1



(a) Our study (with LSS)



(b) Luyben's study (without LSS)

Table 5.1 The initial values of the controlled and manipulated variables for HDA process alternative 1

controlled variable (CV)		manipulated variable (MV)	
process variable	initial value	process variable	initial value
total toluene flow rate	168.62 kgmole/hr	fresh feed toluene flow rate	130 kgmole/hr
gas recycle pressure	4171.3 kPa	fresh feed hydrogen flow rate	222.7 kgmole/hr
methane in gas recycle	0.5894 mole-frac	purge gas	219.4 kgmole/hr
quenched temperature	621.1 ^{o}C	quench flow rate	49.00 kgmole/hr
reactor inlet temperature	621.1 ^{o}C	furnace duty (qfur)	1383 kW
separator temperature	45 ^{o}C	cooler duty (qcooler)	3186 kW
furnace inlet temperature	584 ^{o}C	FEHE1 bypass flow	108.1 kgmole/hr
cooler inlet temperature	119.6 ^{o}C	FEHE1 bypass flow	108.1 kgmole/hr
separator liquid level	50 % level	column C1 feed flow rate	171.9 kgmole/hr
column C1 pressure	1034 kPa	column C1 gas flow rate	8.9 kgmole/hr
column C1 tray-6 temp.	153.9 ^{o}C	column C1 reboiler duty (qr1)	1253 kW
column C1 base level	50 %-level	column C2 feed flow rate	163.0 kgmole/hr
column C1 reflux drum level	50 %-level	column C1 condenser duty (qc1)	177.3 kW
column C2 pressure	206.8 kPa	column C2 condenser duty (qc2)	3995 kW
column C2 tray-12 temp.	120.5 ^{o}C	column C2 reboiler duty (qr2)	3401 kW
column C2 base level	50 %-level	column C3 feed flow rate	41 kgmole/hr
column C2 reflux drum level	50 %-level	column C2 product flow rate	122.1 kgmole/hr
column C3 pressure	206.8 kPa	column C3 condenser duty (qc3)	422.1 kW
avg. C3-tray 1, 2, 3, 4 temp.	228.7 ^{o}C	column C3 bottom flow rate	2.8 kgmole/hr
column C3 base level	50 %-level	column C3 reboiler duty (qr3)	466.5 kW
column C3 reflux drum level	50 %-level	toluene recycle flow rate	38 kgmole/hr

5.2.2 Implementation of Heat Pathway Manipulator in HDA Alternative 1

Figure 5.1 shows the plantwide control structure of HDA process alternative 1. The major loops in HDA process alternative 1 are the same as those used in Luyben et al. (1999), except for the outlet temperature control in FEHE1 and the tray temperature control in the recycle column (C3). For comparison, the previous temperature control in FEHE1 given by Luyben et al. (1999) is also designed (Fig. 5.1.b). In Luyben's control system, the furnace inlet temperature is controlled by manipulating the valve on the bypass line (Fig. 5.1.b).

Based on the heat pathway heuristics for plantwide control, a selective controller with low selector switch (LSS) for FEHE1 is now employed in the current study to select an appropriate heat pathway (Fig. 5.1.a). This control system involves one manipulated variable and two controlled variables and works as follows: The hot outlet temperature of FEHE1 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP1). At the same time, the cold outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the furnace duty at a good level. Whenever the cold outlet temperature of FEHE1 drops below the allowable limit due to, for example, a disturbance load entering the process, the LSS switches the control action from the hot temperature control (TCE1h) to the cold temperature control (TCE1c), and closes the valve VBP1. As a result, the cold outlet temperature of FEHE1 will rise to its normal temperature and the hot outlet temperature of FEHE1 will be further decreased, so the cooler duty will also be decreased. Whenever the cold outlet temperature of FEHE1 increases above a lower limit, i.e. a desired-condition during operation, due to the disturbance load entering the process, the LSS switches the control action from TCE1c to TCE1h. Consequently, the hot outlet temperature of FEHE1 will drop to its normal temperature and the cold outlet temperature of FEHE1 will be further increased, so the furnace duty will also be decreased. In order to apply this LSS control strategy in HYSYS, a selector block can be added to the process flow diagram. On the connections page tab, all input signals are specified. On the parameter page tab, the mode of selector is set; in this case the minimum of all input should be selected.

Since the temperature profile in the recycle column is very sharp because of the large difference in boiling point between toluene and diphenyl, this produces large temperature changes from tray to tray. This means that the process gain is very large when a single tray temperature is controlled. The standard solution for this problem is to use an average (AVG) temperature of several trays instead of a single tray (Luyben, 2002).

A heat exchanger (i.e. as a heat source or a heat sink) is artificially installed in the hot-side stream (i.e. the exchanger X1 in Fig. 5.1) in order to make the disturbance loads of the hot stream (i.e. the hot reactor product). Note that, this exchanger is not used in the real plant, and the temperature controller TCX1 is set to be “off” whenever it is not used to make the disturbances.

The initial values of the controlled and manipulated variables for HDA process alternative 1 are listed in Table 5.1. The control structure and controller parameters for HDA plant alternative 1 are given in Table 5.2. P controllers are employed for the level loops, and PI controllers for the remaining loops. Auto tune variation available tuning method in the HYSYS is first used to estimate these tuning parameters, and then detuning is carried out through trial and error.

Table 5.2 Control structure and controller parameters for HDA process alternative 1

controller	controlled variable	manipulated variable	type	K_C	τ_I [min]	controlled variable range
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	PI	0.1	0.1	0 - 300 kgmole/hr
PCG	gas recycle stream pressure	fresh feed hydrogen valve (V1)	PI	1.2	0.1	3447.38 - 4826.33 kPa
CCG	methane in gas recycle	purge valve (V4)	PI	0.2	15	0.4 - 0.7 mole-fraction
TCQ	quenched temperature	quench valve (V11)	PI	0.15	0.1	593.33 – 648.89 ^oC
TCR	reactor inlet temperature	furnace duty (qfur)	PI	0.0887	0.1	593.33 – 648.89 ^oC
TCS	separator temperature	cooler duty (qcooler)	PI	0.154	0.1	30 – 100 ^oC
TCE1c	furnace inlet temperature	FEHE1 bypass valve (VBP1)	PI	0.4	0.1	530 – 630 ^oC
TCE1h	cooler inlet temperature	FEHE1 bypass valve (VBP1)	PI	0.87	1.05	50 – 150 ^oC
LSS	output of TCE1c and TCE1h	FEHE1 bypass valve (VBP1)	Minimum	-	-	-
LCS	separator liquid level	column C1 feed valve (V5)	P	2	-	0 – 100 %-level
PC1	column C1 pressure	column C1 gas valve (V6)	PI	1	10	689.48 – 1378.95 kPa
TC1	column C1 tray-6 temperature	column C1 reboiler duty (qr1)	PI	1	10	100 – 200 ^oC
LC11	column C1 base level	column C2 feed valve (V7)	P	2	-	0 – 100 %-level
LC12	column C1 reflux drum level	column C1 condenser duty (qc1)	P	1	-	0 – 100 %-level
PC2	column C2 pressure	column C2 condenser duty (qc2)	PI	1	10	137.89 – 275.79 kPa
TC2	column C2 tray-12 temperature	column C2 reboiler duty (qr2)	PI	2	8	93.33 – 148.89 ^oC
LC21	column C2 base level	column C3 feed valve (V9)	P	2	-	0 – 100 %-level
LC22	column C2 reflux drum level	column C2 product valve (V8)	P	2	-	0 – 100 %-level
PC3	column C3 pressure	column C3 condenser duty (qc3)	PI	1	15	137.89 – 275.79 kPa
AVG	avg. temp. of C3-tray 1, 2, 3, and 4	-	Average	-	-	-
TC3	output of AVG	column C3 bottom valve (V10)	PI	0.8	20	175 – 275 ^oC
LC31	column C3 base level	column C3 reboiler duty (qr3)	P	3	-	0 – 100 %-level
LC32	column C3 reflux drum level	toluene recycle valve (V3)	P	2	-	0 – 100 %-level
TCX1	FEHE1 hot inlet temperature	exchanger X1 duty (qx1)	PI	0.08	0.3	600 – 650 ^oC

5.2.3 Implementation of Heat Pathway Manipulator in HDA Alternative 4

The new plantwide control structure for energy-integrated HDA process alternative 4 is shown in Figure 5.2. Its major loops are the same as those used in the HDA process alternative 1, except for the tray temperature control in the product distillation columns (TC2) and pressure control in the recycle column (PC3).

Since the hot reactor product is used to drive the product distillation column, part of this stream in process-to-process exchanger (R2) is bypassed and manipulated to control the tray temperature in the product column (TC2). The hot outlet temperature of FEHE2 (the temperature at the entrance of the reboilers R2) is controlled by manipulating bypass valve in the cold stream to prevent the propagation of thermal disturbance to the separation section (TCE2h).

Since heat-integrated distillation system was used for both the product and recycle columns, the pressure in the two columns should be adjusted so that there is a reasonable differential temperature driving force for heat transfer in the heat exchangers. In this case, the pressure required in the recycle column is 540 kPa to provide a reasonable temperature differential in Condenser/Reboiler (CR). In the recycle column, the cold inlet stream of CR is bypassed and manipulated to control its pressure column. The averaging tray temperature control in the recycle column is used instead of a single tray temperature control. But its set point increases due to the effect of pressure shifting in the recycle column. In order to select an appropriate heat pathway, the LSS is applied in FEHE1 as shown in Figure 5.2.

In order to test the disturbances rejection, the disturbance loads of the hot stream (the hot reactor product stream) and of the cold stream from the bottoms of the product column are made. Two heat exchangers are artificially installed (see exchangers X1 and X2 in Figure 5.2). Again, the temperature controllers TCX1 and TCX2 are set to be “off” whenever these are not used to make the disturbances. The initial values of all the controlled and manipulated variables are listed in Table 5.3. The control structure and controller parameters are given in Table 5.4. P controllers are employed for the level loops, and PI controller for the remaining loops.

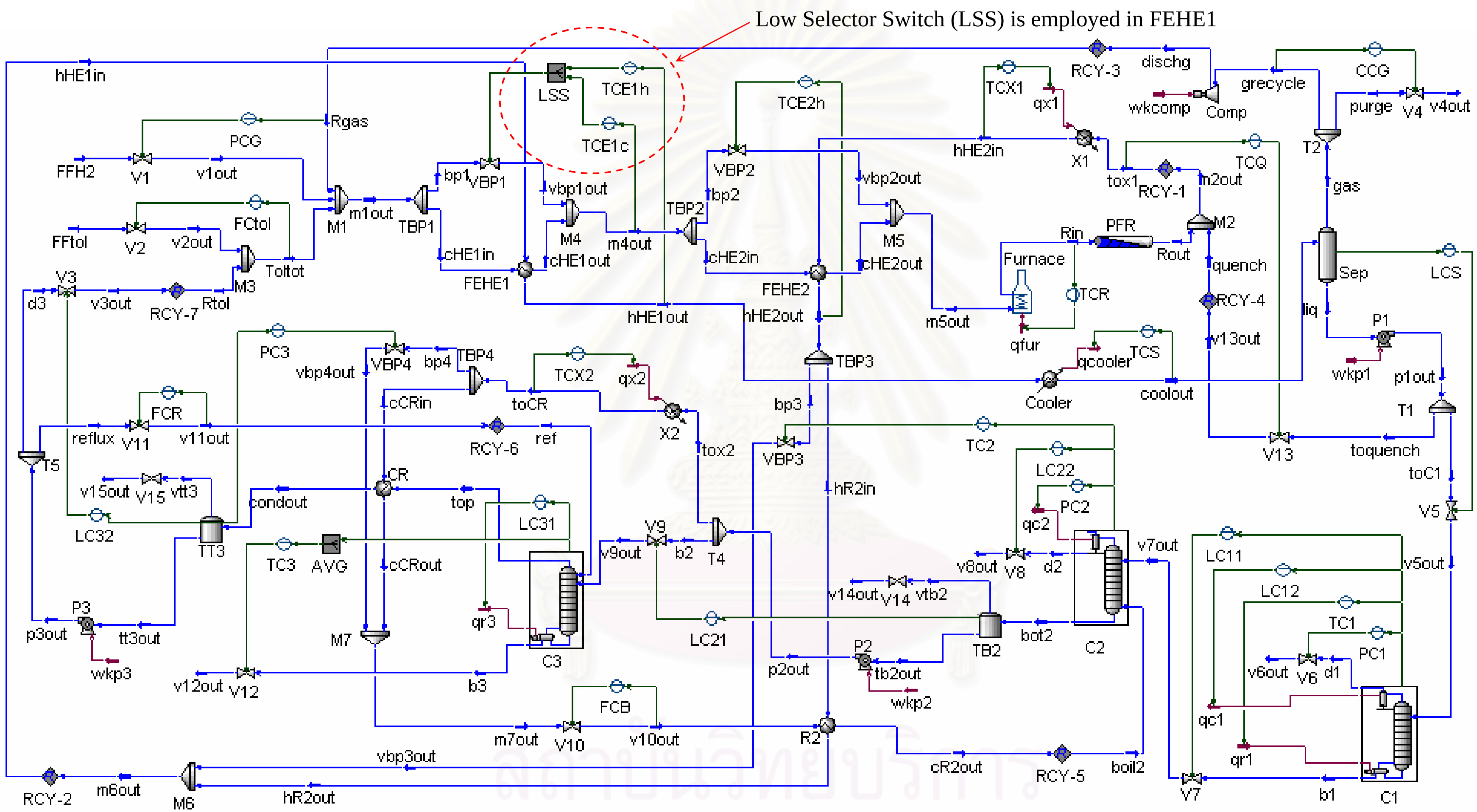


Figure 5.2 Plantwide control structure of the HDA process alternative 4

Table 5.3 The initial values of controlled and manipulated variables for HDA process alternative 4

controlled variable (CV)		manipulated variable (MV)	
process variable	initial value	process variable	initial value
total toluene flow rate	168.6 kgmole/hr	fresh feed toluene flow rate	130 kgmole/hr
gas recycle stream pressure	4171 kPa	fresh feed hydrogen flow rate	221.3 kgmole/hr
methane in gas recycle	0.5904 mole-frac	purge flow rate	218.3 kgmole/hr
quenched temperature	621.1 ^oC	quench flow rate	49 kgmole/hr
reactor inlet temperature	621.1 ^oC	furnace duty (qfur)	3967 kW
separator temperature	45 ^oC	cooler duty (qcooler)	1879 kW
FEHE2 cold inlet temperature	148.5 ^oC	FEHE1 bypass flow rate	103.8 kgmole/hr
cooler inlet temperature	93.6 ^oC	bypass flow rate FEHE1	103.8 kgmole/hr
FEHE2 hot outlet temperature	313.6 ^oC	FEHE2 bypass flow	131 kgmole/hr
separator liquid level	50 %-level	column C1 feed flow rate	171.7 kgmole/hr
column C1 pressure	1034 kPa	column C1 gas flow rate	8.7 kgmole/hr
column C1 tray-6 temperature	154.15 ^oC	column C1 reboiler duty (qr1)	1253 kW
column C1 base level	50 %-level	column C2 feed flow rate	163 kgmole/hr
column C1 reflux drum level	50 %-level	column C1 condenser duty (qc1)	175.9 kW
column C2 pressure	206.8 kPa	column C2 condenser duty (qc2)	5012 kW
column C2 tray-12 temperature	129.75 ^oC	R2 bypass flow	129.1 kgmole/hr
column C2 base level	50 %-level	column C3 feed flow rate	41.3 kgmole/hr
column C2 reflux drum level	50 %-level	column C2 product flow rate	121.6 kgmole/hr
column C2 boilup flow rates	385 kgmole/hr	R2 cold inlet flow rate	385 kgmole/hr
column C3 pressure	526.2 kPa	CR bypass flow rate	25 kgmole/hr
avg. C3-tray 1, 2, 3, and 4 temp.	313 ^oC	column C3 bottom flow rate	2.8 kgmole/hr
column C3 base level	50 %-level	column C3 reboiler duty (qr3)	547.6 kW
column C3 reflux drum level	50 %-level	toluene recycle flow rate	38.5 kgmole/hr
column C3 reflux flow rate	9.94 kgmole/hr	column C3 reflux flow rate	9.94 kgmole/hr

Table 5.4 Control structure and controller parameters for HDA process alternative 4

controller	controlled variable	manipulated variable	type	K_C	τ_I [min]	controlled variable range
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	PI	0.1	0.1	0 - 300 kgmole/hr
PCG	gas recycle stream pressure	fresh feed hydrogen valve (V1)	PI	1.2	0.1	3447.38 - 4826.33 kPa
CCG	methane in gas recycle	purge valve (V4)	PI	0.2	15	0.4 - 0.7 mole-fraction
TCQ	quenched temperature	quench valve (V13)	PI	0.15	0.5	593.33 – 648.89 ^oC
TCR	reactor inlet temperature	furnace duty (qfur)	PI	0.0887	0.1	593.33 – 648.89 ^oC
TCS	separator temperature	cooler duty (qcooler)	PI	0.154	0.1	30 – 100 ^oC
TCE1c	cold inlet temperature of FEHE2	FEHE1 bypass valve (VBP1)	PI	1	1	100 – 200 ^oC
TCE1h	cooler inlet temperature	FEHE1 bypass valve (VBP1)	PI	0.87	1.05	50 - 150 ^oC
LSS	output of TCE1c and TCE1h	FEHE1 bypass valve (VBP1)	Min	-	-	-
TCE2h	hot outlet temperature of FEHE2	FEHE2 bypass valve (VBP2)	PI	0.5	0.1	250 –350 ^oC
LCS	separator liquid level	column C1 feed valve (V5)	P	2		0 – 100 %-level

Table 5.4 *Continued*

controller	controlled variable	manipulated variable	type	Kc	τ_I	range
PC1	column C1 pressure	column C1 gas valve (V6)	PI	1	10	689.48 - 1378.95 kPa
TC1	column C1 tray-6 temperature	column C1 reboiler duty (qr1)	PI	1	10	100 – 200 ^oC
LC11	column C1 base level	column C2 feed valve (V7)	P	2		0 – 100 %-level
LC12	column C1 reflux drum level	column C1 condenser duty (qc1)	P	1		0 – 100 %-level
PC2	column C2 pressure	column C2 condenser duty (qc2)	PI	1	10	137.89 - 275.79 kPa
TC2	column C2 tray-12 temperature	R2 bypass valve (VBP3)	PI	30	5	93.33 – 148.89 ^oC
LC21	column C2 base level	column C3 feed valve (V9)	P	2		0 – 100 %-level
LC22	column C2 reflux drum level	column C2 product valve (V8)	P	2		0 – 100 %-level
FCB	column C2 boilup flow rates	R2 cold inlet valve (V10)	PI	0.05	0.1	300 – 400 kgmole/hr
PC3	column C3 pressure	CR bypass valve (VBP4)	PI	30	20	344.74 – 689.46 kPa
AVG	avg. temp. of C3-tray 1, 2, 3, and 4	-	Avg	-	-	-
TC3	output of AVG	column C3 bottom valve (V12)	PI	0.2	30	250 – 350 ^oC
LC31	column C3 base level	column C3 reboiler duty (qr3)	P	3		0 – 100 %-level
LC32	column C3 reflux drum level	toluene recycle valve (V3)	P	2		0 – 100 %-level
FCR	column C3 reflux flow rates	column C3 reflux valve (V11)	PI	0.2	0.1	0 – 20 kgmole/hr
TCX1	FEHE2 hot inlet temperature	exchanger X1 duty (qx1)	PI	0.08	0.3	600 – 650 ^oC
TCX2	column C2 bottom temperature	exchanger X2 duty (qx2)	PI	0.05	1.0	125 – 175 ^oC

5.2.4 Implementation of Heat Pathway Manipulator in HDA Alternative 6

The plantwide control structure of HDA process alternative 6 is shown in Figure 5.3. Its major loops are the same as those used in HDA process alternative 1, except for the tray temperature controls in the three distillation columns (TC1, TC2 and TC3), the temperature controls in FEHE2 and FEHE3 (TCE2h and TCE3h), and pressure control in the recycle column (PC3). Since the hot reactor product is used to drive all reboilers in the three columns, part of this stream is bypassed and manipulated to control the tray temperatures in the three columns. The hot outlet temperatures of FEHE2 and FEHE3 (the temperature at the entrance of the reboilers, R2 and R3) are controlled by manipulating the bypass valves VBP2 and VBP3, respectively, in order to prevent the propagation of thermal disturbance to the separation section. In the recycle column, the cold stream of condenser/reboiler (CR) is bypassed and manipulated to control its pressure column. The LSS is employed in FEHE1 in order to select an appropriate heat pathway to carry the associated load to a utility unit.

In HDA process alternative 6, the disturbance loads of the hot stream and of the cold streams from the bottoms of the three columns are made to test the disturbances rejection. Four heat exchangers are artificially installed (see exchangers X1, X2, X3, and X4 in Fig. 5.3). Again, the temperature controllers TCX1, TCX2, TCX3, and TCX4 are set to be "off" whenever these are not used to make the disturbances.

Table 5.5 The initial values of controlled and manipulated variables for HDA process alternative 6

controlled variable		manipulated variable	
process variable	initial value	process variable	initial value
total toluene flow rate	168.2 kgmole/hr	fresh toluene feed flow rate	130 kgmole/hr
gas recycle stream pressure	4171 kPa	fresh hydrogen feed flow rate	222 kgmole/hr
methane in gas recycle	0.5876 mole-frac	purge flow rate	219.9 kgmole/hr
quenched temperature	621.1 ^oC	quench flow rate	49 kgmole/hr
reactor inlet temperature	621.1 ^oC	furnace duty (qfur)	5998 kW
separator temperature	45 ^oC	cooler duty (qcooler)	1953 kW
FEHE2 cold inlet temperature	148.5 ^oC	FEHE1 bypass flow rate	108.3 kgmole/hr
cooler inlet temperature	94.9 ^oC	FEHE1 bypass flow rate	108.3 kgmole/hr
FEHE2 hot-outlet temperature	358 ^oC	FEHE2 bypass flow rate	110.2 kgmole/hr
FEHE3 hot-outlet temperature	450 ^oC	FEHE3 bypass flow rate	109.8 kgmole/hr
separator liquid level	50 %-level	column C1 feed flow rate	170.9 kgmole/hr
column C1 pressure	1034 kPa	column C1 gas flow rate	8.4 kgmole/hr
column C1 tray-6 temperature	166.3 ^oC	R1 bypass flow rate	118.8 kgmole/hr
column C1 base level	50 %-level	column C2 feed flow rate	162.5 kgmole/hr
column C1 reflux drum level	50 %-level	column C1 condenser duty (qc1)	383.7 kW
column C1 boil up flowrate	183 kgmole/hr	R1 cold-inlet flow rate	183 kgmole/hr
column C2 pressure	206.8 kPa	column C2 condenser duty (qc2)	5017 kW
column C2 tray-12 temperature	129.78 ^oC	R2 bypass flow rate	122.5 kgmole/hr
column C2 base level	50 %-level	column C3 feed flow rate	40.8 kgmole/hr
column C2 reflux drum level	50 %-level	column C2 product flow rate	121.6 kgmole/hr
column C2 boil up flowrate	385 kgmole/hr	R2 cold-inlet flow rate	385 kgmole/hr
column C3 pressure	526.2 kPa	CR bypass flow rate	22.8 kgmole/hr
avg. C3-tray 1, 2, 3, and 4 temp.	326.7 ^oC	R3 bypass flow rate	123.2 kgmole/hr
column C3 base level	50 %-level	column C3 bottom flow rate	2.78 kgmole/hr
column C3 reflux drum level	50 %-level	toluene recycle flow rate	38 kgmole/hr
column C3 boil up flowrate	47.26 kgmole/hr	R3 cold-inlet flow rate	47.26 kgmole/hr
column C3 reflux flow rate	9.94 kgmole/hr	column C3 reflux flow rate	9.94 kgmole/hr

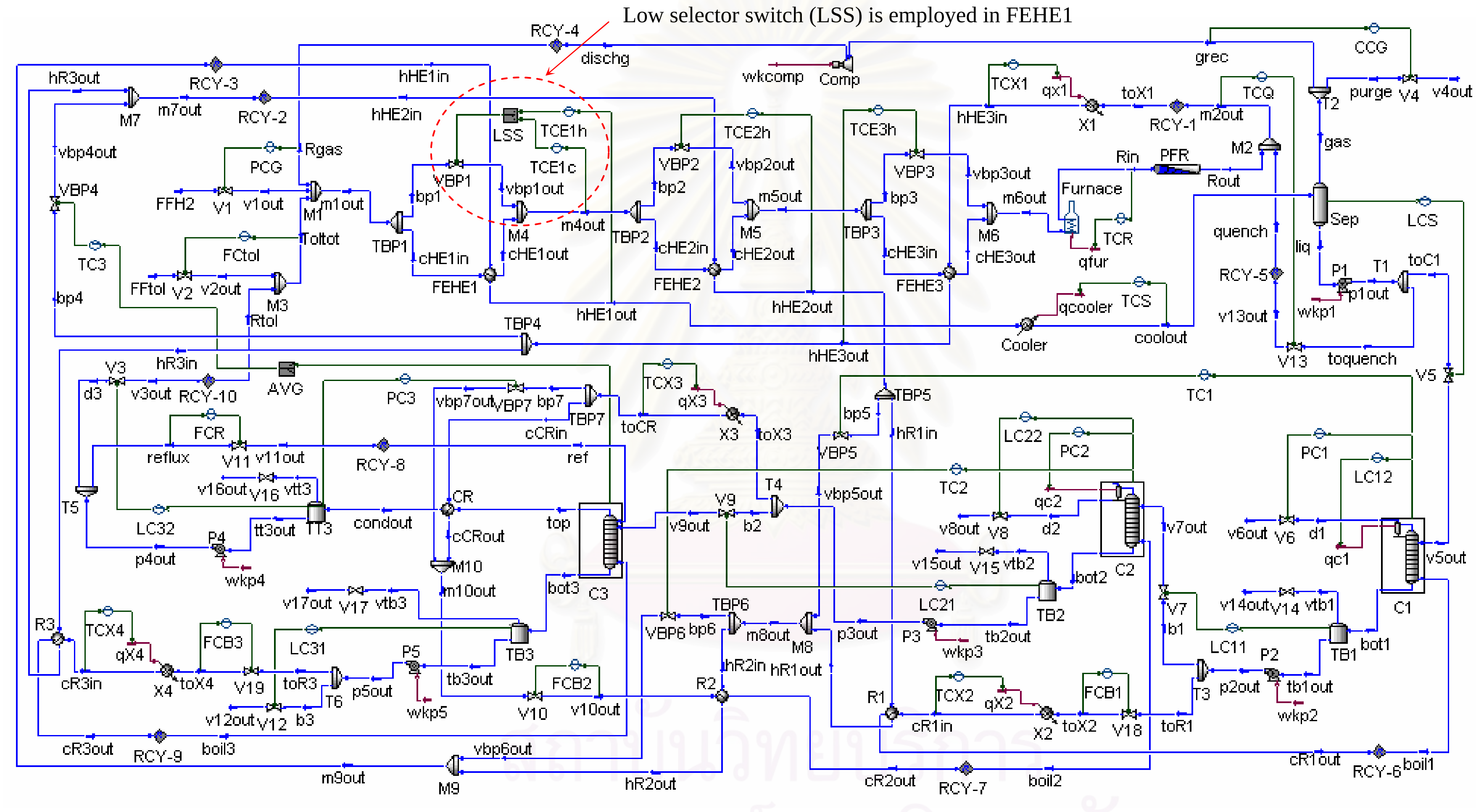


Figure 5.3 Plantwide control structure of the HDA process alternative 6

Table 5.6 Control structure and controller parameters for HDA process alternative 6

controller	controlled variable	manipulated variable	type	K_C	τ_I [min]	controlled variable Range
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	PI	0.01	0.1	0 - 300 kgmole/hr
PCG	gas recycle stream pressure	fresh feed hydrogen valve (V1)	PI	1.2	0.1	3792.1 – 4481.6 kPa
CCG	methane in gas recycle	purge valve (V4)	PI	0.2	15	0.4 - 0.7 mole-fraction
TCQ	quenched temperature	quench valve (V13)	PI	0.15	0.5	593.33 - 648.89 ^oC
TCR	reactor inlet temperature	furnace duty (qfur)	PI	0.0887	0.1	593.33 - 648.89 ^oC
TCS	separator temperature	cooler duty (qcooler)	PI	0.154	0.1	30 - 100 ^oC
TCE1c	FEHE2 cold inlet temperature	FEHE1 bypass valve (VBP1)	PI	1	1	100 – 200 ^oC
TCE1h	cooler inlet temperature	FEHE1 bypass valve (VBP1)	PI	0.9	1	50 - 150 ^oC
LSS	output of TCE1c and TCE1h	FEHE1 bypass valve (VBP1)	Min	-	-	-
TCE2h	FEHE2 hot-outlet temperature	FEHE2 bypass valve (VBP2)	PI	3	1	300 - 400 ^oC
TCE3h	FEHE3 hot-outlet temperature	FEHE3 bypass valve (VBP3)	PI	3	1	400 - 500 ^oC
LCS	separator liquid level	column C1 feed valve (V5)	P	2	-	0 - 100 %-level
PC1	column C1 pressure	column C1 gas valve (V6)	PI	0.1	10	689.48 - 1378.95 kPa
TC1	column C1 tray-6 temperature	R1 bypass valve (VBP5)	PI	20	5	100 - 200 ^oC
LC11	column C1 base level	column C2 feed valve (V7)	P	2	-	0 - 100 %-level
LC12	column C1 reflux drum level	column C1 condenser duty (qc1)	P	1	-	0 - 100 %-level
FCB1	column C1 boil up flowrate	cold-inlet valve of R1 (V18)	PI	0.2	0.1	130 - 230 kgmole/hr
PC2	column C2 pressure	column C2 condenser duty (qc2)	PI	1	10	137.89 - 275.79 kPa
TC2	column C2 tray-12 temperature	R2 bypass valve (VBP6)	PI	30	5	93.33 - 148.89 ^oC
LC21	column C2 base level	column C3 feed valve (V9)	P	2	-	0 - 100 %-level
LC22	column C2 reflux drum level	column C2 product valve (V8)	P	2	-	0 - 100 %-level
FCB2	column C2 boil up flowrate	R2 cold-inlet valve (V10)	PI	0.2	0.1	300 - 400 kgmole/hr
PC3	column C3 pressure	CR bypass valve (VBP7)	PI	30	20	344.74 - 689.48 kPa
AVG	avg. temp. of C3-tray 1, 2, 3, and 4	-	Avg	-	-	-
TC3	output of AVG	R3 bypass valve (VBP4)	PI	4	10	275 - 375 ^oC
LC31	column C3 base level	column C3 bottom valve (V12)	P	2	-	0 - 100 %-level
LC32	column C3 reflux drum level	toluene recycle valve (V3)	P	2	-	0 - 100 %-level

Table 5.6. *Continued*

controller	controlled variable	manipulated variable	type	K_C	τ_I	range
FCB3	column C3 boil up flowrate	R3 cold-inlet valve (V19)	PI	0.2	0.1	20 - 80 kgmole/hr
FCR	column C3 reflux flow rate	column C3 reflux valve (V11)	PI	0.2	0.1	0 - 20 kgmole/hr
TCX1	FEHE1 hot inlet temperature	exchanger X1 duty (qx1)	PI	0.08	0.3	600 – 650 ^oC
TCX2	column C1 bottoms temperature	exchanger X2 duty (qx2)	PI	0.08	1.0	165 – 215 ^oC
TCX3	column C2 bottoms temperature	exchanger X3 duty (qx3)	PI	0.05	1.2	125 – 175 ^oC
TCX4	column C3 bottoms temperature	exchanger X4 duty (qx4)	PI	0.01	2.0	325 – 375 ^oC

The initial values of all of the controlled and manipulated variables are listed in Table 5.5. The control structure and controller parameters are given in Table 5.6. P controllers are employed for the level loops, and PI controller for the remaining loops.

5.3 Dynamic Simulation Results of HDA Process Alternative 1

In order to evaluate the dynamic performances of the new designed plantwide control in HDA process alternative 1, several disturbance loads were made. The dynamic responses of the control systems for the HDA process alternative 1 are shown in Figures 5.4 to 5.6. The dynamic responses of our control structure and the previous control structure (Luyben et al., 1999) are shown in the left side and the right side in Figures 5.4 to 5.6, respectively. In general, better responses of the furnace and cooler utility consumptions are achieved here compared to the Luyben's control structure, since the duties for both furnace and cooler utilities could be decreased. Therefore, the proposed HPH is very useful in terms of heat load or disturbance management to achieve the highest possible dynamic MER. Results for the disturbance load changes are as follows:

Our study (with LSS) Luyben’s study (without LSS)

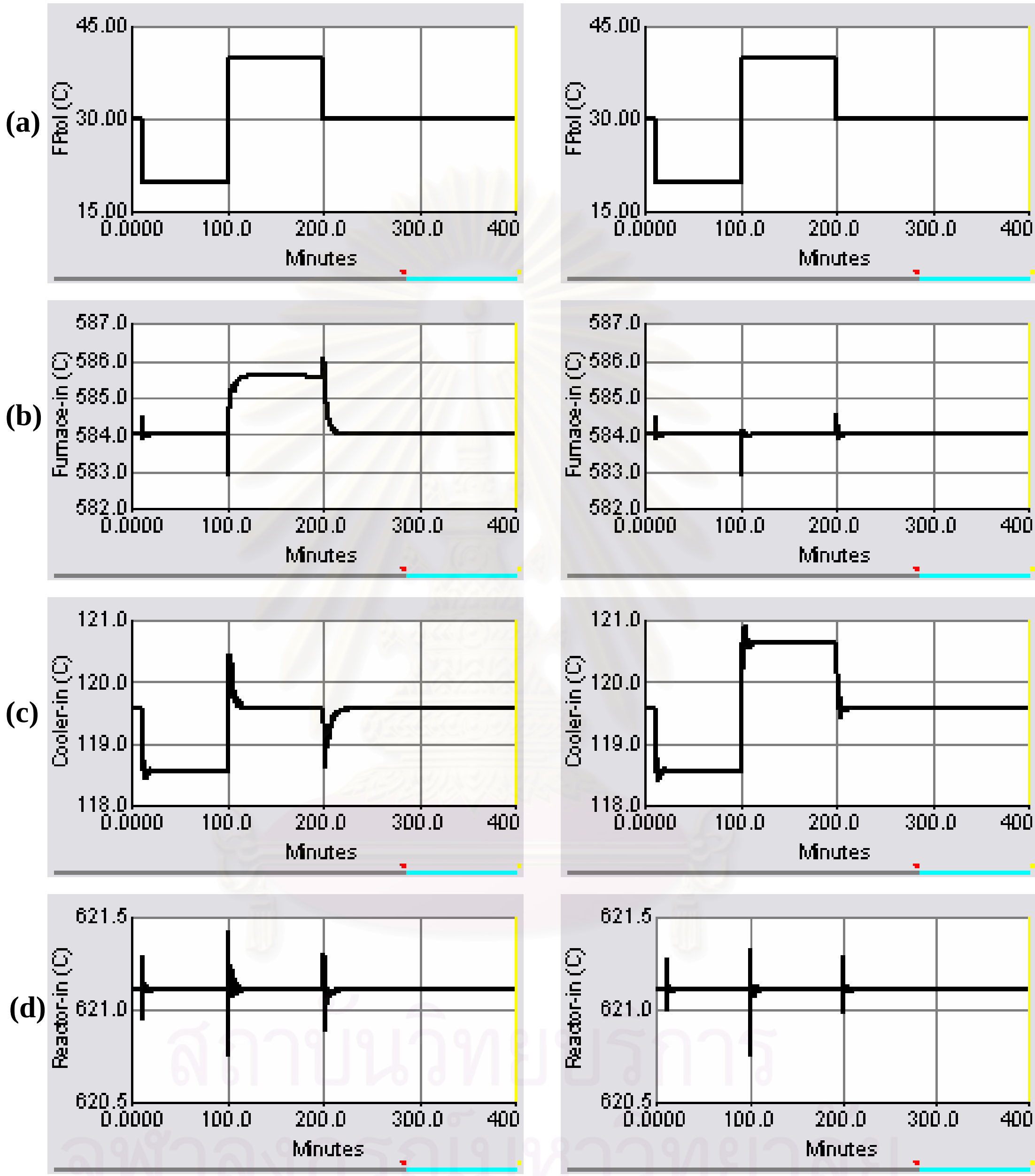


Figure 5.4 Dynamic responses of the HDA process alternative 1 to a change in the disturbance load of cold stream (reactor feed stream); where, (a) fresh feed toluene temperature, (b) furnace inlet temperature, (c) cooler inlet temperature, (d) reactor inlet temperature, (e) separator temperature, (f) C1-tray temperature, (g) C2-tray temperature, (h) C3-tray temperature, (i) furnace duty, (j) cooler duty; comparison between the current study (left side) and the previous study (right side).

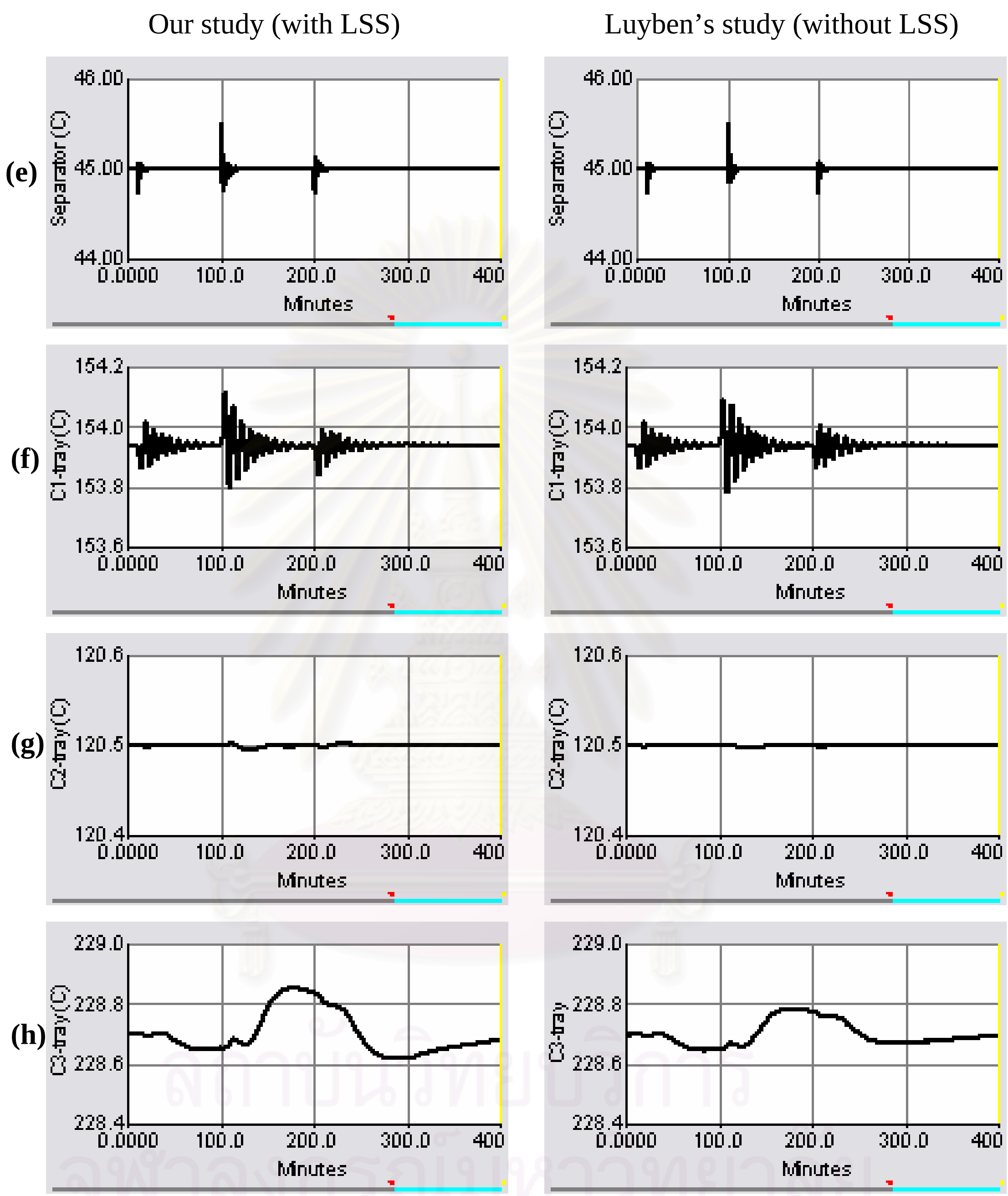


Figure 5.4 *Continued.*

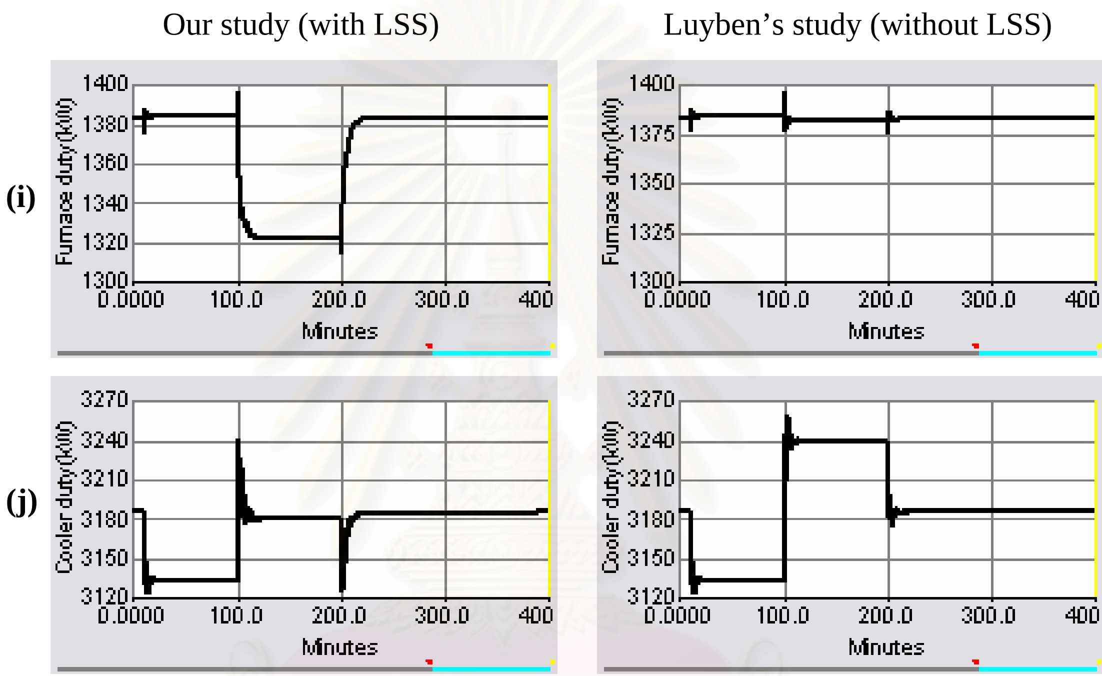


Figure 5.4 *Continued.*

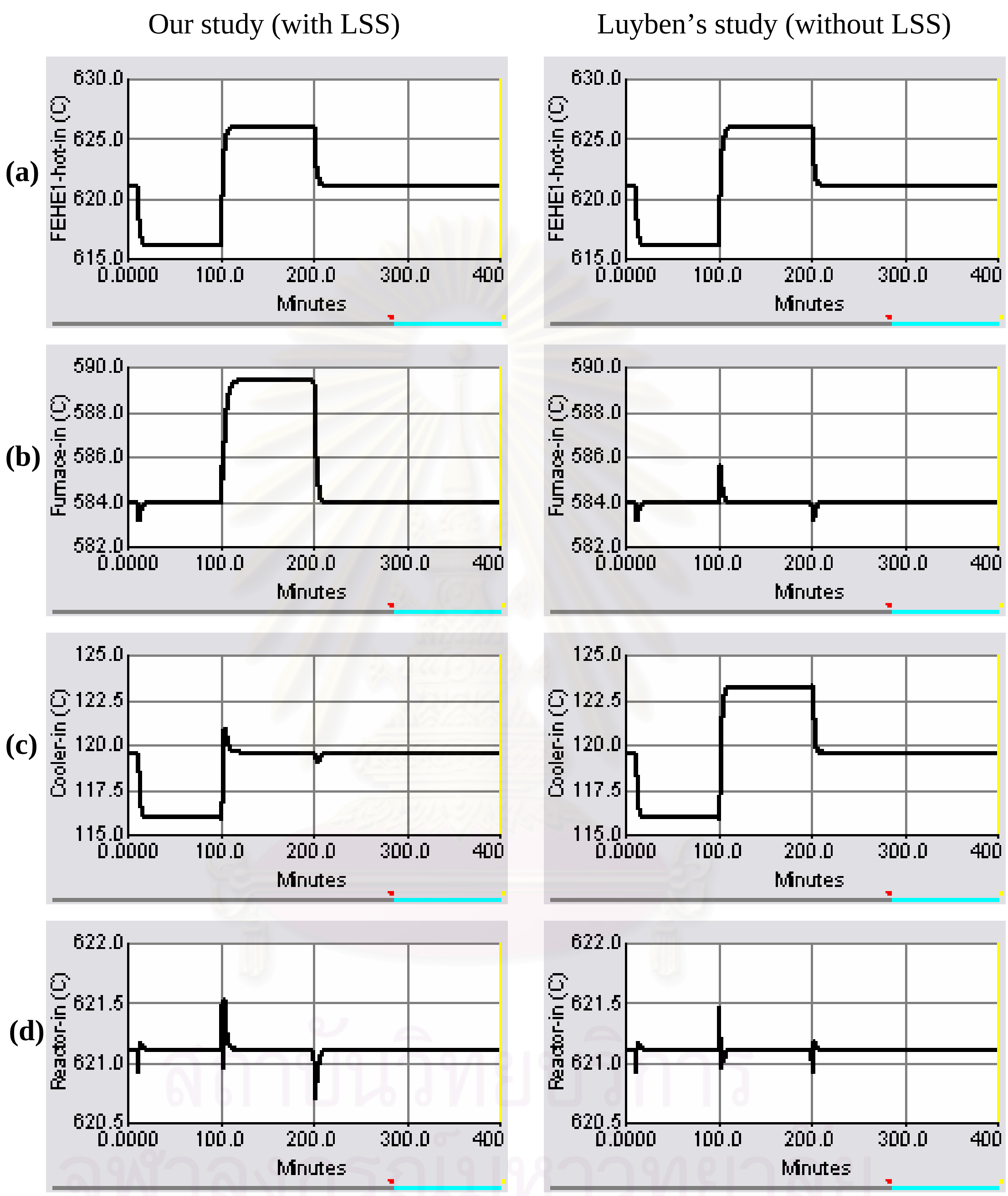
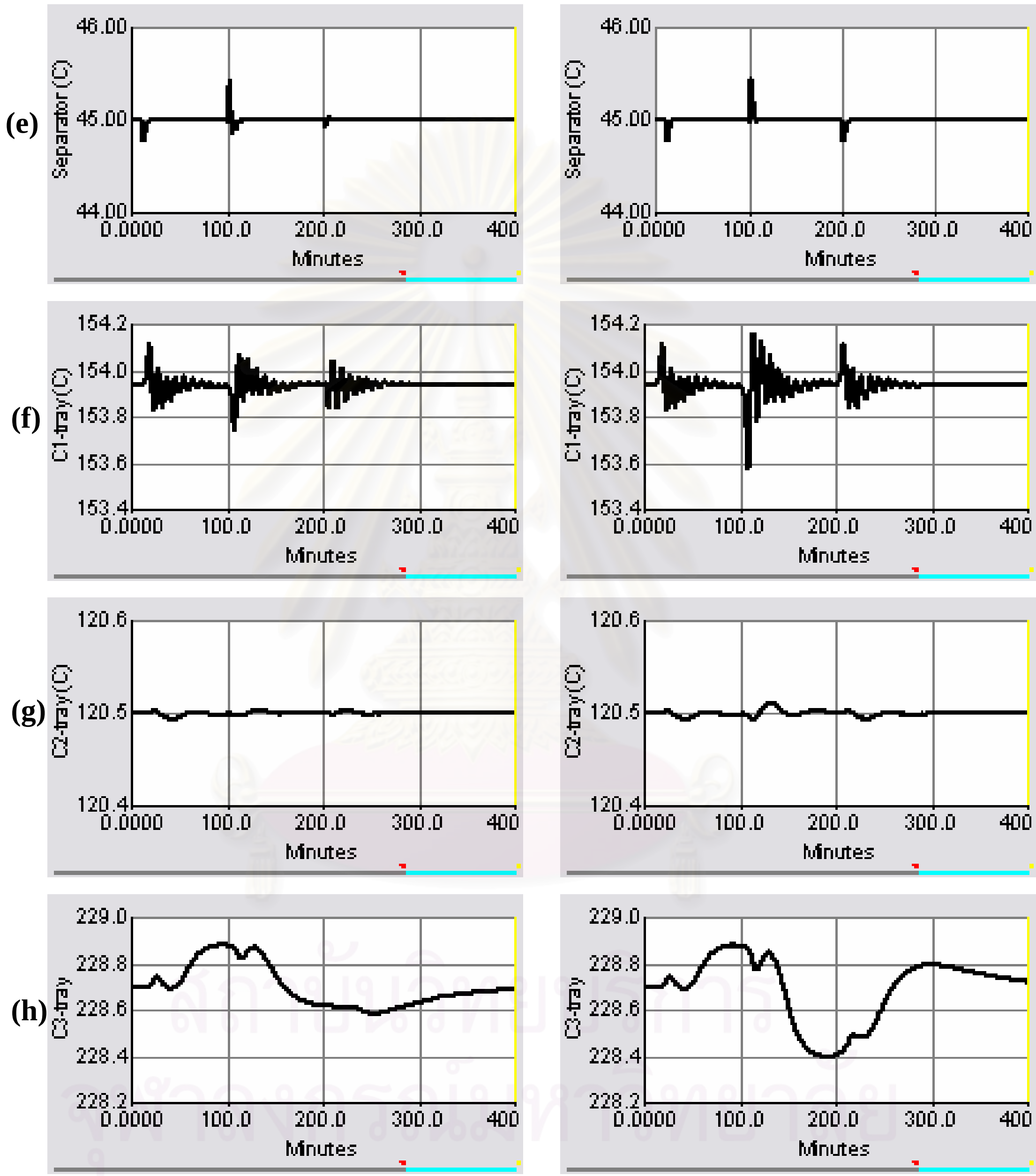


Figure 5.5 Dynamic responses of the HDA process alternative 1 to a change in the disturbance load of hot stream (reactor product stream); where, (a) FEHE1 hot inlet temperature, (b) furnace inlet temperature, (c) cooler inlet temperature, (d) reactor inlet temperature, (e) separator temperature, (f) C1-tray temperature, (g) C2-tray temperature, (h) C3-tray temperature, (i) furnace duty, (j) cooler duty; comparison between the current study (left side) and the previous study (right side).

Our study (with LSS) Luyben's study (without LSS)



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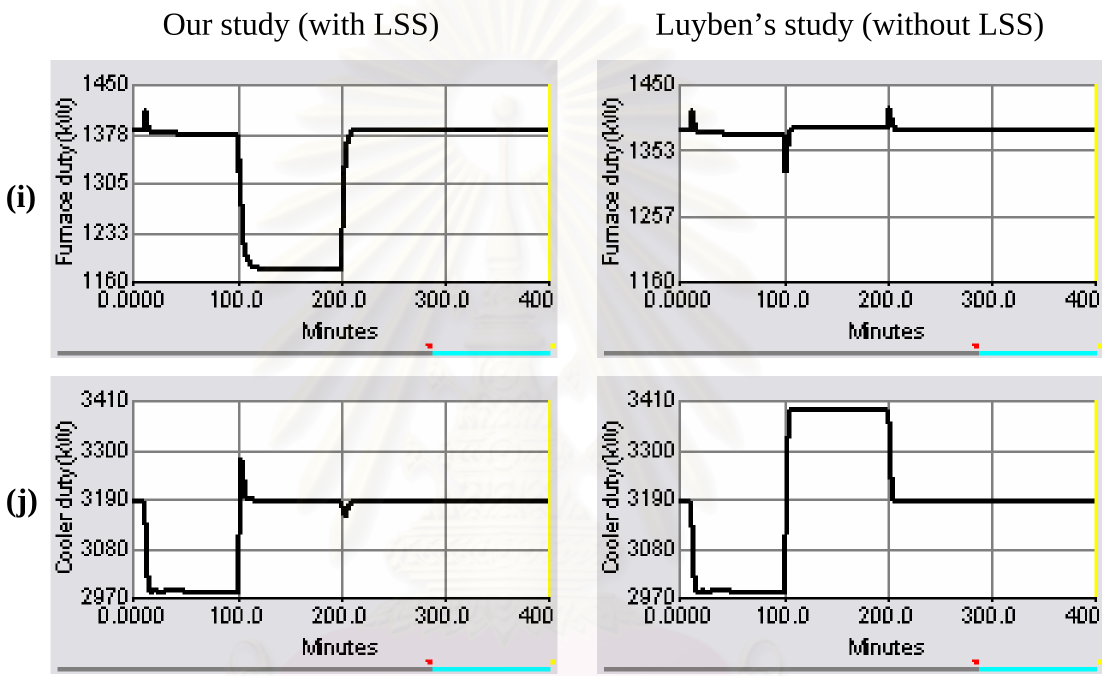

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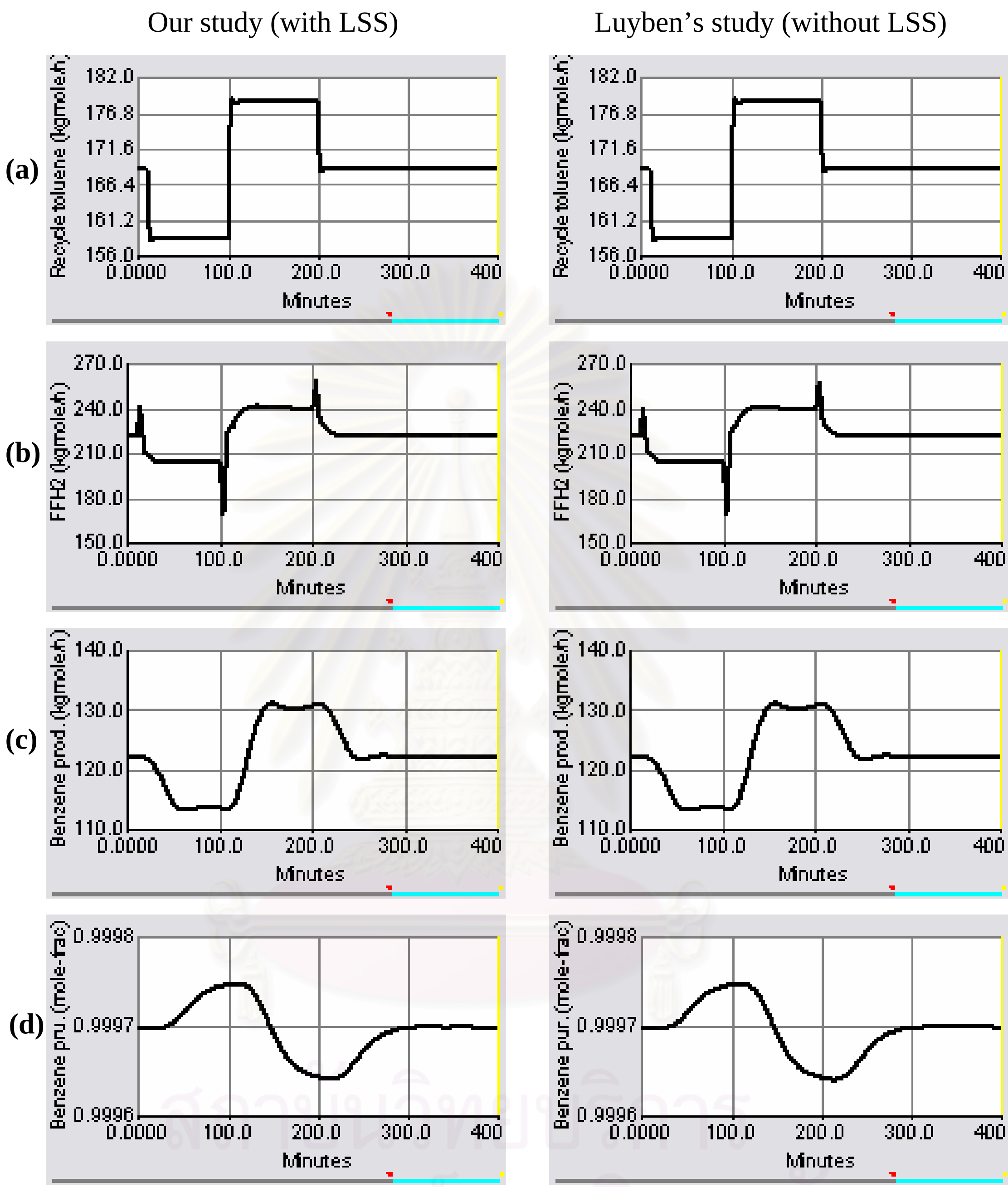
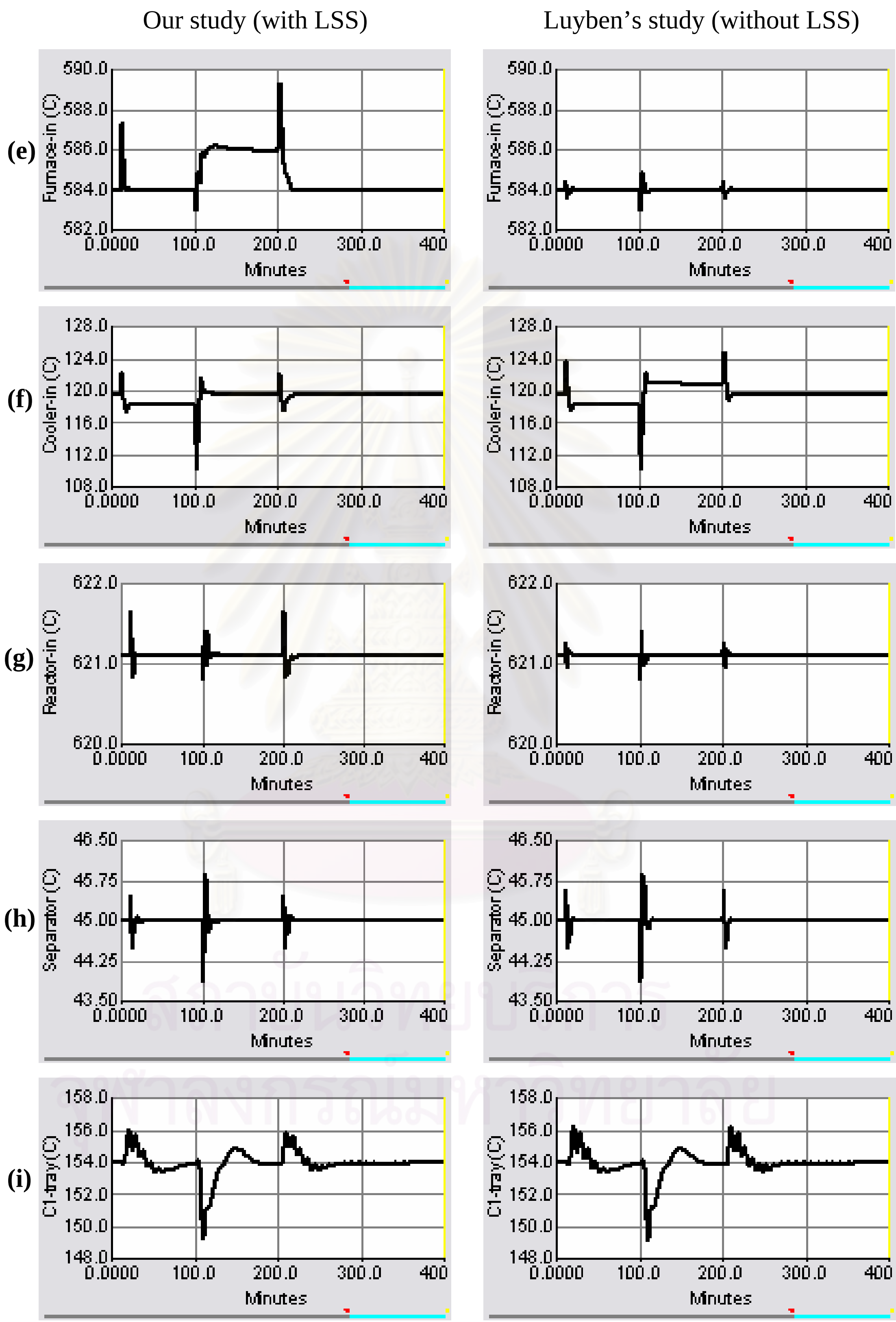


Figure 5.6 Dynamic responses of the HDA process alternative 1 to a change in the recycle toluene flowrates; where, (a) recycle toluene flowrates, (b) fresh feed hydrogen flowrates (c) benzene product flowrates (d) benzene purity (e) furnace inlet temperature, (f) cooler inlet temperature, (g) reactor inlet temperature, (h) separator temperature, (i) C1-tray temperature, (j) C2-tray temperature, (k) C3-tray temperature, (l) furnace duty, (m) cooler duty; comparison between the current study (left side) and the previous study (right side).



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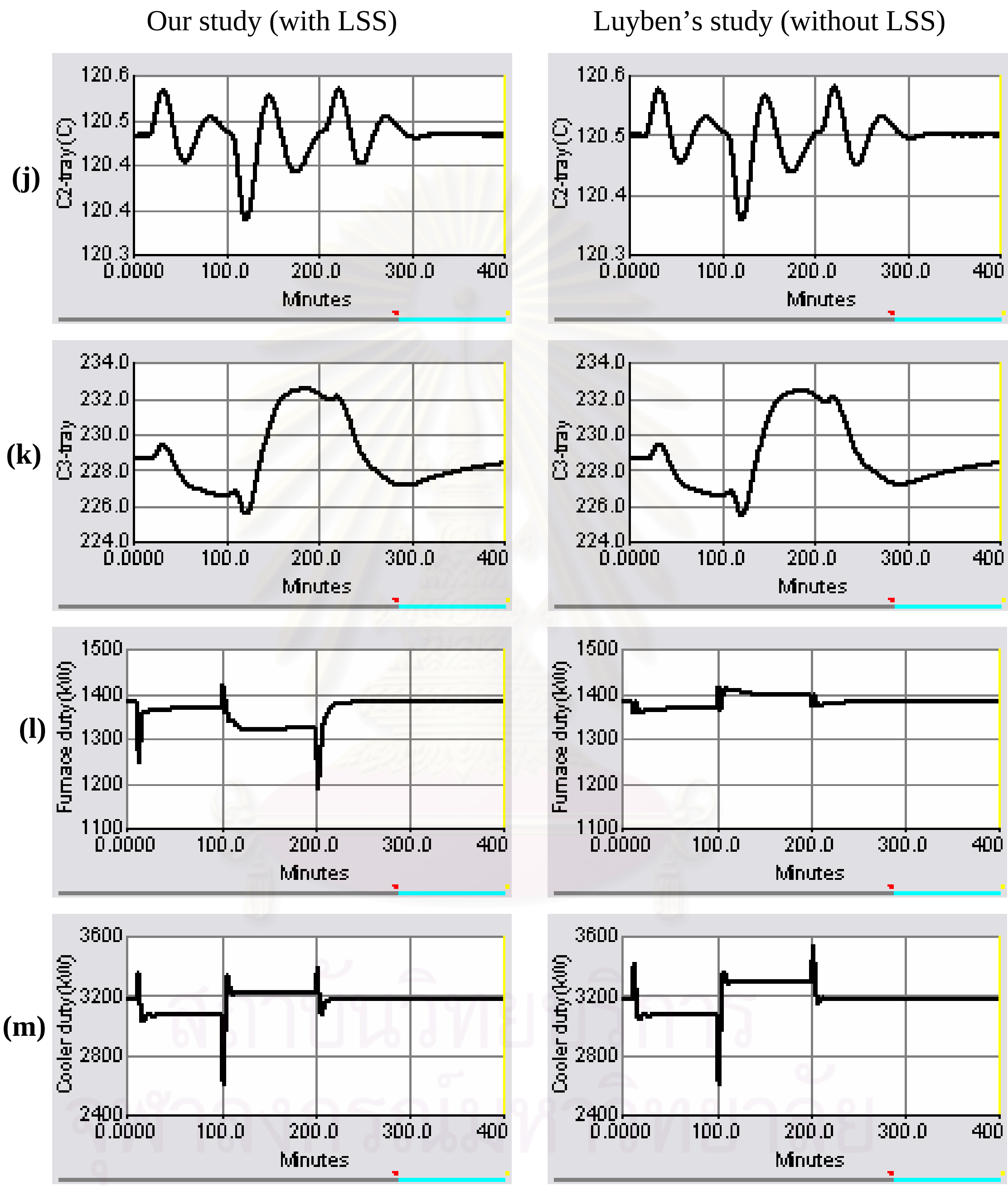


Figure 5.6 *Continued.*

5.3.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Figure 5.4 shows the dynamic responses of the control systems of HDA process alternative 1 to a change in the disturbance load of cold stream (reactor feed stream). In order to make this disturbance, first the fresh toluene feed temperature is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes (Figure 5.4.a).

As can be seen, when the cold inlet temperature of FEHE1 decreases, the LSS will take an action to control the cold outlet temperature of FEHE1 (i.e. furnace inlet temperature as shown in left side in Figure 5.4.b). The cooler inlet temperature quickly drops to a new steady state value (left side in Figure 5.4.c). Therefore, the cooler duty decreases (left side Figure 5.4.j).

When the cold inlet temperature of FEHE1 increases, this leads to the reduction of furnace duty, so the LSS switches the control action from the cold temperature control (TCE1c) to the hot temperature control (TCE1h). Following this action, the furnace inlet temperature rises to a new steady state value (left side in Figure 5.4.b); therefore, the furnace duty decreases (left side in Figure 5.4.i). The cooler inlet temperature drops to its set point quickly (left side in Figure 5.4.c), so the cooler duty also drops to its nominal value quickly (left side in Figure 5.4.j).

Since the furnace inlet temperature in the previous study (Luyben et al., 1999) is always maintained at its nominal value (right side in Figure 5.4.b), the furnace duty is slightly well controlled at the nominal value (right side in Figure 5.4.i). When the cold inlet temperature of FEHE1 increases, the cooler inlet temperature quickly rises to a new steady state value (right side in Figure 5.4.c), therefore the cooler duty in the previous study increases quickly (right side in Figure 5.4.j).

For both our study and Luyben's study, the reactor inlet temperature (Figure 5.4.d), and the separator temperature (Figure 5.4.e) are slightly well controlled. But, the oscillations occur in the tray temperature of the stabilizer column (Figure 5.4.f). The tray temperature in the product column is well controlled (Figure 5.4.g). Tighter control of the average tray temperature in the recycle column is achieved here in the LSS control than in Luyben's work (Figure 5.4.h).

5.3.2 Change in the Disturbance Load of Hot Stream (Reactor Product Stream)

Figure 5.5 shows the dynamic responses of the HDA process alternative 1 to a change in the heat load disturbance of the hot stream (reactor product stream). This disturbance is made as follows: first the set point of FEHE1-hot-inlet temperature controller (i.e. TCX1 in Figure 5.1) is decreased from 621.1 to 616.1 ^{o}C at time equals 10 minutes, the temperature is increased from 616.1 to 626.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 621.1 ^{o}C at time equals 200 minutes (Figure 5.5.a). As can be seen, the FEHE1-hot-inlet temperature response is very rapid, and the new steady state is achieved quickly (Figure 5.5.a).

The dynamic responses to the disturbance load of the hot stream are similar with those to the disturbance load of the cold stream. Again better responses of the furnace and cooler utility consumptions are achieved here compared to the Luyben's control system, since both the furnace (left side in Figure 5.5.i) and cooler (left side in Figure 5.5.j) duties in the current work could be decreased according to the input heat load disturbances.

5.3.3 Change in the Recycle Toluene Flowrates

On the other case, a disturbance in the production rate is also made for this study. Figure 5.6 shows the dynamic responses of the HDA process alternative 1 to a disturbance in the recycle toluene flowrates from 168.6 to 158.6 kgmole/h at time equals 10 minutes, and the flowrates is increased from 158.6 to 178.6 kgmole/h at time equals 100 minutes, then its flowrates is returned to its nominal value of 168.6 kgmole/h at time equals 200 minutes (Figure 5.6.a). Again, the recycle toluene flowrates response is very rapid; the new steady state is reached very quickly.

The dynamic responses of our control system are slightly similar with those in the earlier control system. The drop in toluene feed flowrates reduces the reaction rate, so the benzene product rate drops (Figure 5.6.c) and the benzene purity in the product stream increases (Figure 5.6.d), and vice versa. However both the furnace and cooler duties are slightly maintained at its good levels (left side in Figures 5.6.l and 5.6.m) compared to the Luyben's control system, since the LSS is able to select proper heat pathway to carry the associated load to a utility unit.

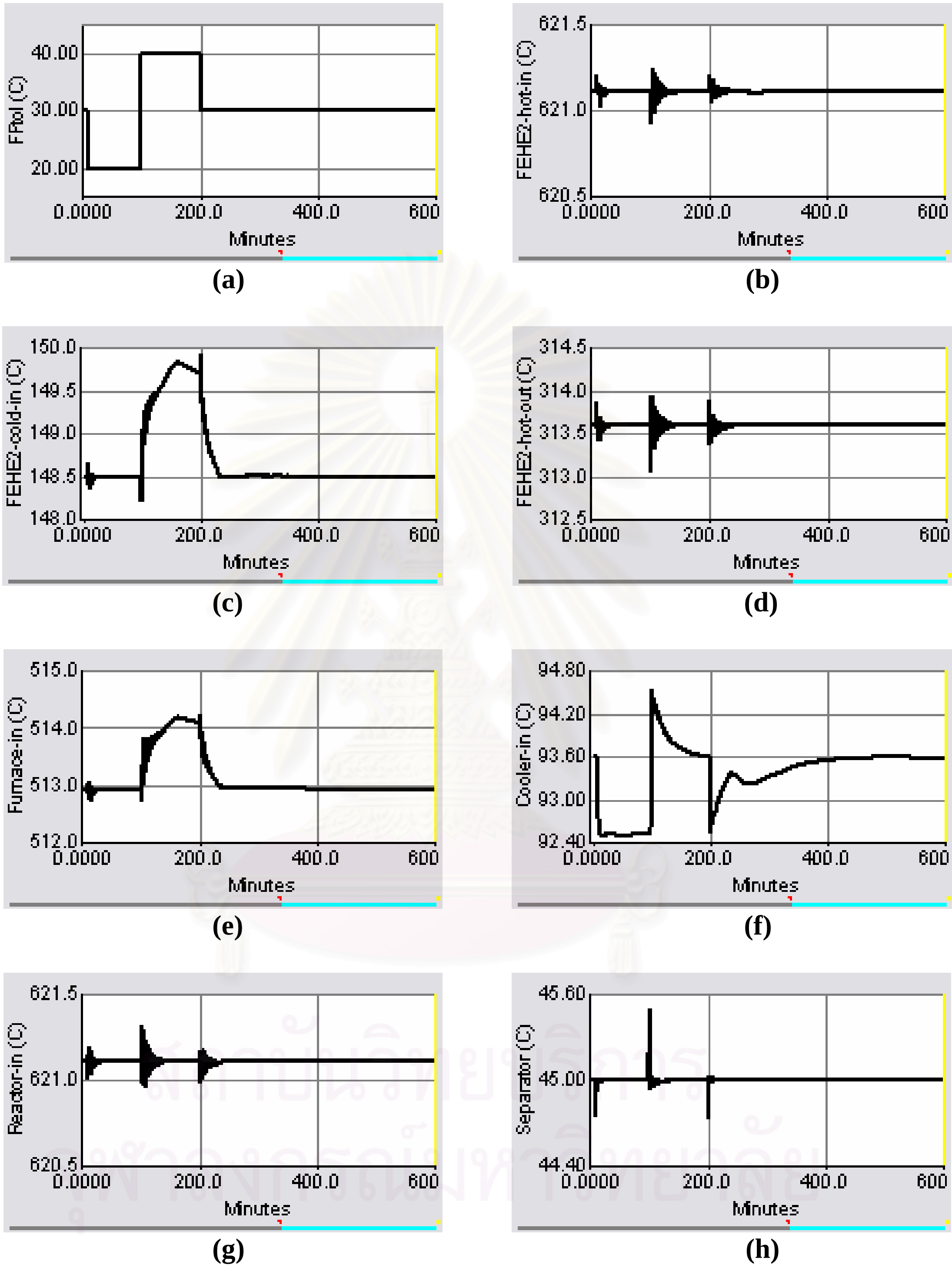
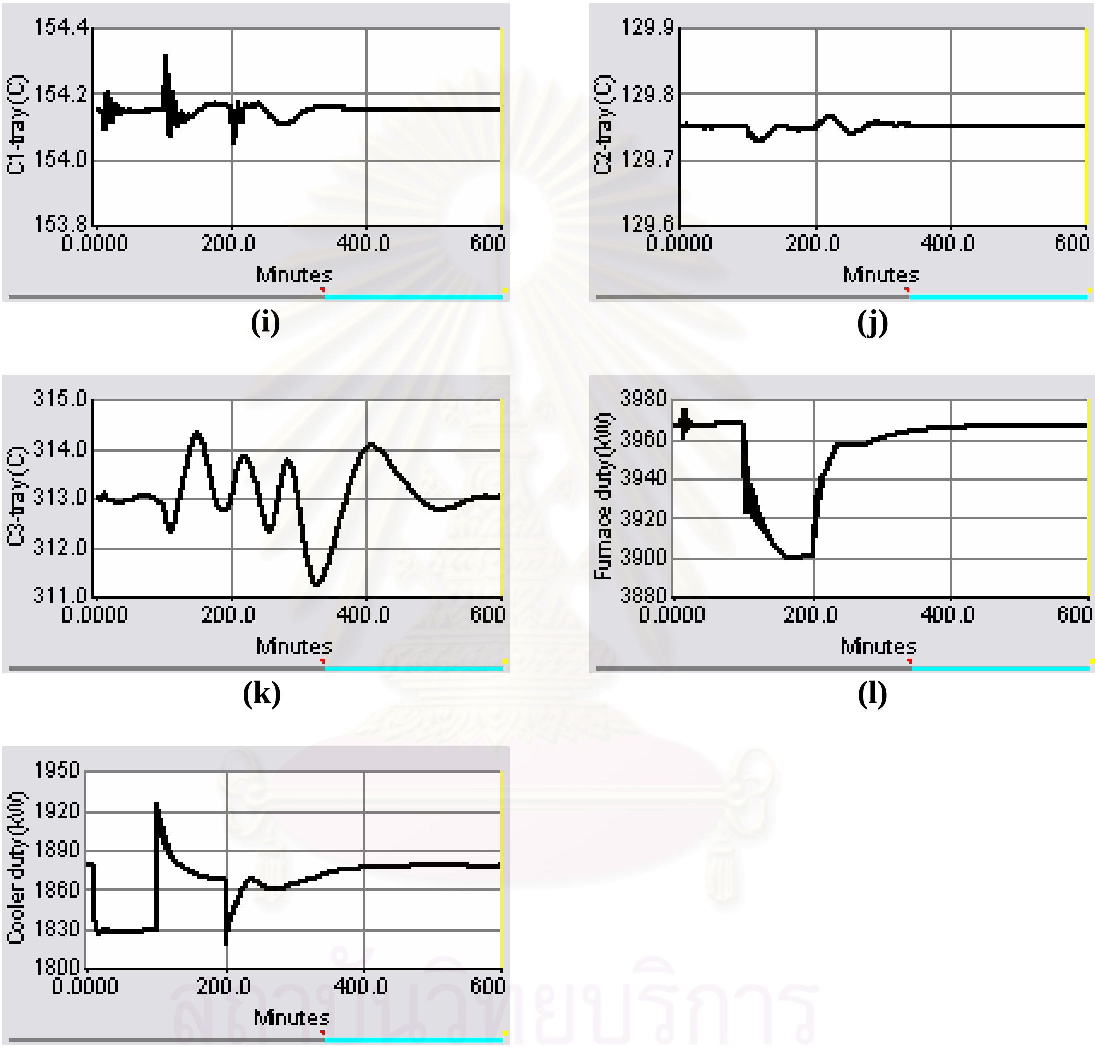


Figure 5.7 Dynamic responses of the HDA process alternative 4 to a change in the disturbance load of cold stream (reactor feed stream); where, (a) fresh feed toluene temperature, (b) FEHE2 hot inlet temperature, (c) FEHE2 cold in temperature, (d) FEHE2 hot out temperature, (e) furnace inlet temperature, (f) cooler inlet temperature, (g) reactor inlet temperature, (h) separator temperature, (i) C1-tray temperature, (j) C2-tray temperature, (k) C3-tray temperature, (l) furnace duty, (m) cooler duty.



(i) (j) (k) (l) (m)

Figure 5.7 *Continued.*

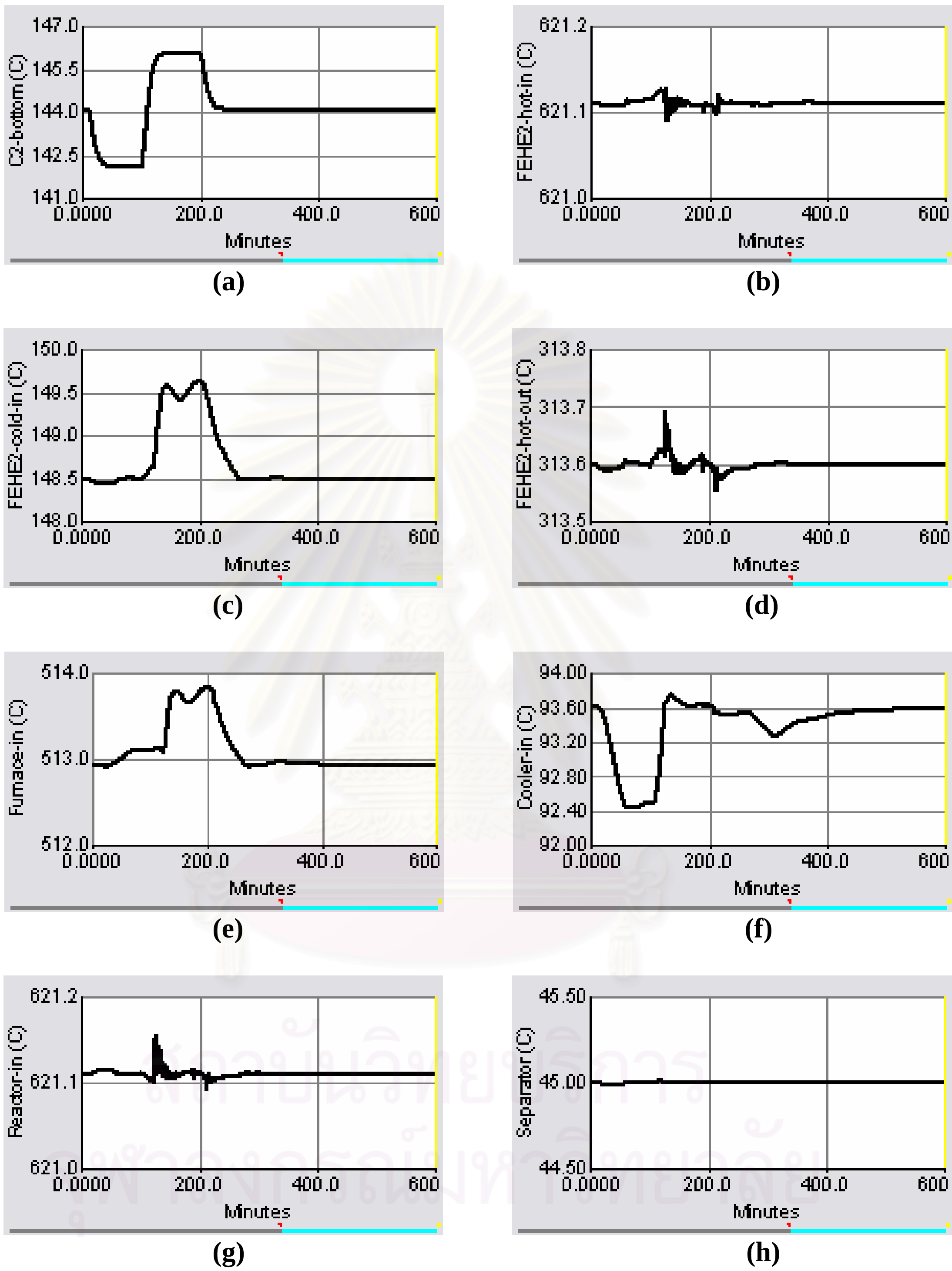
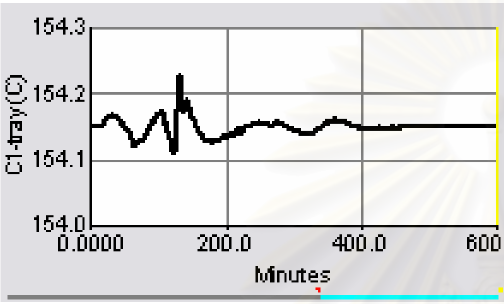
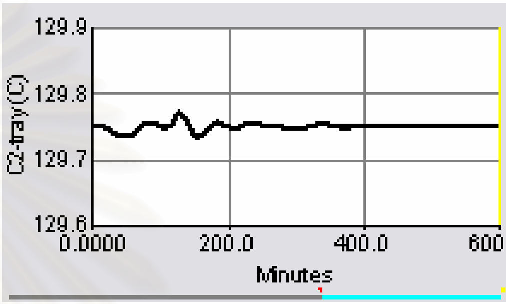


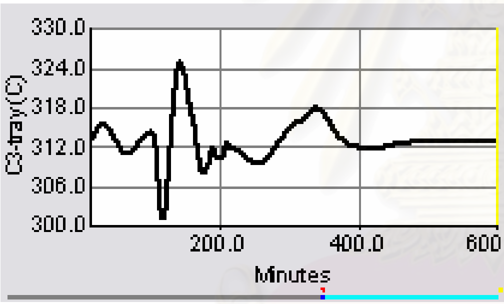
Figure 5.8 Dynamic responses of the HDA process alternative 4 to a change in the disturbance load of cold stream from the bottoms of product column C2; where, (a) C2-bottoms temperature, (b) FEHE2 hot inlet temperature, (c) FEHE2 cold in temperature, (d) FEHE2 hot out temperature, (e) furnace inlet temperature, (f) cooler inlet temperature, (g) reactor inlet temperature, (h) separator temperature, (i) C1-tray temperature, (j) C2-tray temperature, (k) C3-tray temperature, (l) furnace duty, (m) cooler duty.



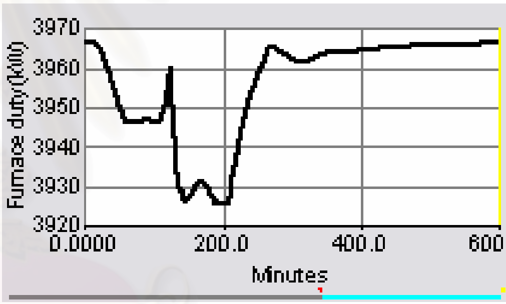
(i)



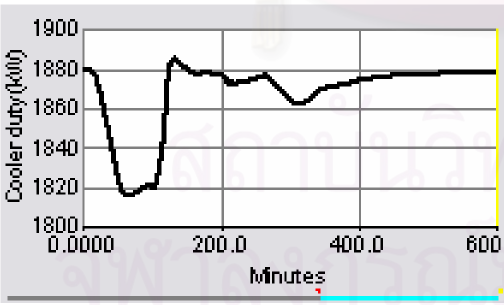
(j)



(k)



(l)



(m)

Figure 5.8 *Continued.*

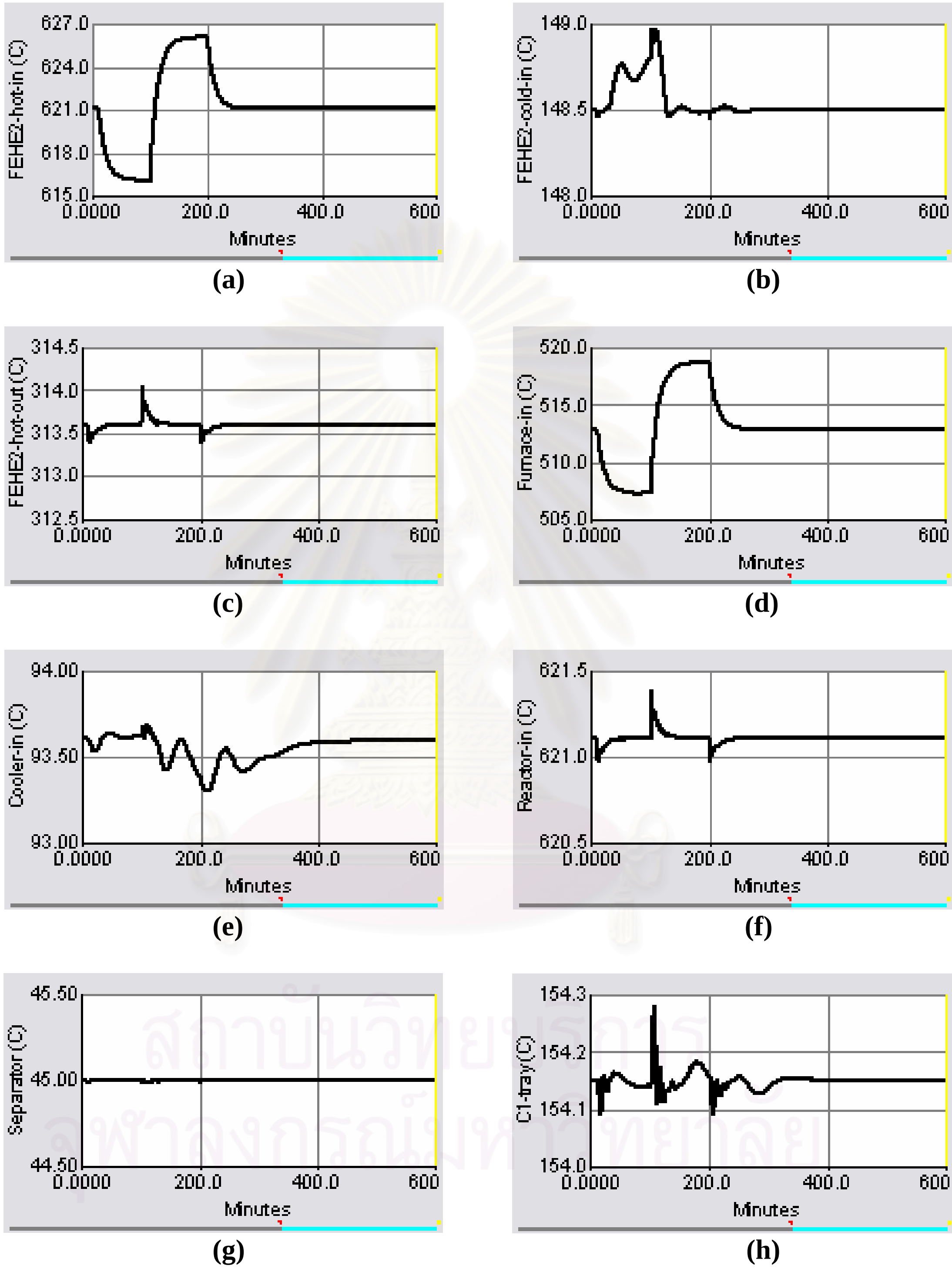
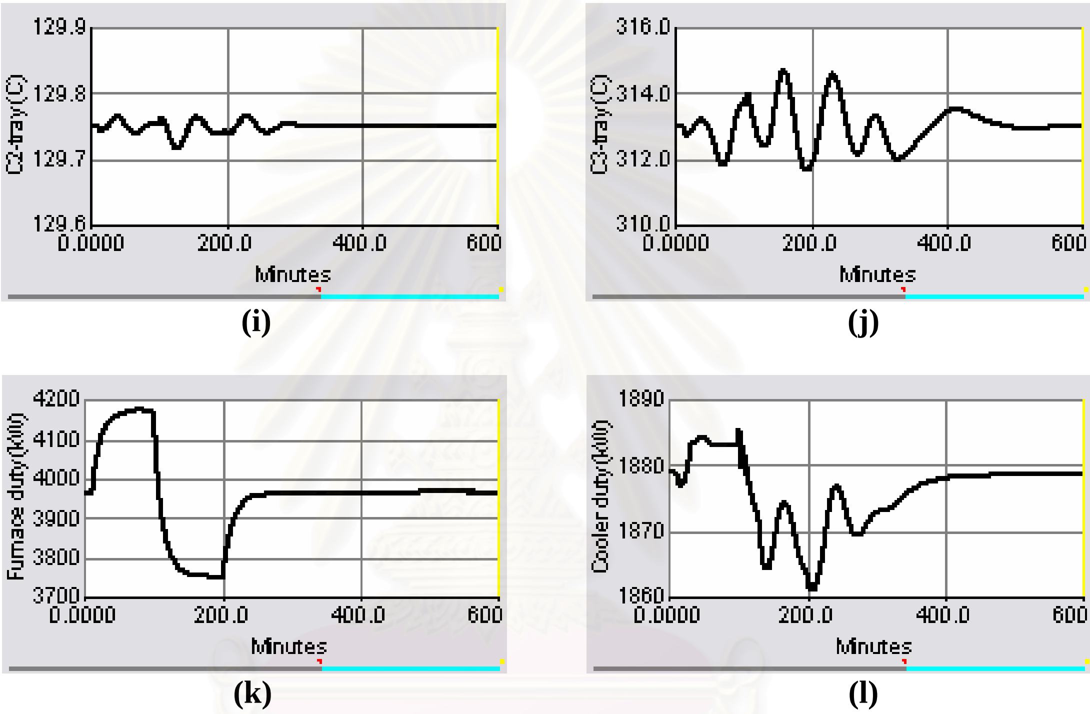


Figure 5.9 Dynamic responses of the HDA process alternative 4 to a change in the disturbance load of hot stream (reactor product stream); where, (a) FEHE2 hot inlet temperature, (b) FEHE2 cold in temperature, (c) FEHE2 hot out temperature, (d) furnace inlet temperature, (e) cooler inlet temperature, (f) reactor inlet temperature, (g) separator temperature, (h) C1-tray temperature, (i) C2-tray temperature, (j) C3-tray temperature, (k) furnace duty, (l) cooler duty.



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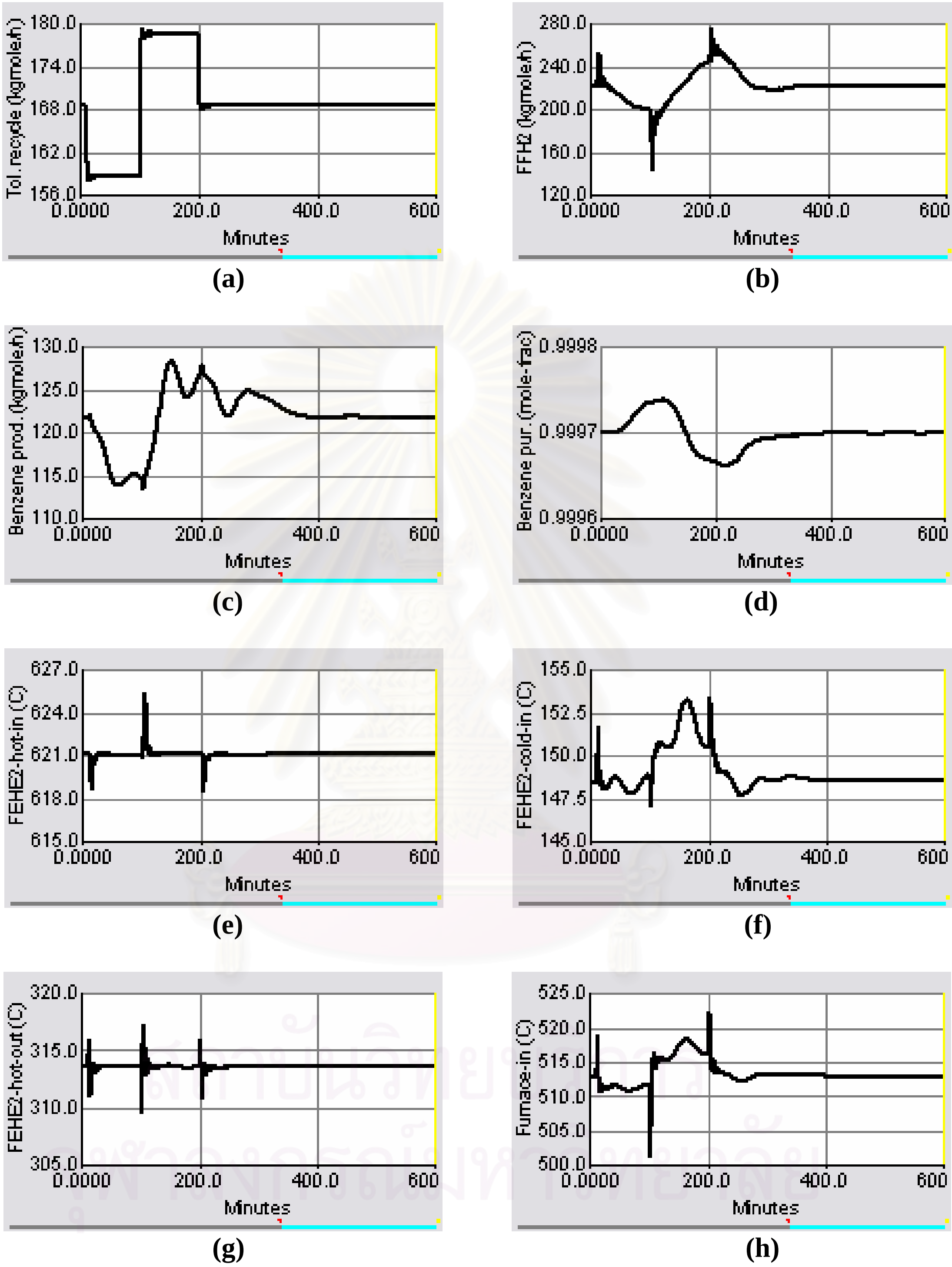


Figure 5.10 Dynamic responses of the HDA process alternative 4 to a change in the recycle toluene flowrates; where, (a) recycle toluene flowrates, (b) fresh feed hydrogen flowrates, (c) benzene product flowrates, (d) benzene purity, (e) FEHE2 hot inlet temperature, (f) FEHE2 cold in temperature, (g) FEHE2 hot out temperature, (h) furnace inlet temperature, (i) cooler inlet temperature, (j) reactor inlet temperature, (k) separator temperature, (l) C1-tray temperature, (m) C2-tray temperature, (n) C3-tray temperature, (o) furnace duty, (p) cooler duty.

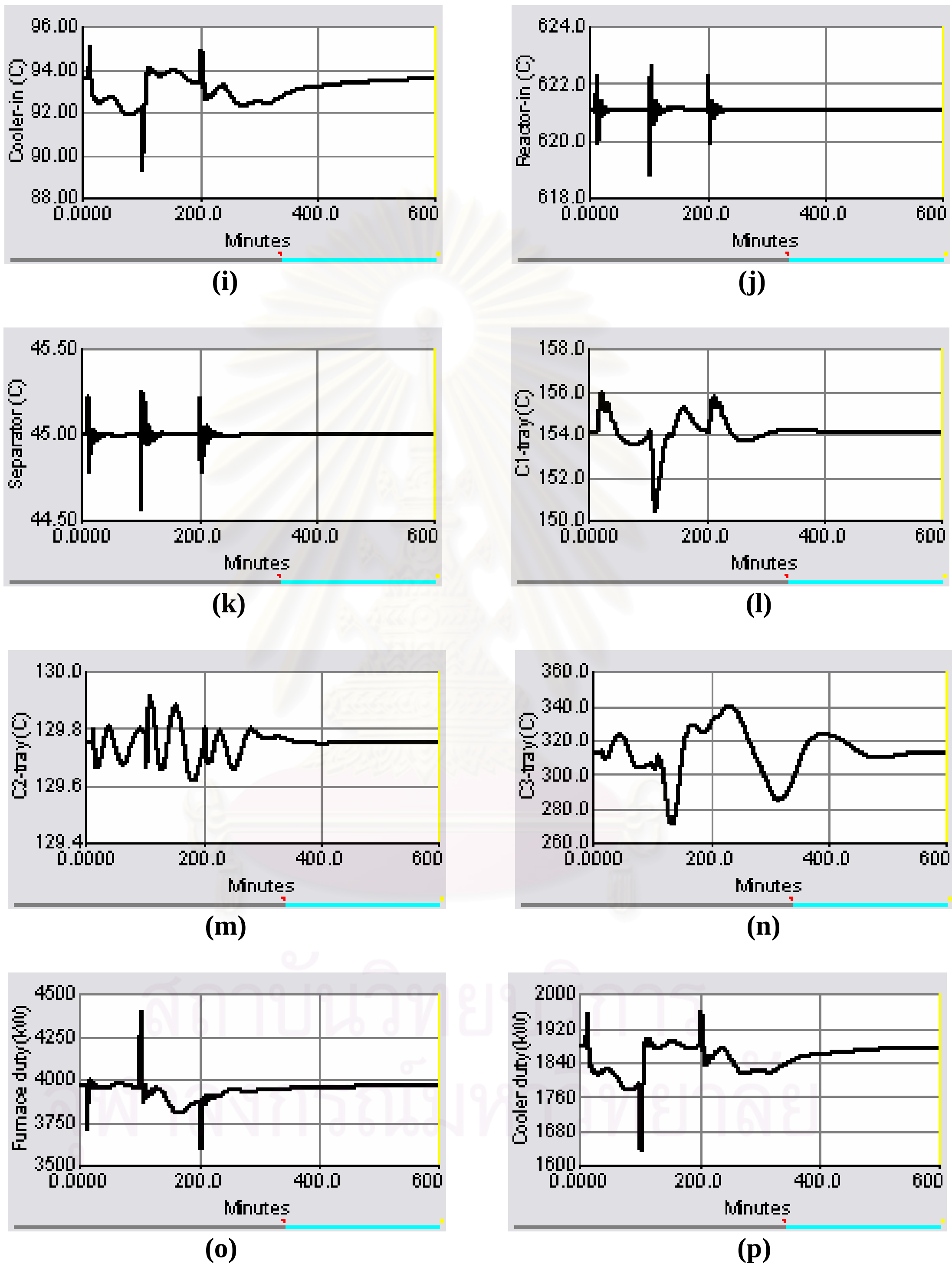


Figure 5.10 *Continued.*

5.4 Dynamic Simulation Results of HDA Process Alternative 4

In order to evaluate the dynamic behaviors of the new control systems in HDA process alternative 4, several disturbance loads were made. The dynamic responses of the control system for the HDA process alternative 4 are shown in Figures 5.7 to 5.10. However, the dynamic responses of the control system in HDA process alternative 4 are slower than those in HDA process alternative 1. Results for individual disturbance load changes are as follows:

5.4.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Figure 5.7 shows the dynamic responses of the HDA process alternative 4 to a change in the heat load disturbance of cold stream (reactor feed stream). In order to make these disturbances, first the fresh toluene feed temperature is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes (Figure 5.7.a).

The dynamic responses in HDA process alternative 4 are slower than those in HDA process alternative 1. The principle work of the LSS in HDA process alternative 4 is the same as that in HDA process alternative 1. When the cold inlet temperature of FEHE2 decreases below its minimum value, the LSS takes an action to control the cold inlet temperature of FEHE2 (figure 5.7.c). As a result, the cooler duty decreases (Figure 5.7.m) since the cooler inlet temperature decreases (Figure 5.7.f). As expected, when the cold inlet temperature of FEHE2 increases above its minimum value, the LSS switches the control action from TCE1c to TCE1h. Therefore, the furnace duty decreases significantly (Figure 5.7.l), since the furnace inlet temperature increases (Figure 5.7.e).

5.4.2 Change in the Disturbance Load of Cold Stream from the Bottoms of Product Column

Figure 5.8 shows the dynamic responses of HDA process alternative 4 to a change in the heat load disturbance of cold stream from the bottoms of product column. This disturbance is made as follows: first the set point of C2-bottom temperature controller (i.e. TCX2 in Figure 5.2) is decreased from 144.1 to 142.1 ^{o}C at time equals 10 minutes, the temperature is increased from 142.1 to 146.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 144.1 ^{o}C at time equals 200 minutes (Figure 5.8.a). The temperature response in the bottoms of product column is somewhat fast (Figure 5.8.a).

The positive disturbance load of cold stream should be shifted to a cooler utility by controlling the cold inlet temperature of FEHE2 (Figure 5.8.c). Therefore, the cooler duty decreases (Figure 5.8.m). Then, the negative disturbance load of cold stream is shifted to a furnace utility by controlling the cooler inlet temperature (Figure 5.8.f). Therefore, the furnace duty decreases (Figure 5.8.l).

5.4.3 Change in the Disturbance Load of Hot Stream (Reactor Product Stream)

Figure 5.9 shows the dynamic responses of HDA process alternative 4 to a change in the heat load disturbance of hot stream (reactor product stream). This disturbance is made as follows: first the set point of FEHE2-hot-inlet-temperature controller (i.e. TCX1 in Figure 5.2) is decreased from 621.1 to 616.1 ^{o}C at time equals 10 minutes, the temperature is increased from 616.1 to 626.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 621.1 ^{o}C at time equals 200 minutes (Figure 5.9.a). Again, the FEHE2-hot-inlet-temperature response is somewhat fast.

Since the hot outlet temperature of FEHE2 (i.e. the hot temperature at the entrance of the reboiler, R2) should be controlled (Figure 5.9.c) at its set point to prevent the propagation of the thermal disturbance, both the positive and negative disturbance loads of the hot stream are shifted to the furnace utility. Therefore, whenever the negative disturbance load is coming with the hot stream (i.e. the hot inlet temperature of FEHE2 decreases), this disturbance load is shifted to the furnace utility. Consequently, the furnace duty will be increased (Figure 5.9.k). Consider the case when the hot inlet temperature of FEHE2 increases (Figure 5.9.a), this is a desired condition to shift the disturbance load to the cold stream. Therefore, the furnace duty decreases to a new steady state value (Figure 5.9.k).

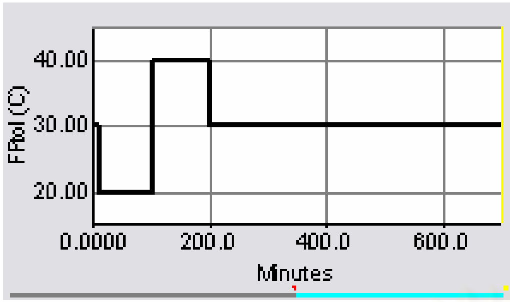
5.4.4 Change in the Recycle Toluene Flowrates

On the other case, a disturbance in the production rate is also made for the HDA process alternative 4. Figure 5.10 shows the dynamic responses of HDA process alternative 4 to a disturbance in the recycle toluene flowrates from 168.2 to 158.2 kgmole/h at time equals 10 minutes, and the flowrates is increased from 158.2 to 178.2 kgmole/h at time equals 100 minutes, then its flowrates is returned to its nominal value of 168.2 kgmole/h at time equals 200 minutes (Figure 5.10.a). The recycle toluene flowrates response is very rapid; the new steady state is reached very quickly (Figure 5.10.a).

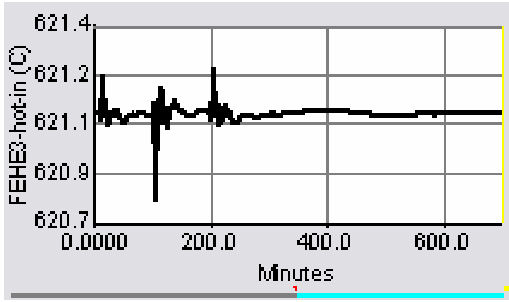
As can be seen that both furnace and cooler duties are slightly maintained at its good levels (Figures 5.10.o and 5.10.p), since the heat load is tightly managed. Again, the drop in toluene feed flowrates reduces the reaction rate, so the benzene product rate drops as shown in Figure 5.10.c, but the benzene product quality increases (Figure 5.10.d), and vice versa. A small deviation of about 0.4 ^{o}C happens on the tray temperature of product column (Figure 5.10.m). But, the tray temperature in recycle column has a large deviation of about 40 ^{o}C, and it takes a long time to slowly return to its nominal value (Figure 5.9.n).

5.5 Dynamic Simulation Results of HDA Process Alternative 6

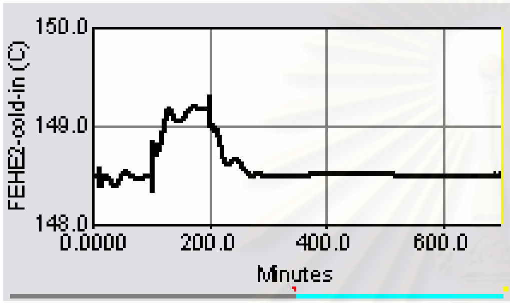
In order to illustrate the dynamic behavior of the developed new control structure in HDA process alternative 6, several disturbance loads were made. The dynamic responses of the new control system in HDA process alternative 6 are shown in Figures 5.11 to 5.16. However, the dynamic responses of the control system in HDA process alternative 6 are the slowest compared with those in alternatives 1 and 4. This study shows that the implementation of complex energy integration to the process deteriorates dynamic performance of the process. Results for individual disturbance load changes are as follows:



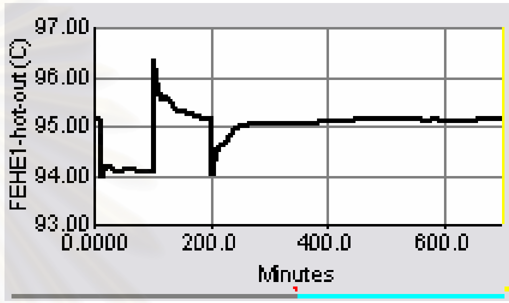
(a)



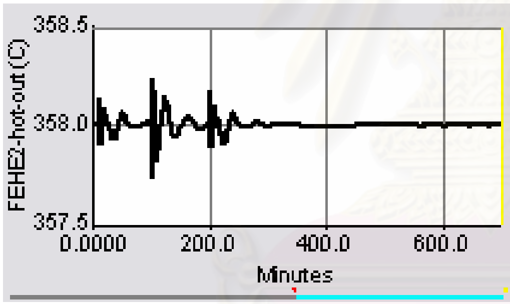
(b)



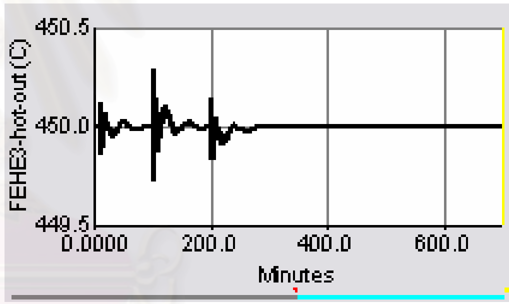
(c)



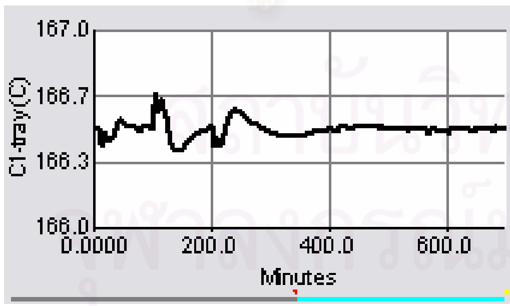
(d)



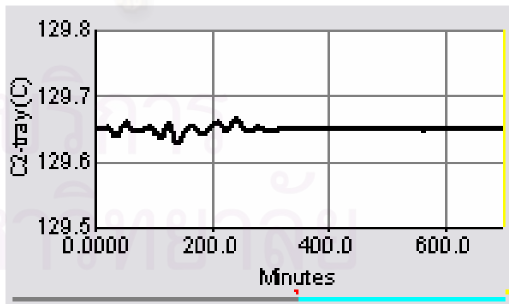
(e)



(f)

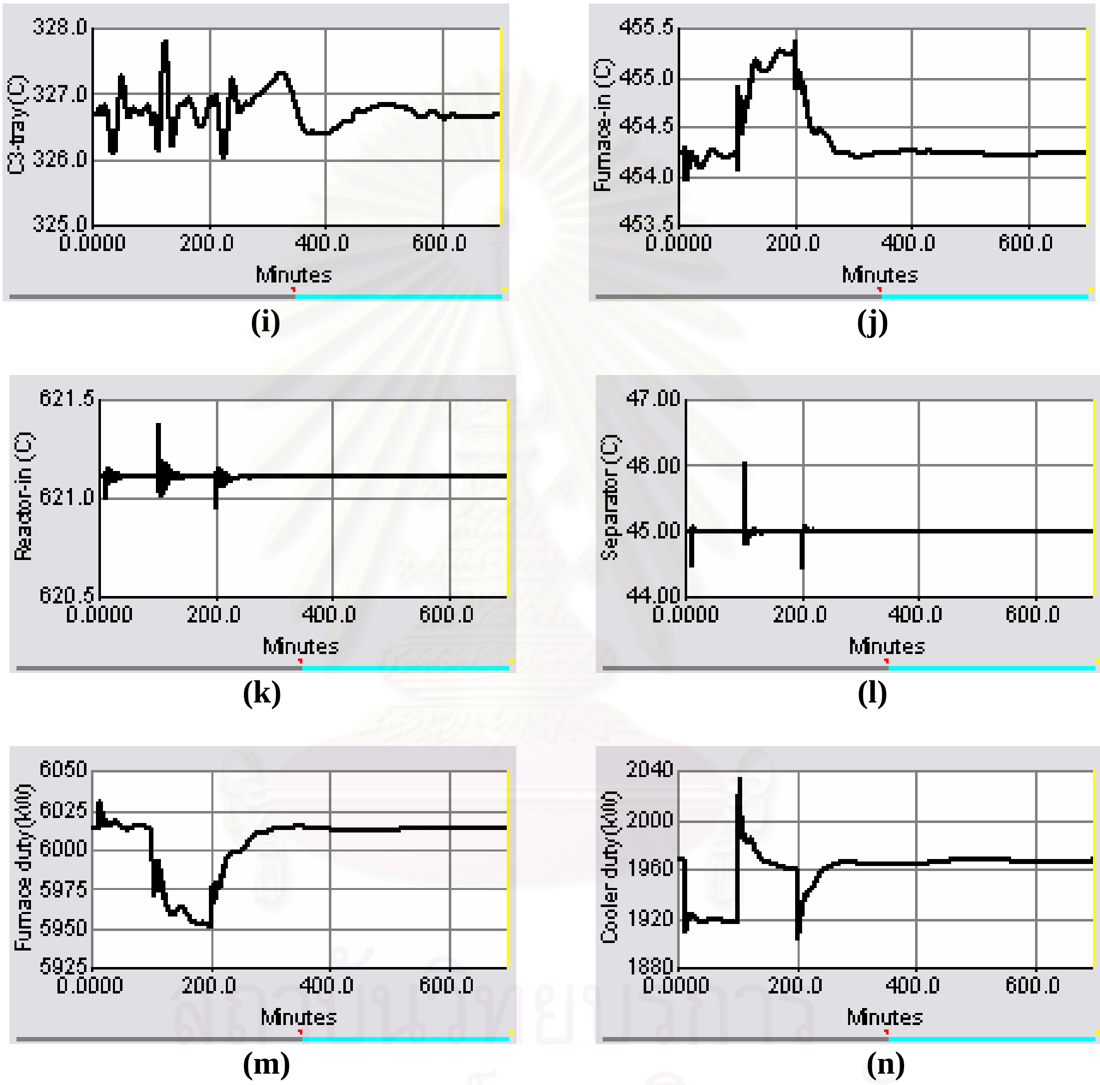


(g)



(h)

Figure 5.11 Dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of cold stream (reactor feed stream), where: (a) fresh feed toluene temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE1 hot outlet temperature, (e) FEHE2 hot outlet temperature, (f) FEHE3 hot outlet temperature, (g) C1-tray temperature, (h) C2-tray temperature, (i) C3-tray temperature, (j) furnace inlet temperature, (k) reactor inlet temperature, (l) separator temperature, (m) furnace duty, (n) cooler duty.



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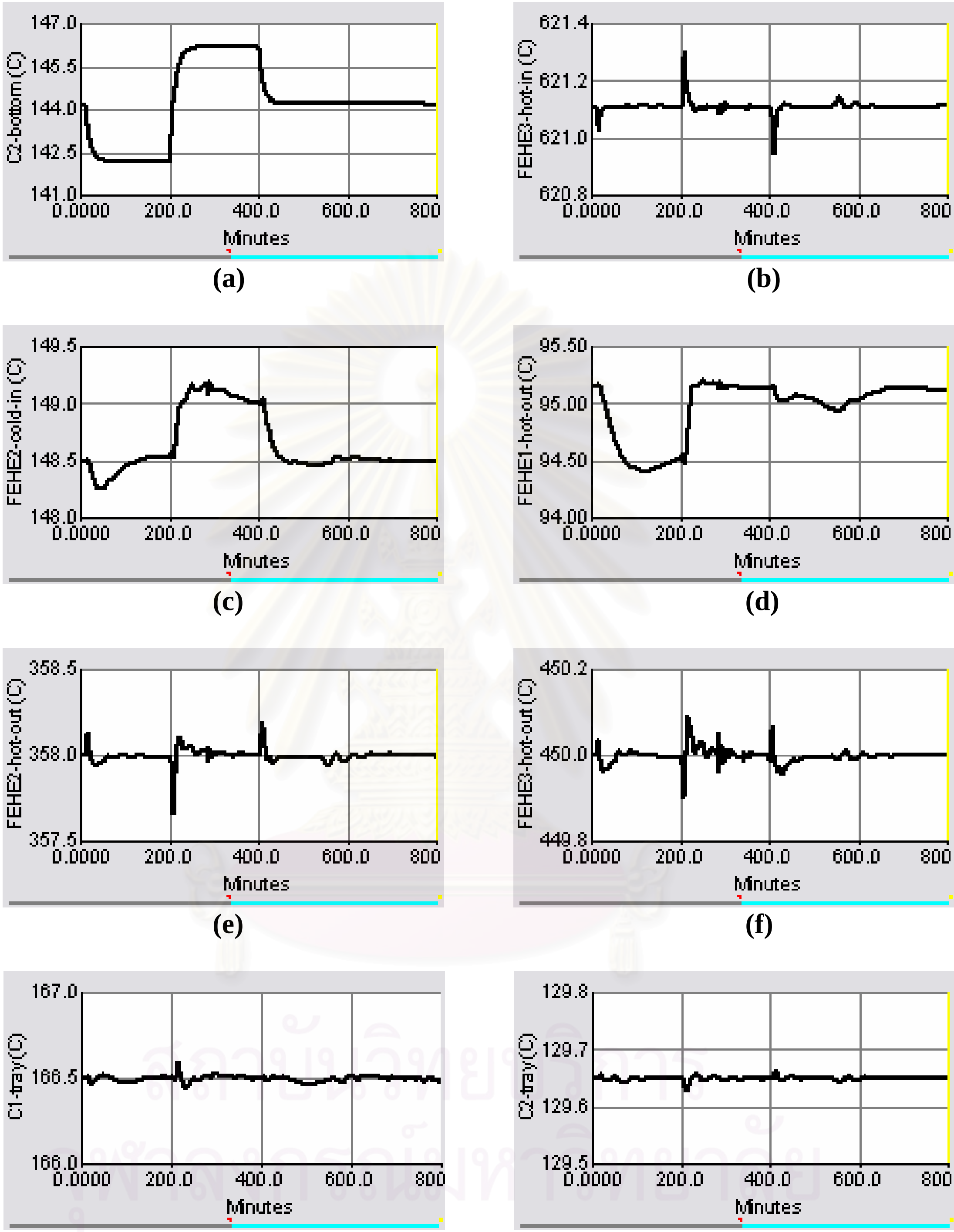


Figure 5.12 Dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of product column C2, where: (a) C2-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE1 hot outlet temperature, (e) FEHE2 hot outlet temperature, (f) FEHE3 hot outlet temperature, (g) C1-tray temperature, (h) C2-tray temperature, (i) C3-tray temperature, (j) furnace inlet temperature, (k) reactor inlet temperature, (l) separator temperature, (m) furnace duty, (n) cooler duty.

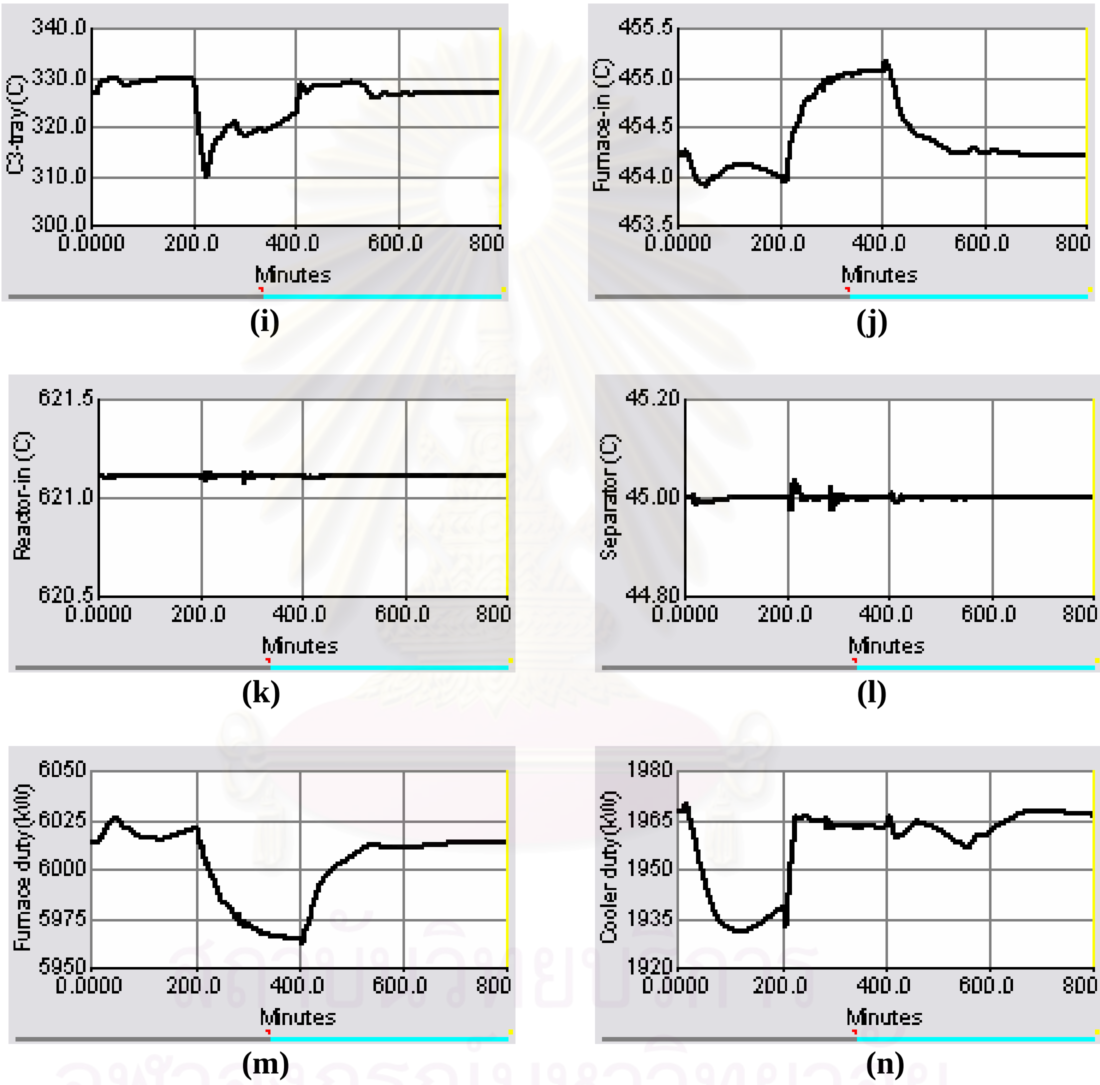
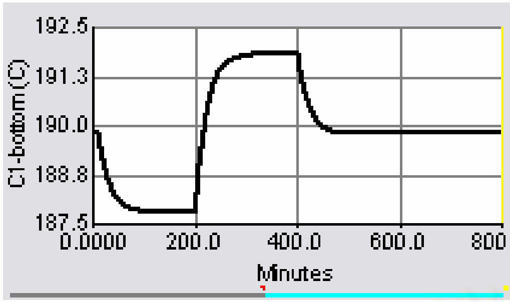
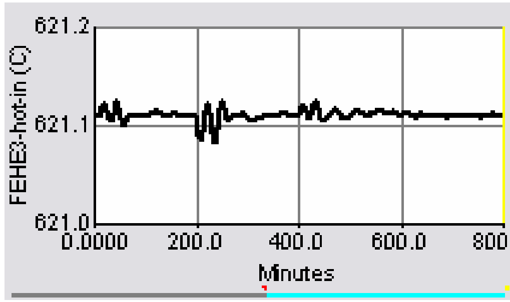


Figure 5.12 *Continued.*



(a)



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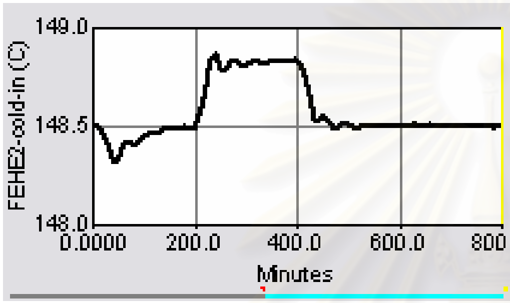

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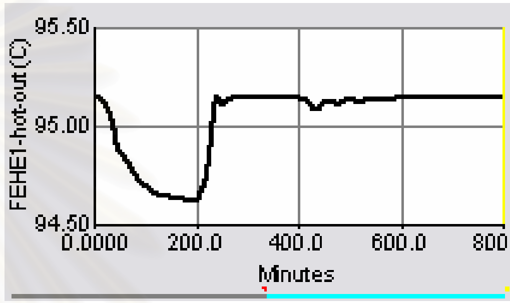

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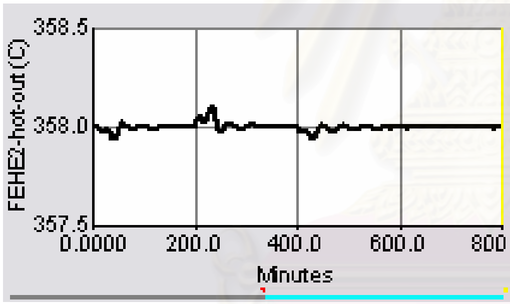

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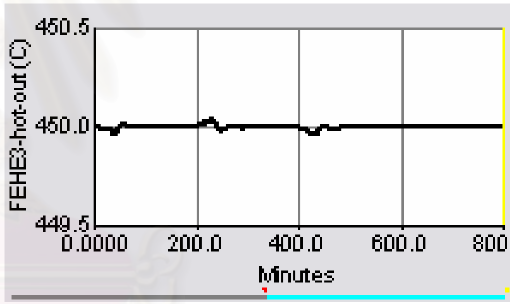
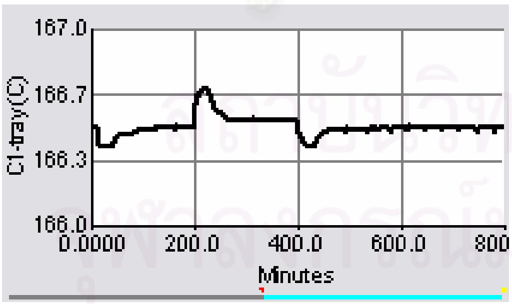


(f)



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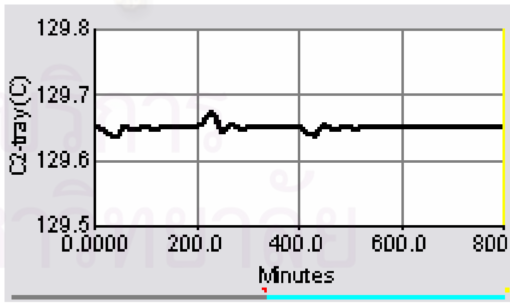
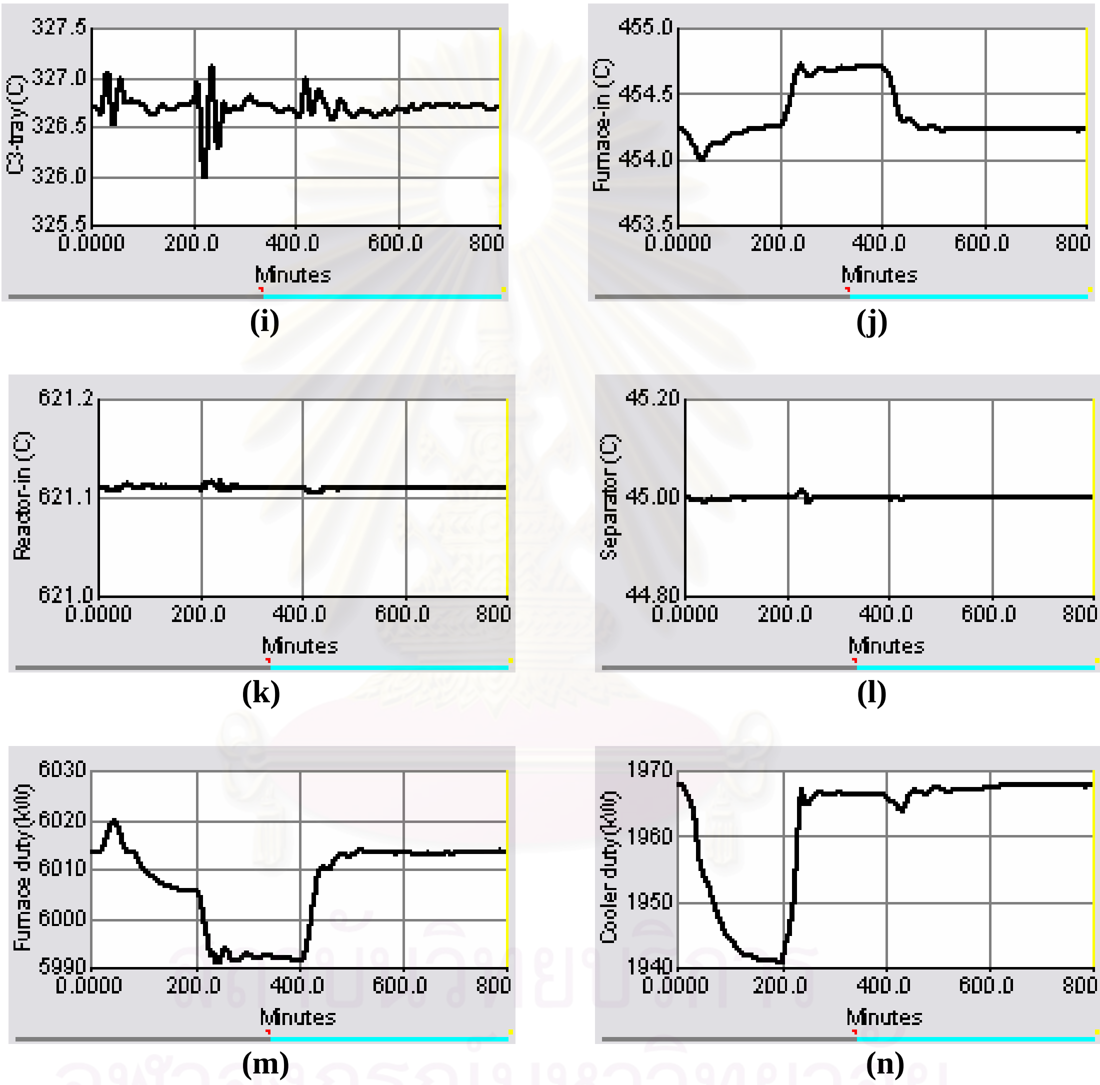


(h)

Figure 5.13 Dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of stabilizer column C1, where: (a) C1-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE1 hot outlet temperature, (e) FEHE2 hot outlet temperature, (f) FEHE3 hot outlet temperature, (g) C1-tray temperature, (h) C2-tray temperature, (i) C3-tray temperature, (j) furnace inlet temperature, (k) reactor inlet temperature, (l) separator temperature, (m) furnace duty, (n) cooler duty.



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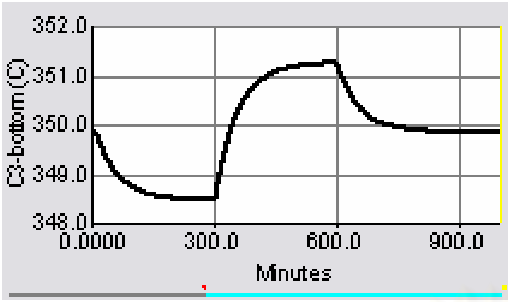

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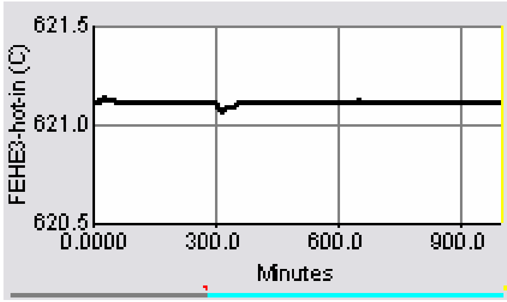

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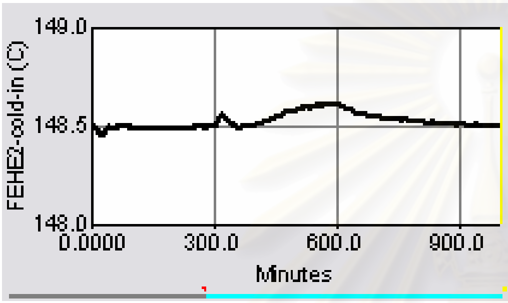

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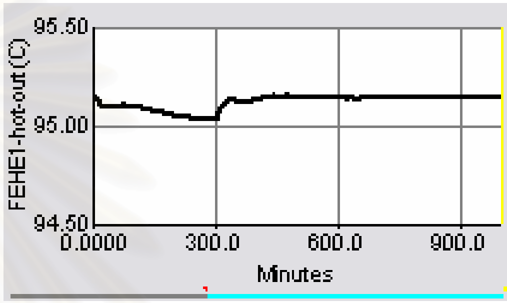

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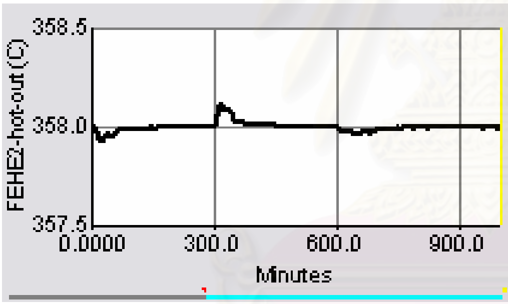

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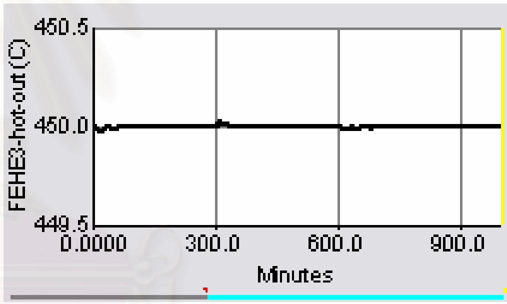

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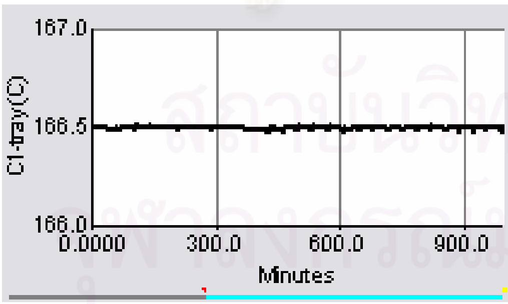

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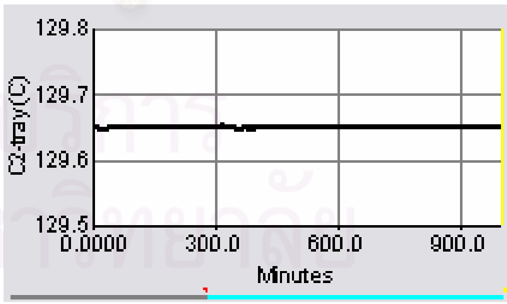
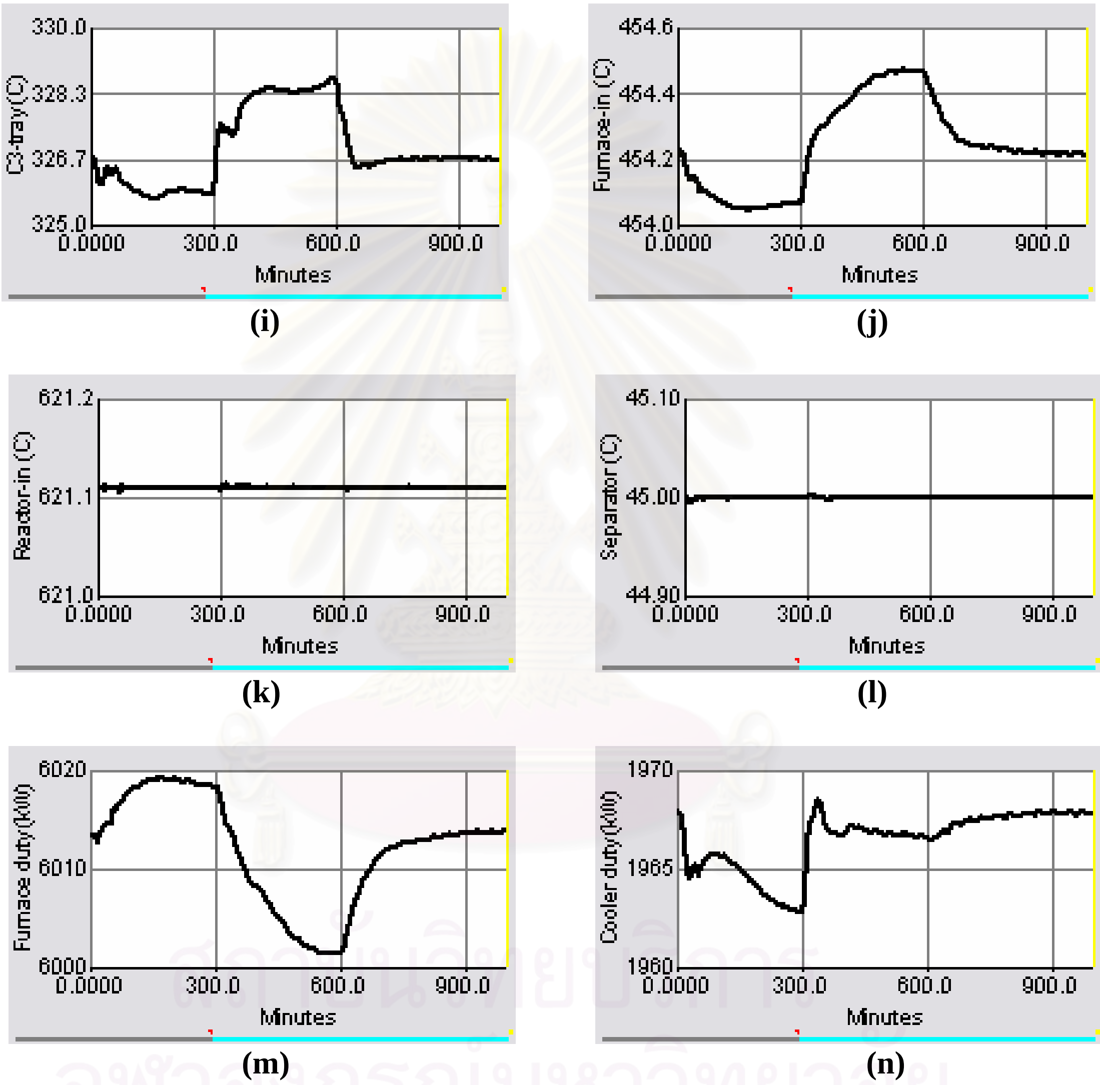


(h)

Figure 5.14 Dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of recycle column C3, where: (a) C3-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE1 hot outlet temperature, (e) FEHE2 hot outlet temperature, (f) FEHE3 hot outlet temperature, (g) C1-tray temperature, (h) C2-tray temperature, (i) C3-tray temperature, (j) furnace inlet temperature, (k) reactor inlet temperature, (l) separator temperature, (m) furnace duty, (n) cooler duty.



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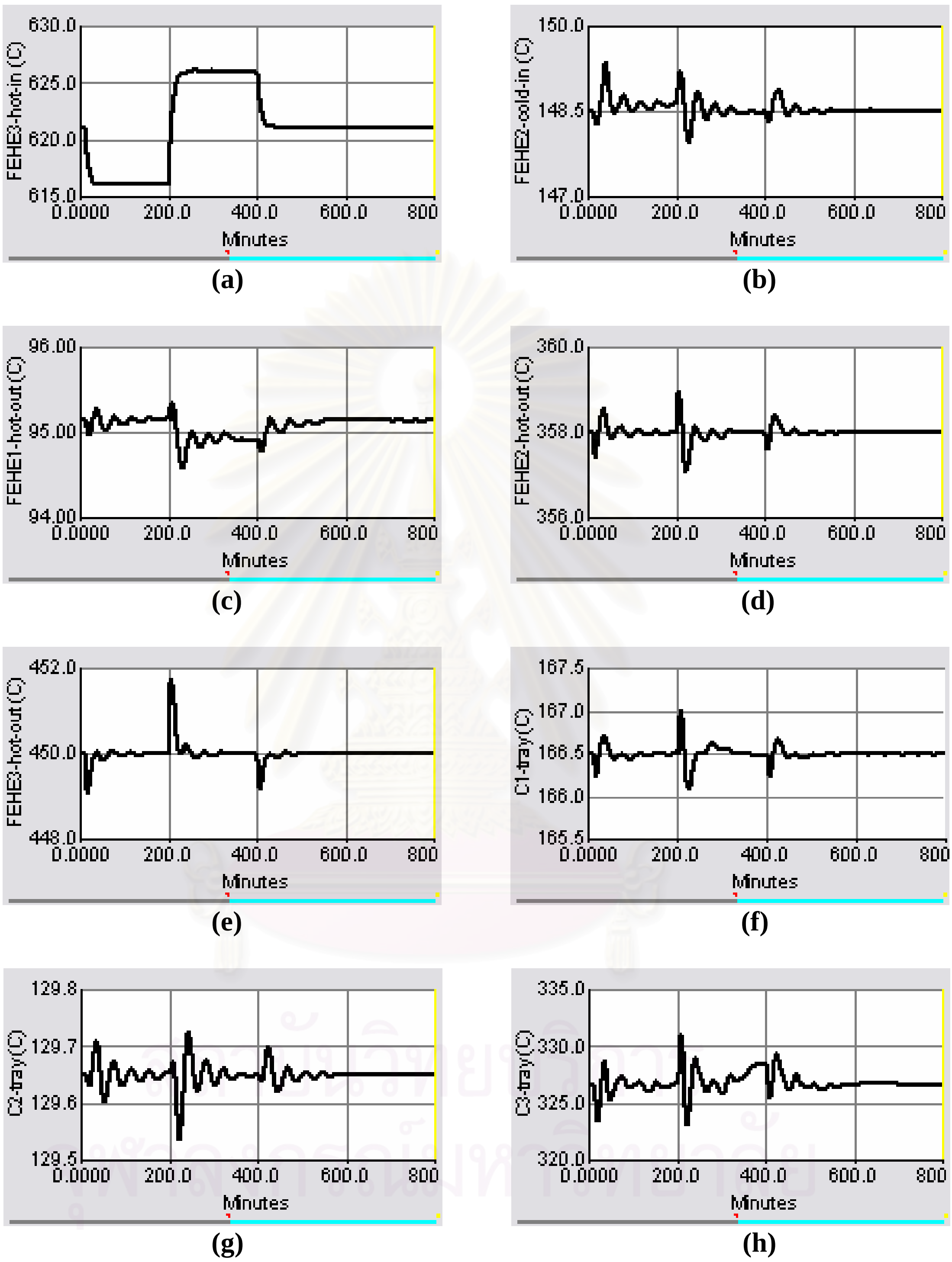
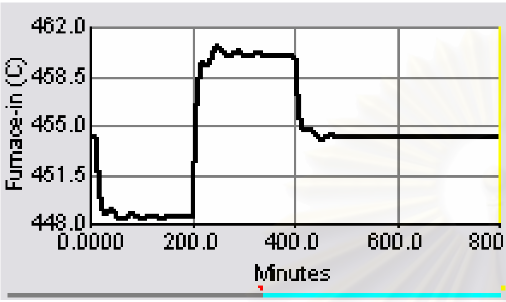


Figure 5.15 Dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of hot stream (reactor product stream), where: (a) FEHE3 hot inlet temperature, (b) FEHE2 cold inlet temperature, (c) FEHE1 hot outlet temperature, (d) FEHE2 hot outlet temperature, (e) FEHE3 hot outlet temperature, (f) C1-tray temperature, (g) C2-tray temperature, (h) C3-tray temperature, (i) furnace inlet temperature, (j) reactor inlet temperature, (k) separator temperature, (l) furnace duty, (m) cooler duty.



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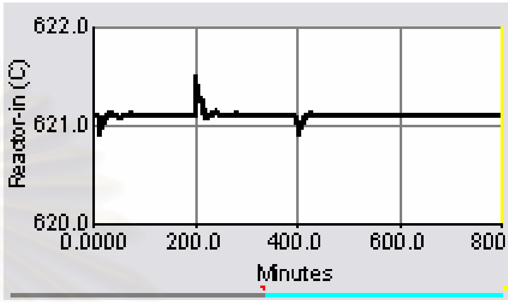

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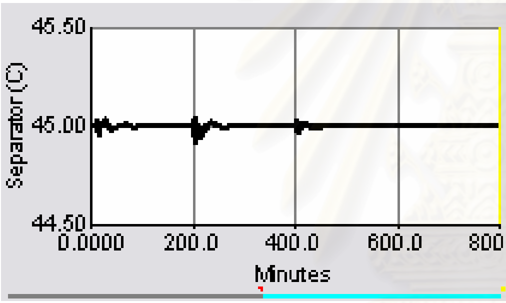

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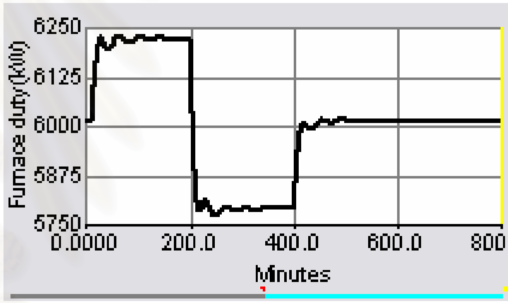

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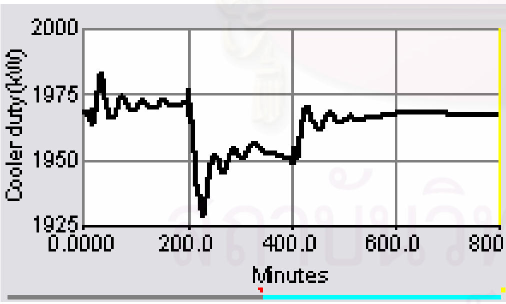

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Figure 5.15 *Continued*

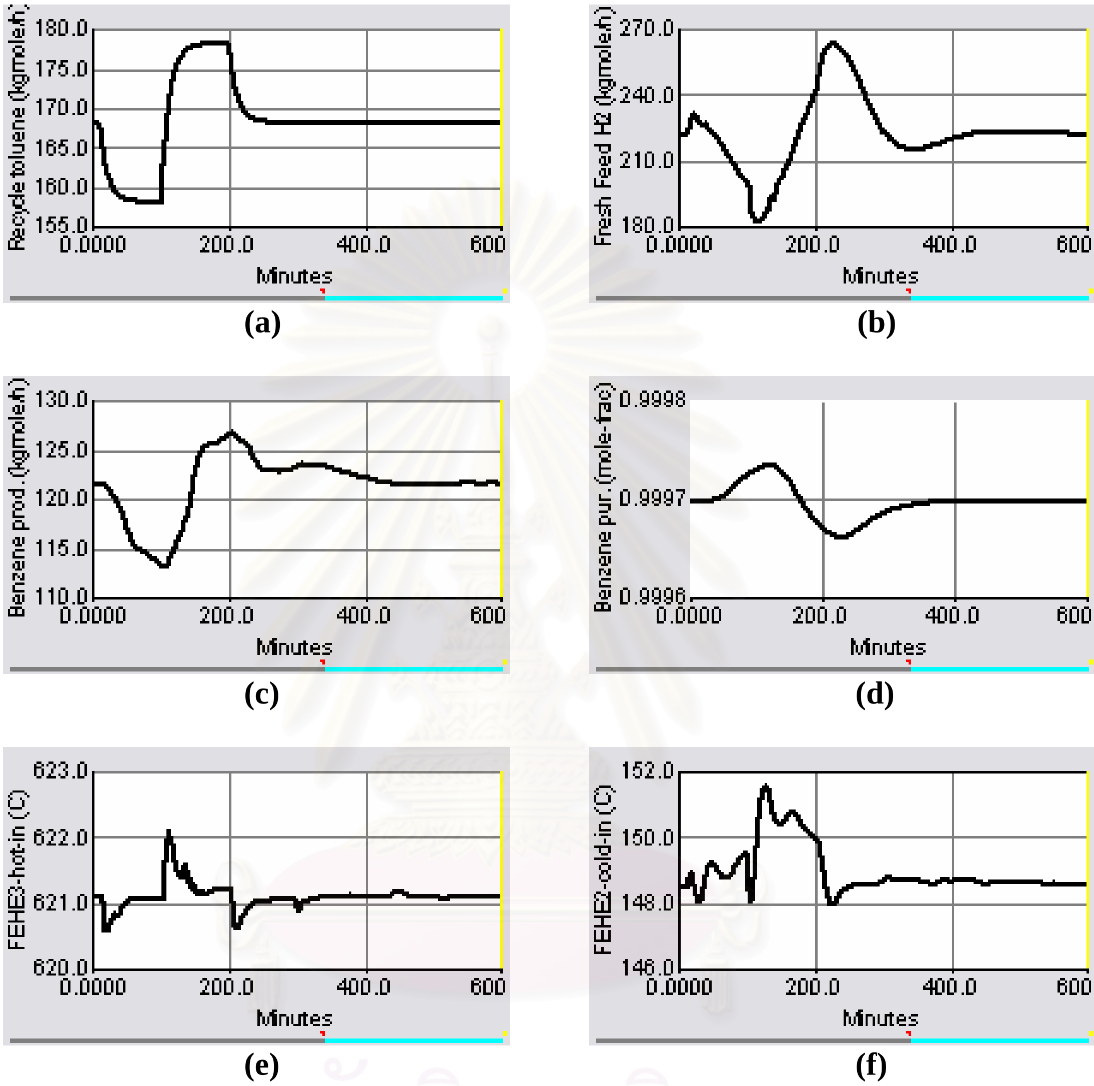
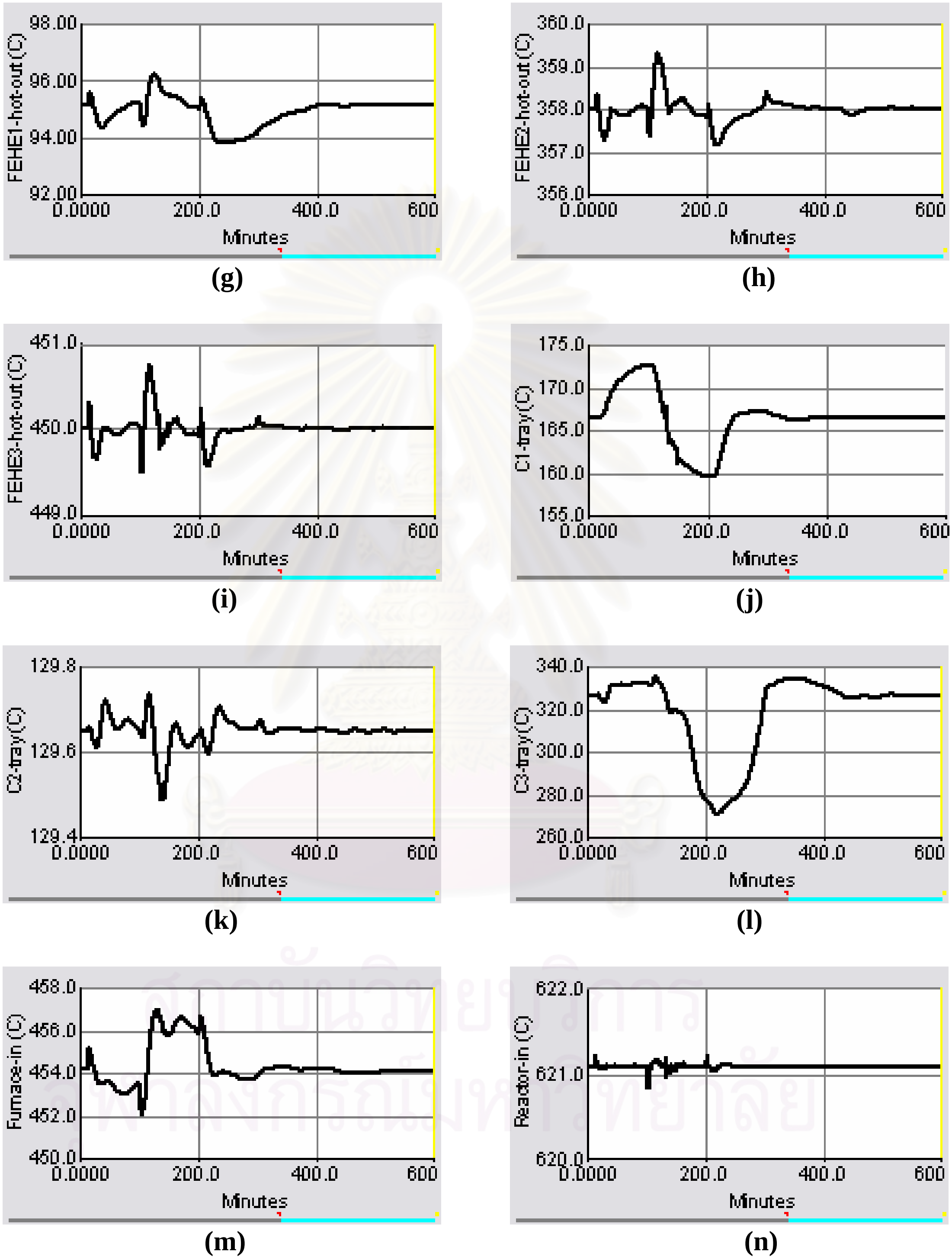


Figure 5.16 Dynamic responses of the HDA process alternative 6 to a change in the recycle toluene flowrates, where: (a) recycle toluene flowrates, (b) fresh feed hydrogen flowrates, (c) benzene product flowrates, (d) benzene purity in the product stream, (e) FEHE3 hot inlet temperature, (f) FEHE2 cold inlet temperature, (g) FEHE1 hot outlet temperature, (h) FEHE2 hot outlet temperature, (i) FEHE3 hot outlet temperature, (j) C1-tray temperature, (k) C2-tray temperature, (l) C3-tray temperature, (m) furnace inlet temperature, (n) reactor inlet temperature, (o) separator temperature, (p) furnace duty, (q) cooler duty.



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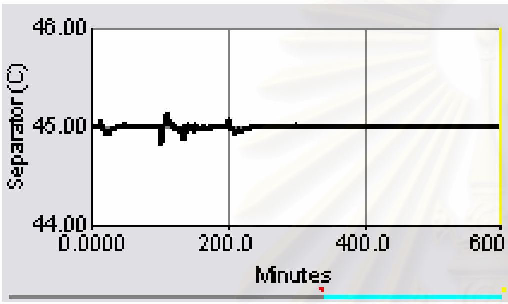

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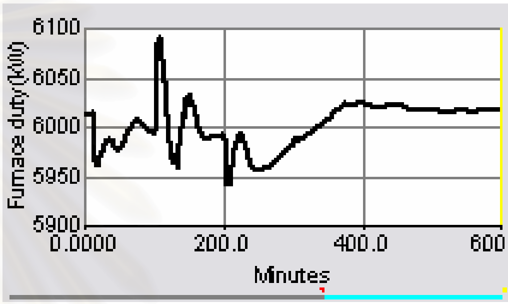

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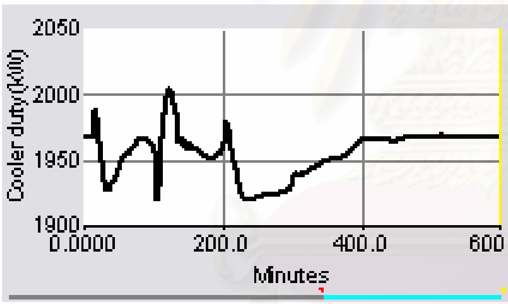


(q)

Figure 5.16 *Continued*

5.5.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Figure 5.11 shows the dynamic responses of the HDA process alternative 6 to a change in the disturbance load of cold stream (reactor feed stream). This disturbance is made as follows: first the fresh toluene feed temperature (stream FFtol in Figure 5.3) is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes (Figure 5.11.a).

Both the cold and hot outlet temperatures of FEHE1 decrease as the cold inlet temperature decreases, this is a desired condition for the hot stream, hence the LSS in FEHE1 switch the control action from TCE1h to TCE1c to control the cold outlet temperature of FEHE1 at its minimum value of 148.5 ^{o}C (i.e. the cold inlet temperature of FEHE2 as shown in Figure 5.11.c). As a result, the hot outlet temperature of FEHE1 (i.e. the cooler inlet temperature) quickly drops to a new steady state value (Figure 5.11.d), and the cooler duty decreases (Figure 5.11.n).

When the cold inlet temperature of FEHE1 increases, first both the cold and hot outlet temperatures of FEHE1 increase, this is an MER choice, as expected the LSS switches the control action from TCE1c to TCE1h. As a result, the hot outlet temperature of FEHE1 drops to its nominal value (Figure 5.11.d). Therefore it is understandable that why the furnace duty decreases significantly (Figure 5.11.m), since the furnace inlet temperature increases (Figure 5.11.j).

The hot outlet temperatures of FEHE2 and FEHE3 (Figures 5.11.e and 10.f) and the tray temperatures in the stabilizer and product columns (Figures 5.11.g and 10.h) are well controlled. But the tray temperature in recycle column has the maximum deviation of about 2 ^{o}C and it takes over 600 minutes to return to its set point (Figure 5.11.i).

5.5.2 Change in the Disturbance Load of Cold Stream from the Bottoms of Product Column

Figure 5.12 shows the dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of product column (C2). This disturbance is made as follows: first the set point of C2-bottom temperature controller (i.e. TCX3 in Figure 5.3) is decreased from 144.18 to 142.18 ^{o}C at time equals 10 minutes, the temperature is increased from 142.18 to 146.18 ^{o}C at time equals 200 minutes, then its temperature is returned to its nominal value of 144.18 ^{o}C at time equals 400 minutes (Figure 5.12.a). As can be seen, the temperature response in the bottoms of product column is somewhat fast (Figure 5.12.a).

When the cold inlet temperature of reboiler R2 (i.e. C2-bottom temperature as shown in Figure 5.12.a) decreases, the hot inlet temperature of FEHE1 decreases, thus the LSS will take a control action to maintain the cold inlet temperature of FEHE2 (Figure 5.12.c). The hot outlet temperature of FEHE1 drops to a new steady state value (Figure 5.12.d). Thus, it will result in decrease of the cooler duty (Figure 5.12.n). On the other hand, when C2-bottom temperature increases (Figure 5.12.a), as expected the LSS switches the control action from TCE1c to TCE1h to maintain the hot outlet temperature of FEHE1 (Figure 5.12.d) at its nominal value. Therefore, the furnace duty decreases significantly (Figure 5.12.m), since the furnace inlet temperature increases (Figure 5.12.j).

5.5.3 Change in the Disturbance Load of Cold Stream from the Bottoms of Stabilizer Column

Figure 5.13 shows the dynamic responses of HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of stabilizer column (C1). This disturbance is made as follows: first the set point of C1-bottom temperature controller (i.e. TCX2 in Figure 5.3) is decreased from 189.9 to 187.9 ^{o}C at time equals 10 minutes, and the temperature is increased from 187.9 to 191.9 ^{o}C at time equals 200 minutes, then its temperature is returned to its nominal value of 189.9 ^{o}C at time equals 400 minutes (Figure 5.13.a). As can be seen, the temperature response in the bottoms of stabilizer column is slower than that in the bottoms of product column.

Principally, shifting of both the positive and negative disturbance loads from the bottoms of stabilizer column are the same as those from the bottoms of product column. When the cold inlet temperature of reboiler R1 (i.e. C1-bottom temperature as shown in Figure 5.13.a) decreases, it will result in decrease of the hot inlet temperature of FEHE1. Thus, the cold inlet temperature of FEHE2 (Figure 5.13.c) is maintained at its minimum value, whereas the hot outlet temperature of FEHE1 drops to a new steady state value (Figure 5.13.d). Therefore, the cooler duty decreases significantly (Figure 5.13.n). When C1-bottom temperature increases (Figure 5.13.a), it will result in increase of the hot inlet temperature of FEHE1. As expected, the LSS switches the control action from TCE1c to TCE1h to maintain the hot outlet temperature of FEHE1 (Figure 5.13.d) at its nominal value. The cold inlet temperature of FEHE2 rises to a new steady state value (Figure 5.13.c). Therefore, the furnace duty decreases significantly (Figure 5.13.m).

5.5.4 Change in the Disturbance Load of Cold Stream from the Bottoms of Recycle Column

Figure 5.14 shows the dynamic responses to a change in the heat load disturbance of cold stream from the bottoms of recycle column (C3). This disturbance is made as follows: first the set point of C3-bottom temperature controller (i.e. TCX4 in Figure 5.3) is decreased from 349.9 to 348.5 ^{o}C at time equals 10 minutes, and the temperature is increased from 348.5 to 351.3 ^{o}C at time equals 300 minutes, then its temperature is returned to its nominal value of 349.9 ^{o}C at time equals 600 minutes (Figure 5.14.a). As can be seen, this set point change is sluggish (Figure 5.14.a).

In a particular case, both the positive and negative disturbance loads of cold the stream from the recycle column is shifted to a furnace utility unit, since the hot outlet temperature of FEHE3, i.e. the hot inlet temperature of reboiler R3 has to be kept at its set point (Figure 5.14.f).

When the cold inlet temperature of reboiler R3 (C3-bottom temperature as shown in Figure 5.14.a) decreases, the hot outlet temperature of reboiler R3 decreases. Consequently, furnace duty increases (Figure 5.14.m), since the furnace inlet decreases (Figure 5.14.j). When C3-bottom temperature increases (Figure 5.14.a), the hot outlet temperature of reboiler R3 is not controlled, i.e. it increases. Therefore, the furnace duty will be decreased (Figure 5.14.m), since the furnace inlet temperature increases (Figure 5.14.j).

5.5.5 Change in the Disturbance Load of Hot Stream (Reactor Product)

Figure 5.15 shows the dynamic responses of the HDA process alternative 6 to a change in the heat load disturbance of hot stream (the hot reactor product). This disturbance is made as follows: first the set point of FEHE3-hot-inlet temperature controller (i.e. TCX1 in Figure 5.3) is decreased from 621.1 to 616.1 ^{o}C at time equals 10 minutes, and the temperature is increased from 616.1 to 626.1 ^{o}C at time equals 200 minutes, then its temperature is returned to its nominal value of 621.1 ^{o}C at time equals 400 minutes (Figure 5.15.a). As can be seen, this temperature response is very fast (Figure 5.15.a), the new steady state is reached quickly (Figure 5.15.a).

Again, the disturbance loads of hot stream is shifted to a furnace utility unit, since the hot outlet temperature of FEHE3 (Figure 5.15.e) has to be kept constant. When the hot inlet temperature of FEHE3 decreases (Figure 5.15.a), it will result in decrease of the furnace inlet temperature (Figure 5.15.i); consequently the furnace duty increases (Figure 5.15.l). When the hot inlet temperature of FEHE3 increases (Figure 5.15.a), the disturbance load is shifted to the cold stream. Therefore, the furnace duty will be decreased (Figure 5.15.l).

5.5.6 Change in the Recycle Toluene Flowrates

Figure 5.16 shows the dynamic responses of the HDA process alternative 6 to a change in the recycle toluene flowrates from 168.2 to 158.2 kgmole/h at time equals 10 minutes, and the flowrates is increased from 158.2 to 178.2 kgmole/h at time equals 100 minutes, then its flowrates is returned to its nominal value of 168.2 at time equals 200 minutes (Figure 5.16.a). Tighter control of the recycle toluene flowrates is achieved in the HDA process alternative 6 than in alternatives 1 and 4 (Figure 5.16.a).

As can be seen that the drop in toluene feed flowrates reduces the reaction rate, so the benzene product flowrates drops (Figure 5.16.c), and the benzene product quality increases (Figure 5.16.d) and vice versa. The tray temperature in the stabilizer column has a maximum deviation of about 7 ^{o}C, and it takes over 300 minutes to return to its nominal value of 166.5 ^{o}C (Figure 5.16.j). But, the tray temperature in the recycle column has a large deviation (Figure 5.16.l), and it takes over 400 minutes to slowly return to its nominal value of 326.7 ^{o}C. The furnace and cooler duties (Figure 5.16.p and Figure 5.16.q) are maintained at its good enough levels.

5.6 Evaluation of the Dynamic Performance

The job of most control loops in a chemical process is one of regulation or load rejection, i.e. holding the controlled variable at its set point in the face of load disturbances. The shape of the complete closed-loop responses, from time t = 0 until steady state has been reached, could be used for the evaluation of the dynamic performance criterion. Unlike the simple criteria that use only isolated characteristics of the dynamic responses (e.g. decay ratio, overshoot, settling time), the criteria of this category are based on the entire response of the process. Integral Absolute Error (IAE) is widely used for the formulation of a dynamic performance as written below:

$$\mathrm{IAE} = \int_0^{\infty} \left|\varepsilon(t)\right| dt \tag{5.1}$$

Note that $\varepsilon(t) = y_{SP}(t) - y(t)$ is the deviation (error) of the response from the desired set point.

In this study, the IAE method is used to evaluate the dynamic performance of the designed control system. Tables 5.7 to 5.9 show the IAE of some temperature controllers in HDA process with different energy integration schemes (i.e. alternatives 1, 4, and 6) for some disturbances. The IAE results for the change in the disturbance loads of cold and hot streams are listed in Tables 5.7 and 5.8, respectively. Table 5.9 shows the IAE results for the change in the total toluene flowrates.

In general, the control system in HDA process alternative 1 is the most effective one compared with those in HDA process alternatives 4 and 6, i.e. the values of IAE in HDA process alternative 1 are smaller than those in alternatives 4 and 6. Thus, these IAE results also reveal that the implementation of complex energy integration to the process deteriorates the dynamic performances of the process.

Table 5.7 The IAE results of the control system to a change in the disturbance load of cold stream (reactor feed stream)

Controller	Integral Absolute Error (IAE)		
	HDA process Alternative 1	HDA process Alternative 4	HDA process Alternative 6
TC1	6.1966	6.3750	11.3125
TC2	0.2530	1.6733	1.2637
TC3	22.9131	182.9202	215.5248
TCE1c	7.2329	15.1917	19.6066
TCE1h	11.9540	67.3376	82.5746
TCE2h	-	6.4417	8.4007
TCE3h	-	-	5.7239
TCQ	0.6604	2.9611	5.2978
TCR	1.5283	3.2800	3.1052
TCS	2.5250	1.6626	4.9324
Total	53.2633	287.8432	357.7422

Table 5.8 The IAE results of the control system to a change in the disturbance load of hot stream (reactor product stream)

Controller	Integral Absolute Error (IAE)		
	HDA process Alternative 1	HDA process Alternative 4	HDA process Alternative 6
TC1	7.5693	4.6492	39.7498
TC2	0.3647	2.5758	9.3419
TC3	29.5399	265.9116	491.9192
TCE1c	17.4755	16.1302	47.2940
TCE1h	20.2402	34.6220	63.9595
TCE2h	-	9.4564	67.1568
TCE3h	-	-	59.4044
TCQ	1.6322	2.5347	17.3824
TCR	3.5679	6.0488	8.7348
TCS	2.6137	0.4252	3.2174
Total	83.0034	342.3539	808.1602

Table 5.9 The IAE results of the control system to a change in the total toluene feed flowrates

Controller	Integral Absolute Error (IAE)		
	HDA process Alternative 1	HDA process Alternative 4	HDA process Alternative 6
TC1	157.5382	196.0117	1061.3814
TC2	10.2029	17.3762	9.9280
TC3	630.1852	5809.8166	6885.7879
TCE1c	42.9002	123.8851	315.9949
TCE1h	63.1619	238.0049	206.0160
TCE2h	-	58.8839	92.5111
TCE3h	-	-	38.5914
TCQ	8.8660	47.6075	56.4657
TCR	5.7998	24.3897	5.7604
TCS	9.8088	5.5640	5.6450
Total	928.4630	6521.5396	8687.9445

5.7 Conclusions

The control strategy for complex energy integrated HDA process has been presented based on the HPH, i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the MER can be obtained with some tradeoffs. In this work, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network.

The new plantwide control structures with the LSS have been applied in the energy-integrated HDA process (i.e. alternatives 1, 4, and 6). The new plantwide control structure of HDA process alternative 1 is compared with the earlier work given by Luyben et al. (1999). Both of the new and earlier control structures are evaluated based on rigorous dynamic simulation using the commercial software HYSYS. In general, better responses of the furnace and cooler utility consumptions are achieved here compared to the Luyben's control structure, since the new control structure in the current study is able to select an appropriate heat pathway. As shown in the dynamic simulation study, the proposed HPH is therefore considered useful to achieve the highest possible DMER.

However, the dynamic responses of the control systems in both HDA process alternatives 4 and 6 are slower than those in HDA process alternative 1. From the steady state point of view, the implementation of complex energy integration in the process can recover more energy. But, it will deteriorate the dynamic performances of the control system as indicated by the values of IAE. The value of IAE in the complex energy-integrated HDA process alternative 6 is the largest one compared with those in HDA process alternatives 1 and 4.

CHAPTER VI
HEN CONTROL CONFIGURATION DESIGN AND OPERATION FOR DYNAMIC MER

The heuristic of selection and manipulation of heat pathways has been implemented in plantwide control for the hydrodealkylation of toluene (HDA) process as given in chapters 4 and 5. Our purpose of this chapter is to present the extended general heuristic design procedure for heat exchanger networks control configuration and operation for dynamic maximum energy recovery (DMER).

6.1 Introduction

The problem of energy recovery to reduce the utility cost has attracted many research attentions. There have been many contributions on design of heat exchanger networks (HENs). For examples, Linnhoff and Hindmarsh (1983) and Linnhoff et al. (1983) have presented a pinch method for the design of HENs and a good integration between distillation and the overall process, respectively. Calandranis and Stephanopoulos (1988) have also provided a comprehensive summary of work on the design of control loop configuration in HENs. Wongsri (1990) have presented a simple but effective systematic synthesis procedure for the design of resilient HENs. His heuristic design procedure is used to design or synthesize HENs with pre-specified resiliency. Terrill and Douglas (1987a, 1987b, 1987c) have proposed six HEN alternatives for the HDA process, in which their energy saving ranges between 29% and 43%.

Although several authors have studied the general design and control of HENs, there is no report on study of the energy management for energy-integrated plants, particularly in manipulating heat pathways in order to achieve the highest possible DMER. Actually, maximum energy recovery (MER) should not be taken as a static value, i.e. its value varies according to the operating conditions, e.g. the input heat load disturbance. Therefore, for the process associated with energy integration, it is important to study the heat pathway control in order to manage the heat load disturbance in such a way that the MER can always be achieved.

As discussed in chapters 4 and 5, a selective controller with low selector switch (LSS) can be used to select an appropriate heat pathway to direct the associated disturbance load to a cooling or heating utility unit, so that its duty will be decreased. This chapter presents the new heuristic design procedure for HENs control configuration and operation. In particular case, multiple LSSs (i.e. more than one LSS) are required for the resilient HEN. The number of LSS can be determined based on the new heuristic design procedure. This heuristic also explains where the LSS should be placed in the designed HEN.

6.2 Process Control of Heat Exchanger Networks

An HEN is widely used in the petroleum and chemical industries to perform heat exchange, so that each process stream attains its specified temperature. Every process is subjected to random disturbances and operator upsets, which require a process control scheme that will maintain all outlet temperatures at their set-point values.

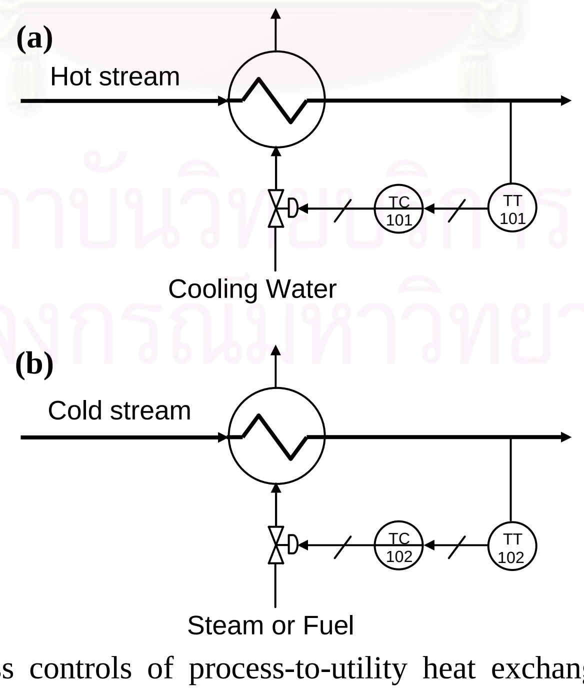


Figure 6.1 Process controls of process-to-utility heat exchangers: (a) use of cold utility, (b) use of hot utility

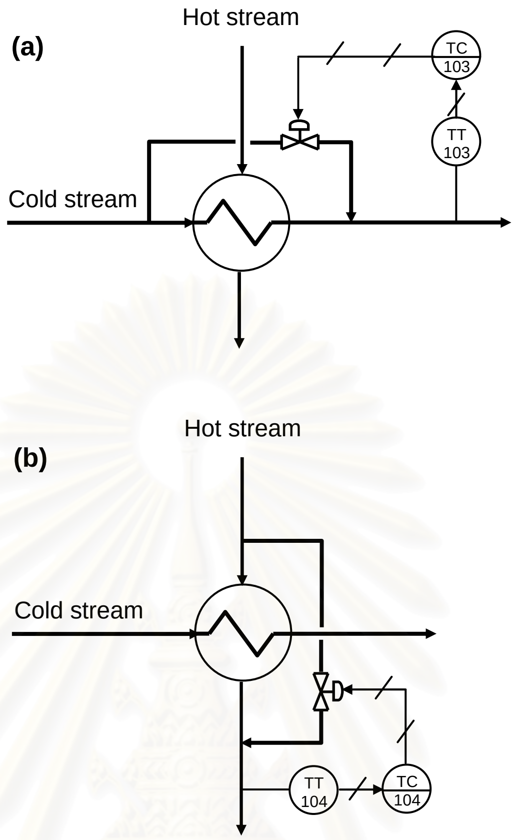


Figure 6.2 Process controls of process-to-process heat exchangers: (a) controlling the cold outlet temperature, (b) controlling the hot outlet temperature

6.2.1 Process-to-Utility Heat Exchangers

Process-to-utility heat exchangers are defined as those heat exchange operations that exchange heat between a process stream and a utility stream as shown in Figure 6.1. Mostly the water flow rate is manipulated to control the outlet temperature of hot stream (Figure 6.1.a). Whereas the steam flow rate is manipulated to control the outlet temperature of cold stream (Figure 6.1.b).

The outlet temperature of the process stream can be easily controlled by manipulating the flow rate of the utility stream. Generally, the utility system of a complex energy-integrated plant is designed to absorb large disturbances in the process, and making process-to-utility exchangers relatively easy to control.

6.2.2 Process-to-Process Heat Exchangers

Process-to-process heat exchangers are defined as those heat exchange operations that exchange heat between two process streams, i.e. the cold and hot streams, as shown in Figure 6.2. The outlet temperature of one process stream can be controlled using the bypass flow of other stream as the manipulated variable. During the operation of heat exchanger, if the bypass flow rate is increased, the mean temperature difference is reduced, resulting in a smaller duty. As a result, the actual manipulated variable is the heat load of the heat exchanger. For that reason, it is not possible to control both outlet temperatures in the same heat exchanger, e.g. using bypass flow on both sides.

Furthermore, a process-to-process heat exchanger that be used to control an outlet temperature must be designed with nonzero bypass flow rate to handle disturbances that require an increase or decrease of the heat load. Good engineering practice would maintain a minimum flow rate of 5-10% through the bypass (Jones, W.E. and Wilson, J.A., 1997). Because the existence of bypass stream results in smaller mean temperature difference, thus larger area must be employed.

Steady state simulations show that, from the economic point of view, the bypass stream should be placed on the stream with largest heat flow rate capacity, because this stream can handle larger disturbances with less additional capital cost compared to the situation in which the bypass is placed on the stream with smallest heat flow rate capacity. On the other hand, Seborg et al., (1989) stated that manipulated variables that rapidly affect the controlled variables should be selected. Using this principle, dynamic simulations indicate that the bypass stream must be placed on the exchanger stream that has its outlet temperature controlled, independently of the heat flow rate capacity values. Thus, the dynamic result should be considered in the design of heat exchanger networks control schemes.

6.3 Heat Pathway Heuristics for Heat Exchanger Networks Control

Since the plant disturbances (e.g. the feed stream temperature, the feed flowrates) are not taken as static values, the heat load changes. Thus, these disturbances can propagate to the whole process. A control strategy is required to manage these disturbance loads, so that MER can always be achieved.

6.3.1 Influence of Disturbance Loads on the Utility Requirements

Several disturbance loads have been defined in Chapter 4. The influence of disturbance loads on the utility requirements is summarized in Table 6.1. Both positive and negative disturbance loads affect the utility requirements; those disturbances can result in either increase or decrease of the utility duties.

In this work, we attempt to shift D^+ of cold stream and D^- of hot stream to the cooler utility, and shift D^+ of hot stream and D^- of cold stream to the heater utility, thus its utility duties will be decreased based upon the input disturbance loads. Since the disturbance load significantly affect the utility requirements, proper heat pathway should be selected to carry the associated load to a utility unit.

6.3.2 Design of Heat Pathways for Dynamic MER

For the plantwide energy management, the heat pathways through the network are designed so that the dynamic MER can always be achieved. In this work, the heat pathways are designed based on the match patterns design and disturbance propagation technique (Wongsri, 1990). Review of resilient HEN design using the match patterns design is given in Appendix C. The disturbance propagation technique is also given in Appendix D for a review.

Table 6.1 Influence of disturbance loads on the utility requirements

disturbance load	source	effects on the utility requirements
positive disturbance load (D^+) of cold stream	the inlet temperature of cold stream decreases	decreases heat duty of cooler or increases heat duty of heater
positive disturbance load (D^+) of hot stream	the inlet temperature of hot stream increases	decreases heat duty of heater or increases heat duty of cooler
negative disturbance load (D^-) of cold stream	the inlet temperature of cold stream increases	decreases heat duty of heater or increases heat duty of cooler
negative disturbance load (D^-) of hot stream	the inlet temperature of hot stream decreases	decreases heat duty of cooler or increases heat duty of heater

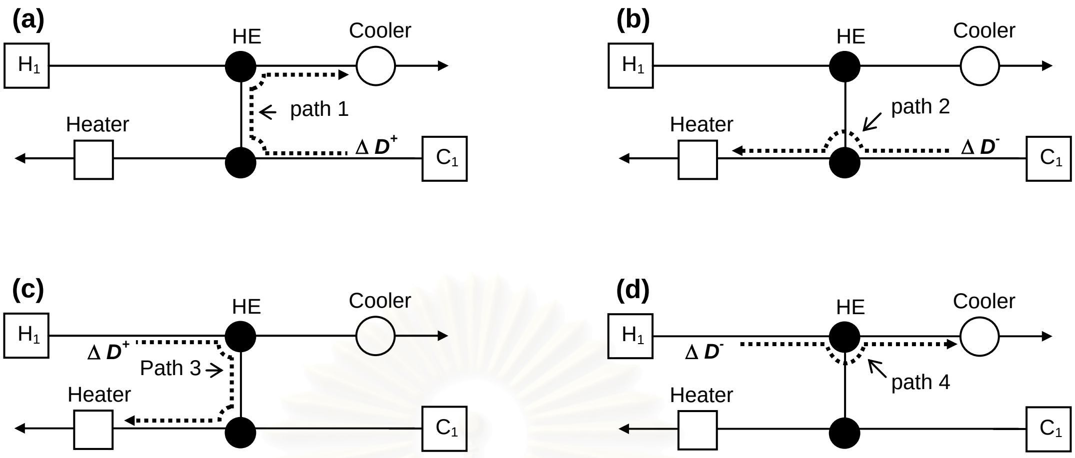


Figure 6.3 Heat pathways in the simplified HEN to achieve DMER, where: (a) path 1 is used to shift D^+ of the cold stream to the cooler, (b) path 2 is used to shift $D^-$of the cold stream to the heater, (c) path 3 is used to shift D^+ of the hot stream to the heater, and path 4 is used to shift D^- of the hot stream to the cooler.

Based on the positive effect of the disturbance load on the utility requirement, we attempt to shift the disturbance load to either cooler or heater utility unit in such a way that DMER is realized. Therefore, the duties of utility units will be decreased as the disturbance is entering the process. A simple HEN that is widely used in the chemical industries (e.g. HDA process alternative 1) as shown in Figure 6.3 is used to explain how an appropriate heat pathway should be activated to carry the associated load to a heating or cooling utility unit. For instance, when the inlet temperature of a disturbed cold stream decreases, path 1 (Figure 6.3.a) should be activated by controlling the cold outlet temperature of the heat exchanger (HE). This will have the effect of shifting D^+ of the cold stream to the cooler. Thus, the cooler duty will be decreased. Consider the case when the inlet temperature of a disturbed cold stream increases, path 2 (Figure 6.3.b) should be activated by controlling the hot outlet temperature of HE to shift D^- of the cold stream to heater. Thus, the heater duty will be decreased.

On the other hand, when the inlet temperature of a disturbed hot stream increases, path 3 (Figure 6.3.c) should be activated by controlling the hot outlet temperature of HE to shift D^+ of the hot stream to heater. As a result, the heater duty will be decreased. Consider the case when the inlet temperature of a disturbed hot stream decreases, path 4 (Figure 6.3.d) should be activated by controlling the cold outlet temperature of HE to shift D^- of the hot stream to cooler. As a result, the cooler duty will be decreased. Hence, the DMER can be obtained.

6.3.3 Control Strategy for Dynamic MER

A control strategy for an HEN is required such as an appropriate designed pathway will be selected at any given time so that DMER will be obtained. Figure 6.4 shows a control strategy for an HEN to obtain DMER. In Figure 6.4, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway to carry the associated load to a utility unit.

The LSS involves one manipulated variable and two controlled variables and works as follows: The hot outlet temperature (T_{Hout}) of HE is controlled at its normal set point by manipulating the valve on the bypass line i.e. loop 1 in Figure 6.4. At the same time, the cold outlet temperature (T_{Cout}) of HE should not be allowed to drop below a lower limit value, which is necessary to keep the heater utility duty at a good level. Whenever the temperature T_{Cout} drops below the allowable limit due to, for example, a disturbance load entering the process, the LSS switches the control action

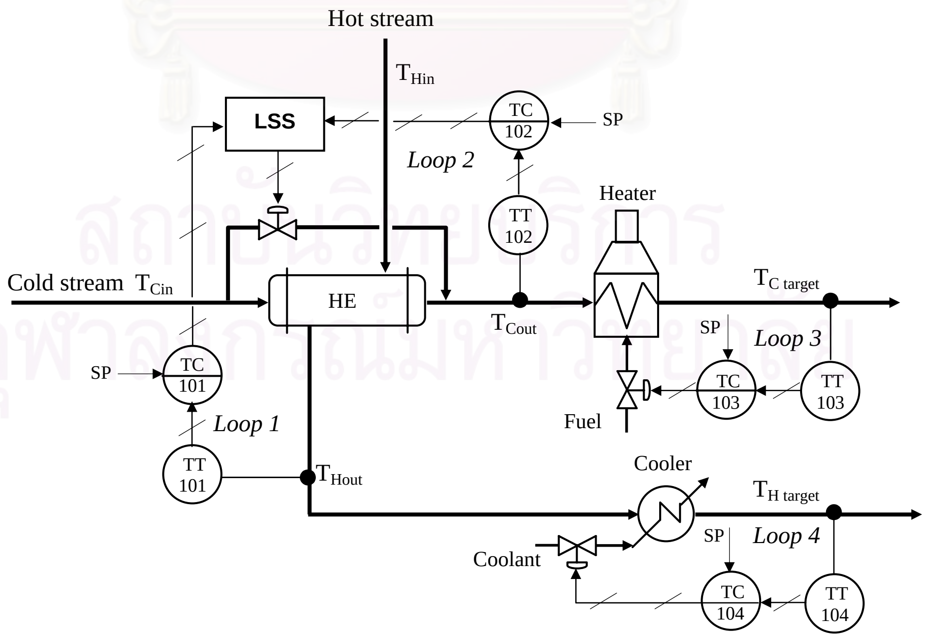


Figure 6.4 A selective controller with the LSS for an HEN to achieve DMER

from the hot temperature control (TC101) to the cold temperature control (TC102), i.e. switches the control action from loop 1 to loop 2, and closes the valve on the bypass line. As a result, T_{Cout} will rise to its normal temperature and T_{Hout} will be further decreased, so the cooler duty will also be decreased.

Whenever the temperature T_{Cout} increases above a lower limit, a desired-condition during operation, due to the disturbance load entering the process, the LSS switches the control action from loop 2 to loop 1, and closes the valve on the bypass line. Consequently, T_{Hout} will drop to its normal temperature and T_{Cout} will be further increased, so the furnace duty will also be decreased.

6.4 Design and Control of Heat Pathways for Heat Exchanger Networks

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

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

- The utility exchangers can handle all variations of heat load.
- The target temperatures are not subject to changes. Only the variation in input conditions is of interest.
- The path for disturbance loads is co-current with all of the process streams.
- Any heat exchanger will have enough heat transfer area to accommodate increases in heat loads of disturbed process stream.
- Bypass lines are provided to all heat exchangers as a standard feature to adjust heat load.

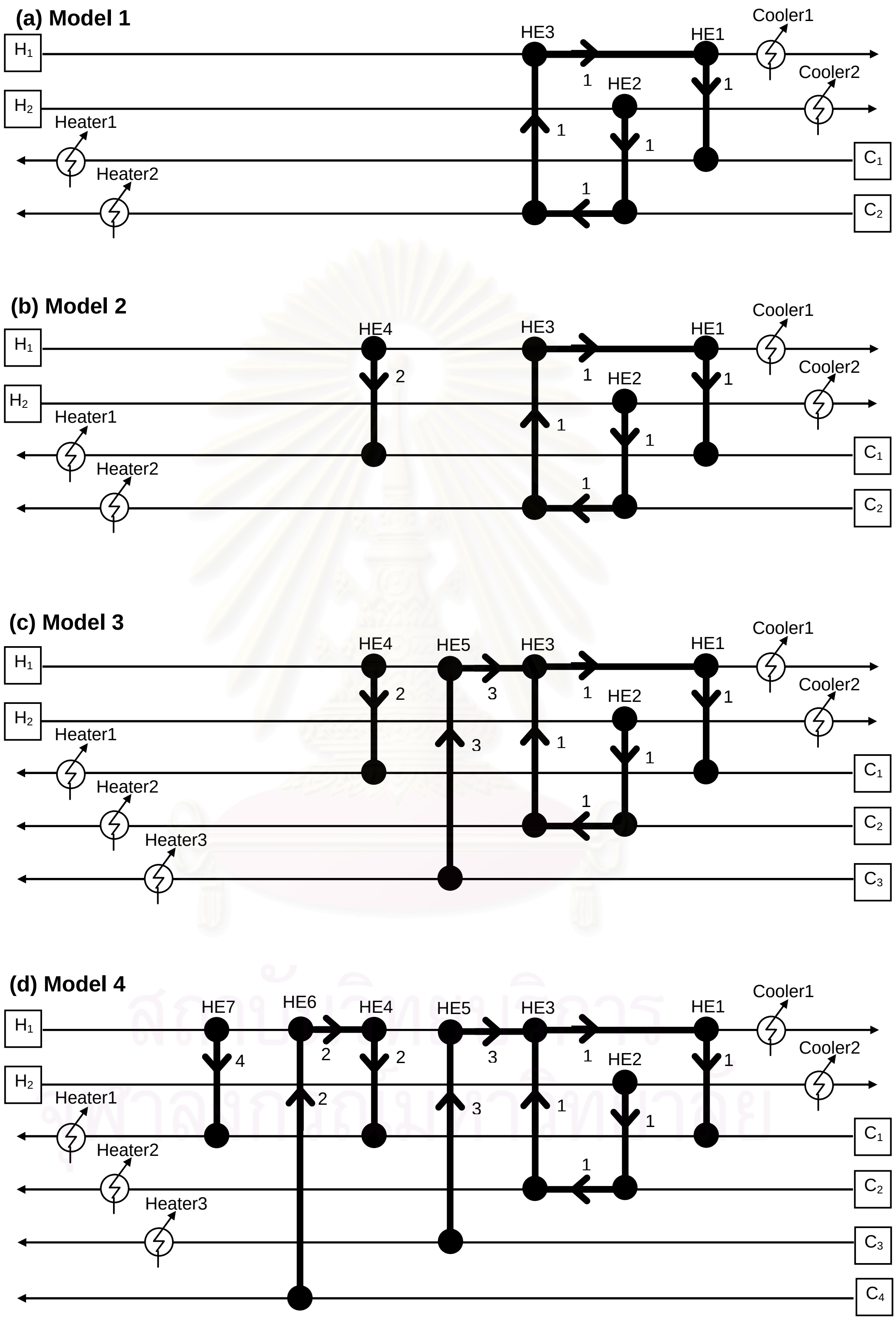


Figure 6.5 Several typical HEN examples with its specified heat links

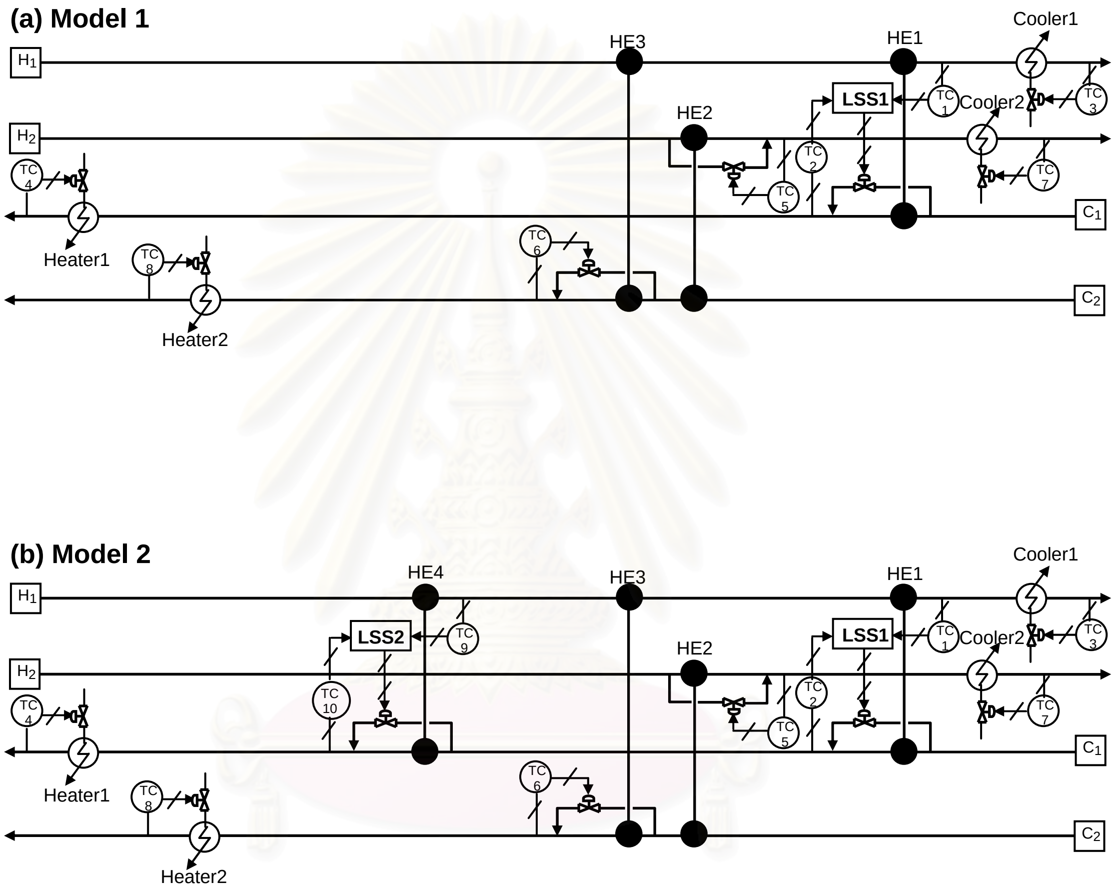


Figure 6.6 Control configurations for the typical HEN examples to achieve DMER

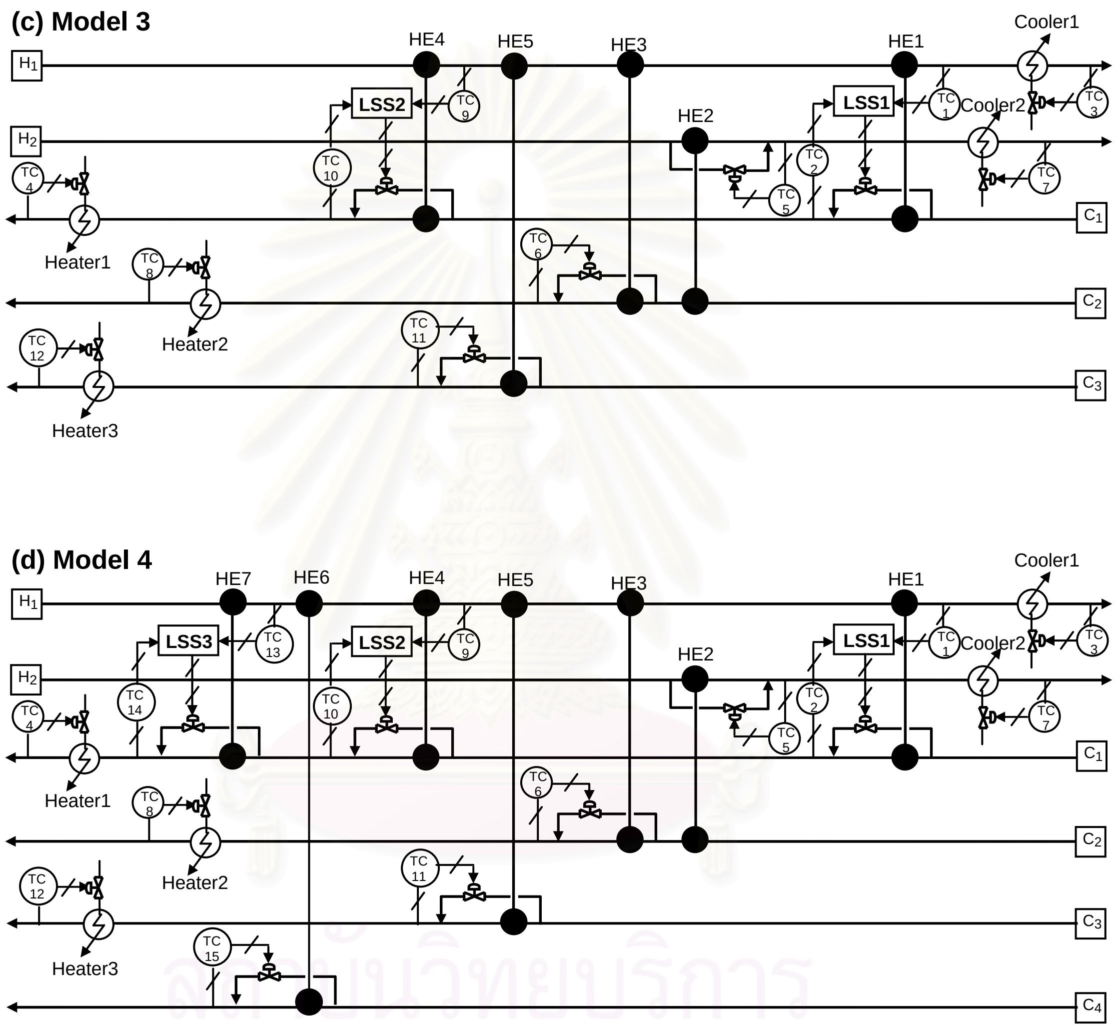


Figure 6.6 *Continued*.

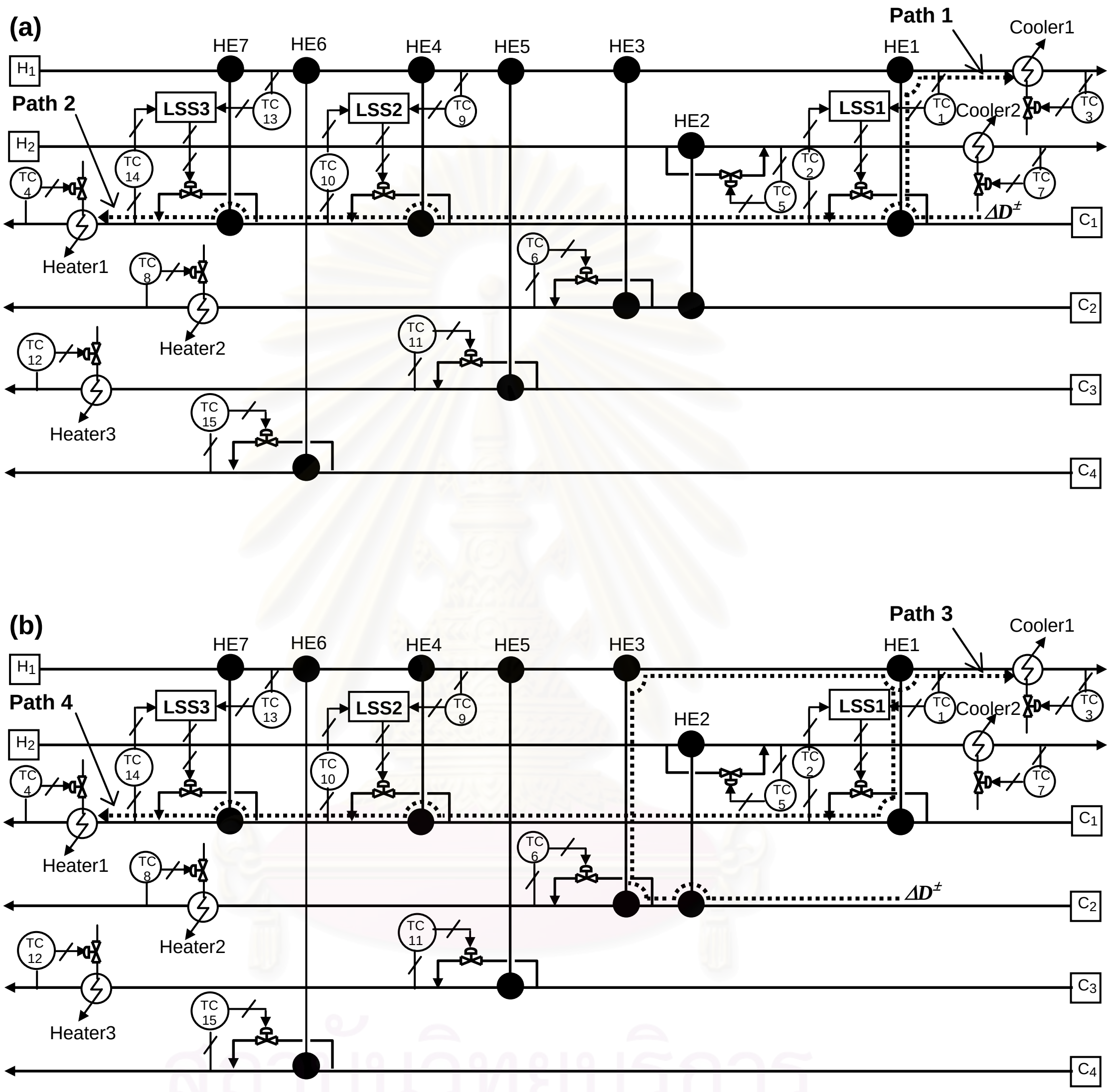


Figure 6.7 Heat pathways through a typical complex HEN example (e.g. HDA process alternative 6) that are designed to direct and manage the disturbance load of: (a) the cold stream C_1, (b) the cold stream C_2, (c) the cold stream C_3, (d) the cold stream C_4, and (e) the hot stream H_1

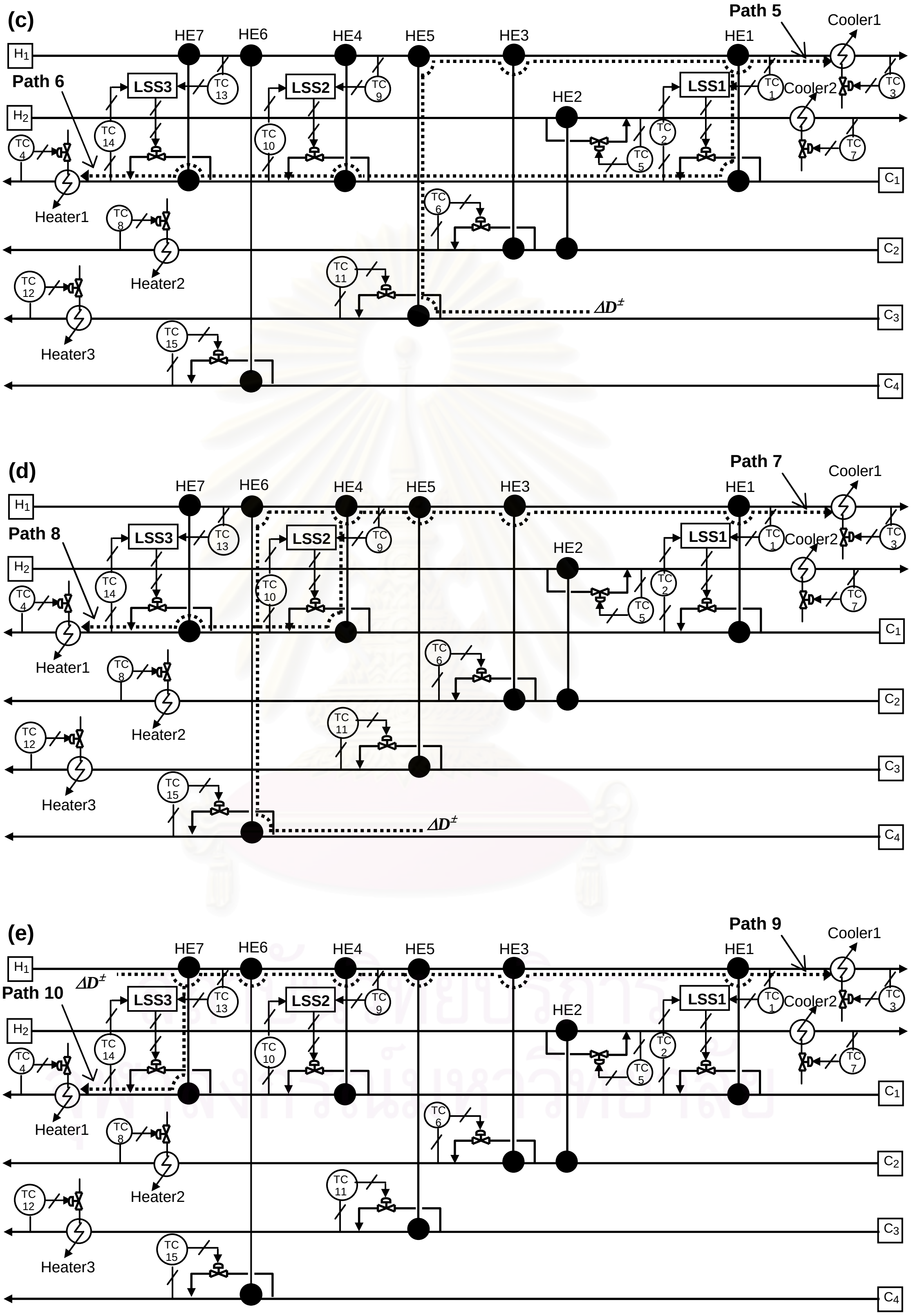


Figure 6.7 *Continued*

6.4.1 Implementation of Heat Pathway Manipulator

For a complex HEN which contains more than one HE unit, some questions may arise such as, where the LSS should be placed and how many LSS should be employed to direct the disturbance load to a utility unit. This section discusses the implementation of heat pathway manipulator for some typical HEN examples and answers those questions.

In order to know how many LSS should be employed and where they should be placed, first we must identify the heat link in HEN i.e. path for heat from one HE to the others, since it can be used for the propagation of the disturbance load. Then, we must find the last HE unit of the identified heat link. The LSS should be placed on the last HE unit. The solid lines in Fig. 6.5 show the identified heat link for the propagation of the disturbance load in some typical HEN examples. Note that the propagation of the disturbance load is co-current with all of the process streams.

HEN Model 1 (Figure 6.5.a) is defined as the HEN contains two cold and two hot streams, and three HE units. As can be seen that, this HEN has only one heat link that starts from HE2, continues to HE3, and finally to the last heat exchanger HE1 (see solid line in Figure 6.5.a). Since HEN Model 1 has only one heat link that ends up at the last heat exchanger HE1, only one LSS is employed and placed on HE1. The cold outlet temperature of HE3 and the hot outlet temperature of HE2 are maintained by using bypass control. The control system of this HEN is given in Figure 6.6.a.

HEN Model 2 (Figure 6.5.b) is the same as HEN Model 1, except, a HE unit (i.e. HE4) is additionally installed to exchange heat between streams H_1 and C_1. HEN Model 2 is similar with HEN alternative 4 of HDA process (Terrill and Douglas, 1987,a,b,c). There are two heat links in this HEN. The first heat link in HEN Model 2 is the same as that in Model 1. The second heat link is on HE4. Thus, two LSSs are employed and placed on both HE1 and HE4. The control configuration for this model is shown in Figure 6.6.b.

HEN Model 3 is the same as HEN Model 2, except, a HE unit (i.e. HE5) is additionally installed to exchange heat between stream H_1 and the additional stream C_3, as shown in Figure 6.5.c. HEN Model 3 is similar with HEN alternative 5 of

HDA process (Terrill and Douglas, 1987a,b,c). There are three heat links in this HEN. The first and second heat links in HEN Model 3 are the same as those in Model 2. Since the new stream C_3 is matched to stream H_1, this gives new heat link, namely heat link 3 (solid line in Figure 6.5.c). In this particular case, i.e. HEN contains more than one heat link, in order to reduce the number of LSS, we design all heat links so that they will end up at the same heat exchanger. In HEN Model 3, it is possible to design the third heat link so that it will end up at the heat exchanger HE1 (see link 3 in Figure 6.5.c). Consequently, we need only one LSS for both heat links 1 and 3, and one LSS for heat link 2. Thus, two LSSs are employed and placed on HE1 and HE4. The other control loops in HEN Model 3 are the same as those in HEN Model 2, except the cold outlet temperature of HE5 is maintained by using bypass control, as shown in Figure 6.6.c.

HEN Model 4 is the same as HEN model 3, except, a HE unit (i.e. HE6) is additionally installed to exchange heat between stream H_1 and the additional stream C4, and HE7 is used to exchange heat between streams H_1 and C1, as shown in Figure 6.5.d. HEN Model 4 is similar with HEN alternative 6 of HDA process (Terrill and Douglas, 1987a,b,c). There are four heat links in this HEN. The first and third heat links in HEN Model 4 are the same as those in Model 3. Since the new stream C_4 is matched to stream H_1, the second heat link starts from HE6 and ends up at HE4. The fourth heat link is on HE7. Three LSSs are employed and placed on HE1, HE4 and HE7. The control configuration for Model 4 is shown in Figure 6.6.d.

6.4.2 Heat Pathways Management for Dynamic MER

Heat pathways management for a typical complex HEN example (e.g. HDA process alternative 6) is shown in Figure 6.7. In this HEN, the disturbance loads must be dissipated as much as possible by shifting it to the streams that are serviced by utility exchangers. Three LSSs are employed and placed on HE1, HE4 and HE7 to direct the disturbance loads to either Cooler 1 or Heater 1 utility, so its utility duties will be decreased based upon the input disturbance loads.

As can be seen, when D^+ is coming from the cold stream C_1 (i.e. the cold inlet temperature decreases), the LSS1 will direct this load via path 1 (Figure 6.7.a) by controlling the cold outlet temperature of HE1 (TC2) at its set point. Following path 1, D^+ of stream C_1 will result in decrease of the Cooler 1 duty. Consider the case when D^- is coming from stream C_1 (i.e. the cold inlet temperature increases), the LSS1 will switch the control action (from TC2 to TC1) to control the hot outlet temperature of HE1 at its set point. As a result, the cold outlet temperature of HE1 will be further increased, thus the LSS2 and LSS3 will take an action to control the hot outlet temperatures of HE4 and HE7, respectively (TC9 and TC13). Following path 2 (Figure 6.7.a), D^- of stream C_1 will result in decrease of the Heater 1 duty.

Since the hot outlet temperature of HE2 and the cold outlet temperature of HE3 are kept constant (TC5 and TC6), both D^+ and D^- of stream C_2 are shifted to stream H_1 to be further directed to heat sink or heat source according to its effects. Consider the case when the supply temperature of stream C_2 decreases, the hot outlet temperature of HE3 will decrease. The LSS1 will take an action to control the cold outlet temperature of HE1 at its set point. Thus, following path 3 (Figure 6.7.b), D^+ of stream C_2 will result in decrease of the Cooler 1 duty. On the other hand, when the supply temperature of stream C_2 increases, the LSS1 will switch the control action from TC2 to TC1 to control the hot outlet temperature of HE1 at its set point. This lets the inlet temperature of Heater 1 to increase. Following this action, path 4 as shown in Figure 6.7.b will result in decrease of the Heater 1 duty.

Figure 6.7.c shows the heat pathways management when the disturbance loads are coming from the cold stream C_3. The heat pathways resulting from these disturbances are similar with those coming from the cold stream C_2. Thus, path 5 (Figure 6.7.c) is used to carry the D^+ of cold stream C_3 to the Cooler 1, and path 6 (Figure 6.7.c) is used to carry the D^- of cold stream C_3 to the Heater 1, hence its duties will be decreased according to the input disturbance loads.

Figure 6.7.d shows the heat pathways management when the disturbance loads are coming from the cold stream C_4. Since the cold outlet temperature of HE6 is maintained constant (TC15), both D^+ and D^- of stream C_4 are shifted to stream H_1 to be further directed to heat sink or heat source according to its effects. Consider the case when the supply temperature of stream C_4 decreases, the hot outlet temperature of HE6 will decrease. The LSS2 will take an action to control the cold outlet temperature of HE4 at its set point (TC10). Thus, following path 7 (Figure 6.7.d), D^+

of stream C_4 will result in decrease of the Cooler 1 duty. On the other hand, when the supply temperature of stream C_4 increases, LSS2 will switches the control action from TC10 to TC9 to maintain the hot outlet temperature of HE4 at its set point. Thus, following path 8 (Figure 6.7.d), D^- of stream C_4 will result in decrease of the heater 1 duty.

Figure 6.7.e shows heat pathways management when the disturbance loads are coming with the hot stream H_1. When the hot inlet temperature of HE7 decreases (D^- of stream H_1), the LSS3 will take an action to control the cold outlet temperature of HE7 (TC14) at its set point. This disturbance load is continued to the down stream units via path 9. As a result, the Cooler 1 duty will be decreased. Consider the case when the hot inlet temperature of HE7 increases (D^+ of stream H_1), LSS3 will switch the control action from TC14 to TC13 to control the hot outlet temperature of HE7 at its set point. Therefore, following path 10 (Figure 6.7.e), the Heater 1 duty will be decreased.

6.5 The New Heuristic Design Procedure for HEN Control Configuration and Operation

For any HEN configurations, based on the method developed for the above models, we propose the outline for the design of control configuration for heat pathways management to achieve DMER as follows:

(1) The heat exchanger network for a particular processing plant should be designed as a resilient HEN following the match pattern proposed by Wongsri (1990) (see Appendix C for a review).

- (1.1) Design the match pattern in HEN as Class A or Class B so that they are considered to be potential resilient match pattern.
- (1.2) If there is the match pattern in HEN as Class C or Class D, they are considered as non-resilient match pattern. For the remedy, any Class C or Class D in the match pattern should be redesigned so that its residual stream must be connected to either Class A or Class B. Hence the only two classes of interests are Class A and Class B.

(2) From the economic point of view, we strongly suggest to:

(2.1) shift D^+ of cold stream or D^- of the hot stream to the cooler utility, thus its duty will be decreased.

(2.2) shift D^- of cold stream or D^+ of the hot stream to the heater utility, thus its duty will be decreased.

(3) A selective controller with low selector switch (LSS) should be employed to select an appropriate heat pathway through the network to carry the associated load to the utility unit.

(4) The number of LSS to be used in a particular case can be determined as follows:

(4.1) Identify the heat link in HEN that can be used for the propagation of disturbance load, note that the propagation is co-current with the process stream (see Figure 6.5).

(4.2) If there is only one heat link (see Figure 6.5.a), the only one LSS is employed and placed on the last heat exchanger (see Figure 6.6.a).

(4.3) If there are more than one heat link (see Figures 6.5.b and 6.5.c):

(4.3.1) Design the heat links so that all of them will end up at the same heat exchanger unit in order to reduce the number of LSS.

(4.3.2) If all the heat links end up at the different heat exchanger units, so the number of LSS is equal to the number of heat link (see Figure 6.5.b) or the number of the last heat exchangers. For instance, based on the HEN model 2 (see Figure 6.5.b), there are 2 heat links, which end up at the different heat exchangers (HE1 and HE4). Thus, the number of LSS is equal to 2 (see Figure 6.6.b).

(4.3.3) If there are some heat links, which end up at the same heat exchanger unit (see Figure 6.5.c), the number of LSS is equal to the number of the last heat exchangers. For instance, based on the HEN model 3 (see Figure 6.5.c); There are three heat links (links 1, 2, and 3). Two of the three heat links (i.e. links 1 and 3) end up at the same heat exchanger unit (i.e. HE1). HE4 is used for link 2. Therefore, there are two last heat exchangers (i.e. HE1 and HE4) for all heat links. Hence, two LSS are required and placed on HE1 and HE4 (see Figure 6.6.c).

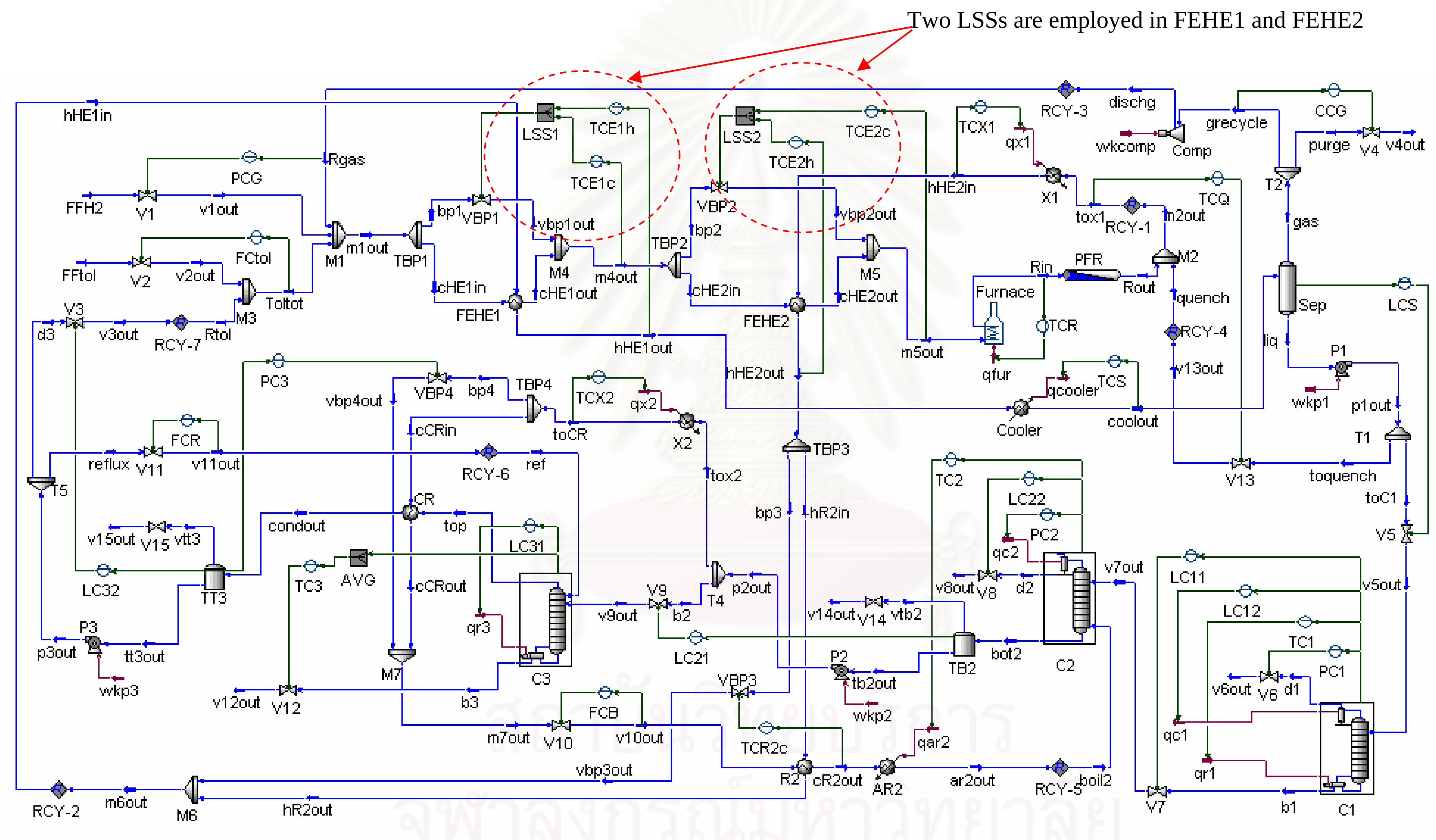


Figure 6.8 Plantwide control structure of the HDA process alternative 4 with 2 LSSs

Table 6.2 The initial values of controlled and manipulated variables for HDA process alternative 4 with two LSSs

controlled variable (CV)		manipulated variable (MV)	
process variable	initial value	process variable	initial value
total toluene flow rate	168.6 kgmole/hr	fresh feed toluene flow rate	128.5 kgmole/hr
gas recycle stream pressure	4171 kPa	fresh feed hydrogen flow rate	218.7 kgmole/hr
methane in gas recycle	0.5904 mole-frac	purge flow rate	215.4 kgmole/hr
quenched temperature	621.1 ^oC	quench flow rate	49 kgmole/hr
reactor inlet temperature	621.1 ^oC	furnace duty (qfur)	3386 kW
separator temperature	45 ^oC	cooler duty (qcooler)	1938 kW
FEHE2 cold inlet temperature	176.1 ^oC	FEHE1 bypass flow rate	232.9 kgmole/hr
cooler inlet temperature	94.4 ^oC	FEHE1 bypass flow rate	232.9 kgmole/hr
furnace inlet temperature	530.4 ^oC	FEHE2 bypass flow rate	122.4 kgmole/hr
FEHE2 hot outlet temperature	316.3 ^oC	FEHE2 bypass flow rate	122.4 kgmole/hr
R2 cold outlet temperature	180 ^oC	R2 bypass flow rate	231.6 kgmole/hr
separator liquid level	50 %-level	column C1 feed flow rate	172.0 kgmole/hr
column C1 pressure	1034 kPa	column C1 gas flow rate	8.8 kgmole/hr
column C1 tray-6 temperature	154.15 ^oC	column C1 reboiler duty (qr1)	1253 kW
column C1 base level	50 %-level	column C2 feed flow rate	163 kgmole/hr
column C1 reflux drum level	50 %-level	column C1 condenser duty (qc1)	176.0 kW
column C2 pressure	206.8 kPa	column C2 condenser duty (qc2)	4996 kW
column C2 tray-12 temperature	129.75 ^oC	auxiliary reboiler duty (qar2)	616.7 kW
column C2 base level	50 %-level	column C3 feed flow rate	42 kgmole/hr
column C2 reflux drum level	50 %-level	column C2 product flow rate	121.0 kgmole/hr
column C2 boilup flow rates	385 kgmole/hr	R2 cold inlet flow rate	385 kgmole/hr
column C3 pressure	526.2 kPa	CR bypass flow rate	25 kgmole/hr
avg. C3-tray 1, 2, 3, and 4 temp.	313 ^oC	column C3 bottom flow rate	2.7 kgmole/hr
column C3 base level	50 %-level	column C3 reboiler duty (qr3)	559.7 kW
column C3 reflux drum level	50 %-level	toluene recycle flow rate	40.1 kgmole/hr
column C3 reflux flow rate	9.94 kgmole/hr	column C3 reflux flow rate	9.94 kgmole/hr

Table 6.3 Control structure and controller parameters for HDA process alternative 4 with two LSSs

controller	controlled variable	manipulated variable	type	K_C	τ_I [min]	controlled variable range
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	PI	0.1	0.1	0 - 300 kgmole/hr
PCG	gas recycle stream pressure	fresh feed hydrogen valve (V1)	PI	1.2	0.1	3447.38 - 4826.33 kPa
CCG	methane in gas recycle	purge valve (V4)	PI	0.2	15	0.4 - 0.7 mole-fraction
TCQ	quenched temperature	quench valve (V13)	PI	0.15	0.5	593.33 – 648.89 ^oC
TCR	reactor inlet temperature	furnace duty (qfur)	PI	0.05	1.0	593.33 – 648.89 ^oC
TCS	separator temperature	cooler duty (qcooler)	PI	0.154	0.1	30 – 100 ^oC
TCE1c	FEHE2 cold inlet temperature	FEHE1 bypass valve (VBP1)	PI	1	1	125 – 225 ^oC

Table 6.3 *Continued*

controller	controlled variable	manipulated variable	type	Kc	τ_I	range
TCE1h	cooler inlet temperature	FEHE1 bypass valve (VBP1)	PI	0.87	1.05	50 - 150 ^oC
LSS1	output of TCE1c and TCE1h	FEHE1 bypass valve (VBP1)	Min	-	-	-
TCE2c	furnace inlet temperature	FEHE2 bypass valve (VBP2	PI	1	2	475 –575 ^oC
TCE2h	FEHE2 hot outlet temperature	FEHE2 bypass valve (VBP2)	PI	1	0.7	250 –350 ^oC
LSS2	output of TCE2c and TCE2h	FEHE2 bypass valve (VBP2)	Min	-	-	-
TCR2c	heat exchanger R2 cold outlet temperature	R2 bypass valve (VBP3)	PI	15	1	130 –230 ^oC
LCS	separator liquid level	column C1 feed valve (V5)	P	2	-	0 – 100 %-level
PC1	column C1 pressure	column C1 gas valve (V6)	PI	1	10	689.48 - 1378.95 kPa
TC1	column C1 tray-6 temperature	column C1 reboiler duty (qr1)	PI	1	10	100 – 200 ^oC
LC11	column C1 base level	column C2 feed valve (V7)	P	2	-	0 – 100 %-level
LC12	column C1 reflux drum level	column C1 condenser duty (qc1)	P	1	-	0 – 100 %-level
PC2	column C2 pressure	column C2 condenser duty (qc2)	PI	1	10	137.89 - 275.79 kPa
TC2	column C2 tray-12 temperature	auxiliary reboiler duty (qar2)	PI	2	8	93.33 – 148.89 ^oC
LC21	column C2 base level	column C3 feed valve (V9)	P	2	-	0 – 100 %-level
LC22	column C2 reflux drum level	column C2 product valve (V8)	P	2	-	0 – 100 %-level
FCB	column C2 boilup flow rates	R2 cold inlet valve (V10)	PI	0.05	0.1	300 – 400 kgmole/hr
PC3	column C3 pressure	CR bypass valve (VBP4)	PI	30	20	344.74 – 689.46 kPa
AVG	avg. temp. of C3-tray 1, 2, 3, and 4	-	Avg	-	-	-
TC3	output of AVG	column C3 bottom valve (V12)	PI	0.2	30	250 – 350 ^oC
LC31	column C3 base level	column C3 reboiler duty (qr3)	P	3	-	0 – 100 %-level
LC32	column C3 reflux drum level	toluene recycle valve (V3)	P	2	-	0 – 100 %-level
FCR	column C3 reflux flow rates	column C3 reflux valve (V11)	PI	0.2	0.1	0 – 20 kgmole/hr
TCX1	FEHE2 hot inlet temperature	exchanger X1 duty (qx1)	PI	0.08	0.3	600 – 650 ^oC
TCX2	column C2 bottom temperature	exchanger X2 duty (qx2)	PI	0.05	1.0	125 – 175 ^oC

6.6 Application to Energy-Integrated HDA Process Alternative 4

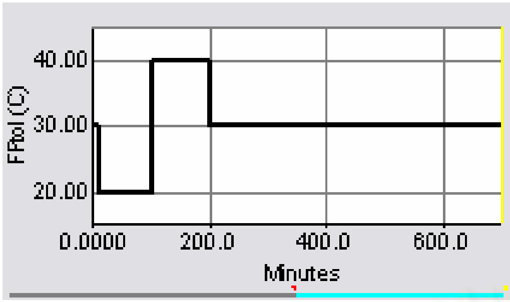
The new proposed heuristic design procedure for HEN control is used in conjunction with Luyben's procedure (Luyben et al., 1999) to design plantwide control structures of energy-integrated HDA process (i.e. alternative 4). The major loops are the same as those used in Luyben et al., (1999), but we have designed two LSSs in FEHE1 and FEHE2 in order for the resilient HEN.

The new plantwide control structure of HDA process alternative 4 with two LSSs is shown in Figure 6.8. The LSS1 and LSS2 are employed in FEHE1 and FEHE2, respectively. An auxiliary reboiler is installed at both steady state and dynamic condition in order to handle any imbalance in reboiling heat duties (AR2 in Figure 6.8). The duty of AR2 is manipulated to control the tray temperature (TC2) in the product column (column C2). The cold outlet temperature of heat exchanger R2 is controlled by manipulating valve on the bypass line (TCR2c). In the recycle column, the cold stream of condenser/reboiler (CR) is bypassed and manipulated to control its pressure column.

In HDA process alternative 4, in order to make the disturbance loads of the hot stream (i.e. stream H_1 in Figure 6.7) and of the cold stream from the bottoms of the product column (i.e. stream C_2 in Figure 6.7), two heat exchangers are artificially installed (see exchangers X1 and X2 in Figure 6.8). Note that, these exchangers are not used in the real plant. The temperature controllers TCX1 and TCX2 are set to be "off" whenever these are not used to make the disturbances. The initial values of all the controlled and manipulated variables are listed in Table 6.2. The control structure and controller parameters are given in Table 6.3. P controllers are employed for the level loops, and PI controllers for the remaining loops.

6.6.1 Dynamic Simulation Results

In order to illustrate the dynamic behaviors of the new control structure with 2 LSSs in HDA process alternative 4, several disturbance loads were made. Figures 6.9 to 6.12 show the dynamic responses of the control structure with 2 LSSs for the HDA process alternative 4. Results for individual disturbance load changes are as follows:



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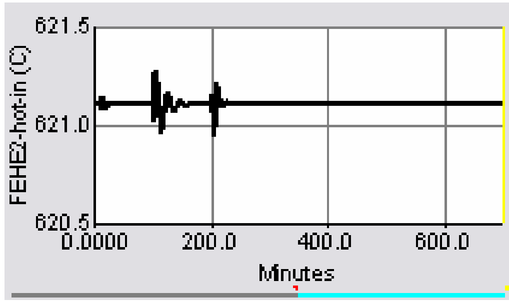

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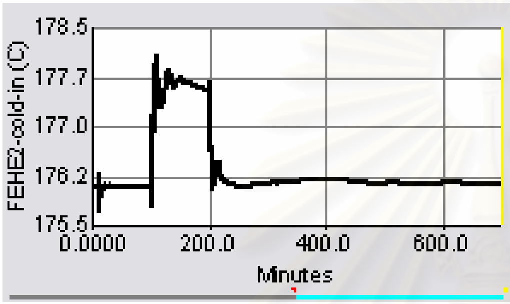

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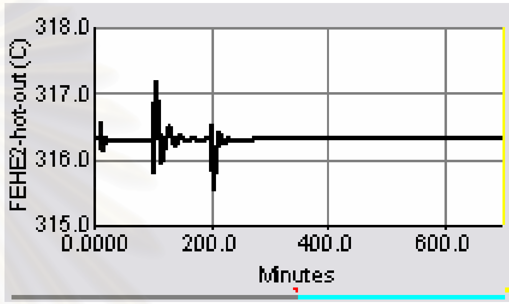

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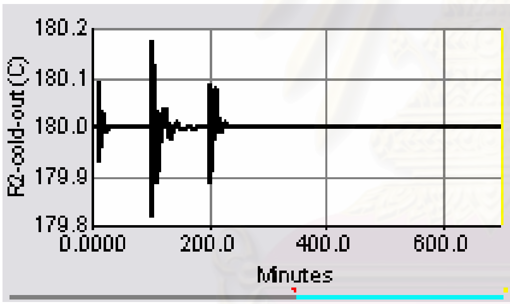

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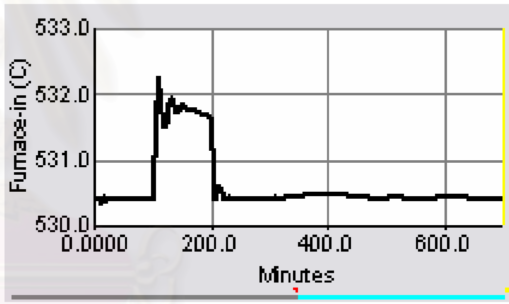
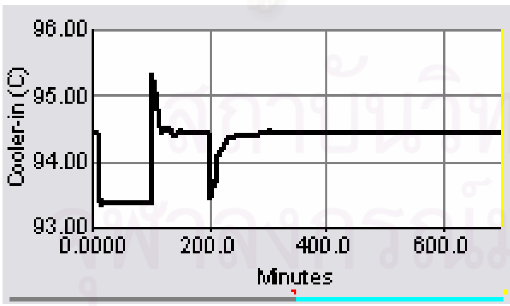
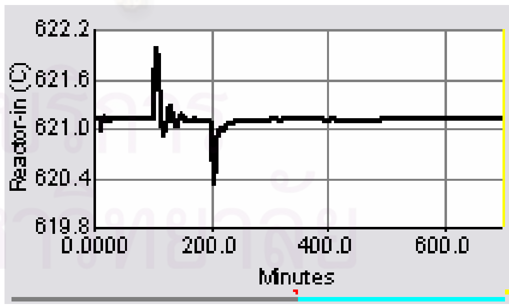


(f)

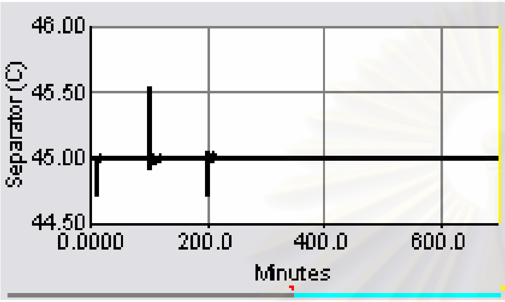


(g)



(h)

Figure 6.9 Dynamic responses of the HDA process alternative 4 with 2 LSSs to a change in the disturbance load of cold stream (reactor feed stream); where, (a) fresh feed toluene temperature, (b) FEHE2 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE2 hot outlet temperature, (e) R2 cold outlet temperature, (f) furnace inlet temperature, (g) cooler inlet temperature, (h) reactor inlet temperature, (i) separator temperature, (j) C1-tray temperature, (k) C2-tray temperature, (l) C3-tray temperature, (m) furnace duty, (n) cooler duty.



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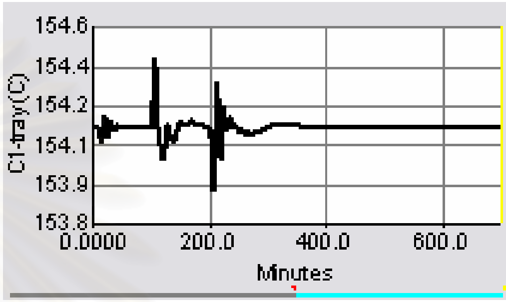

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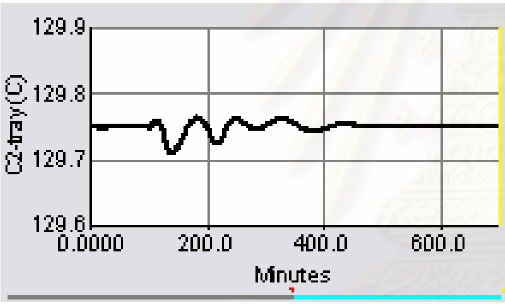

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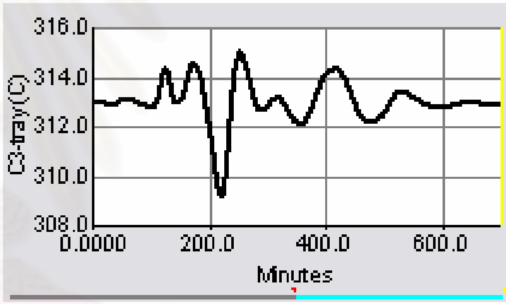

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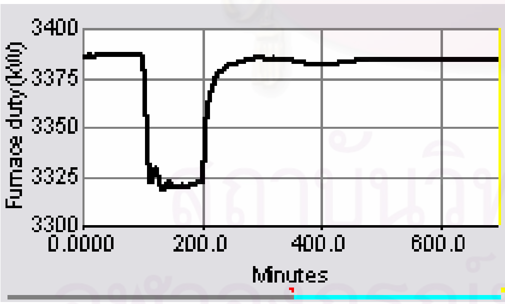
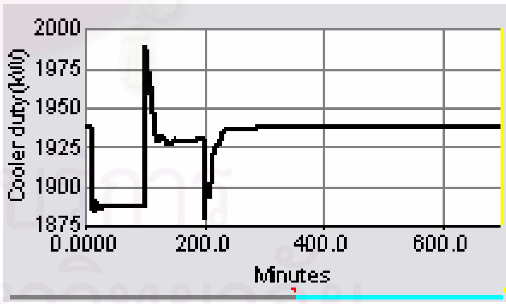


(m)



(n)

Figure 6.9 *Continued.*

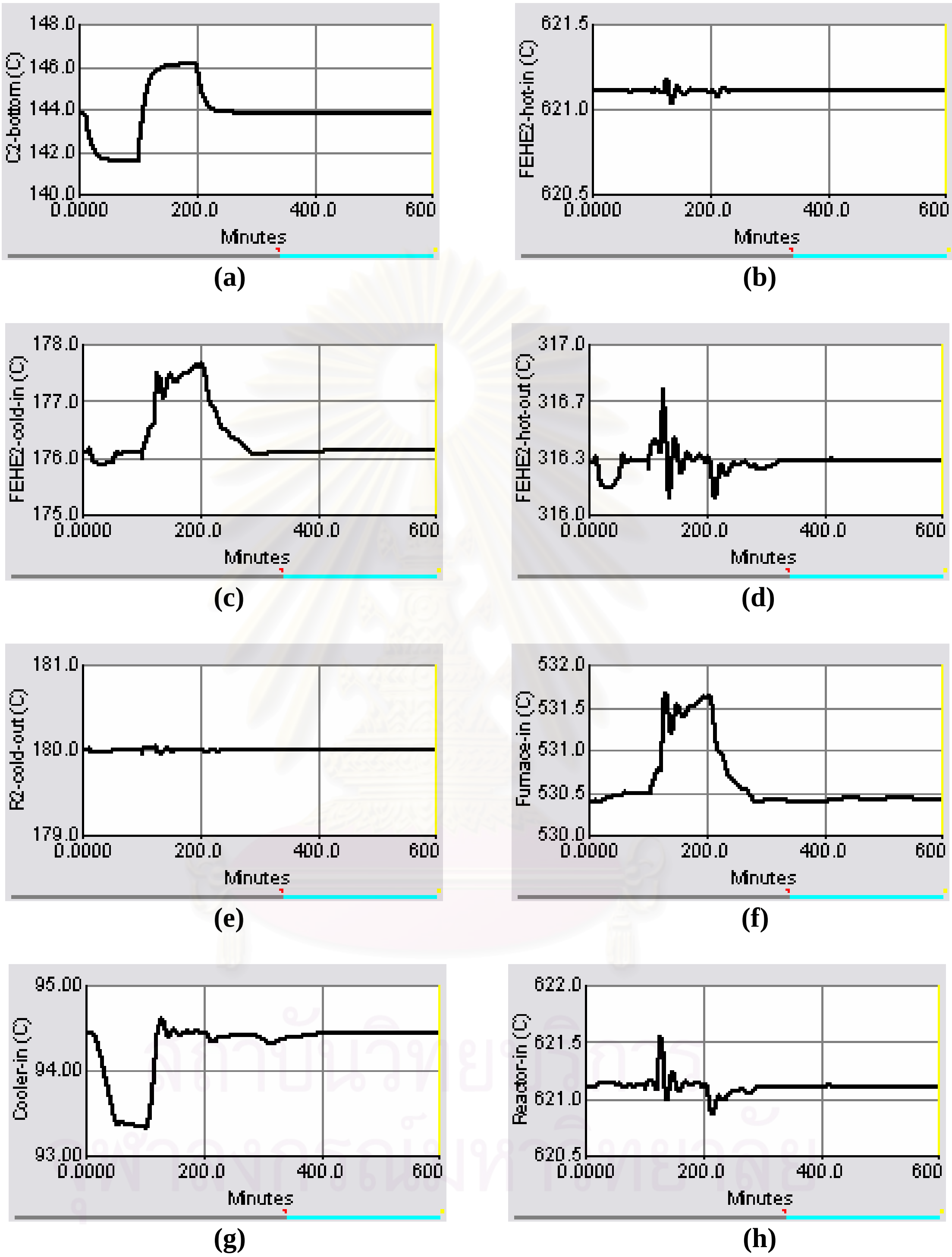
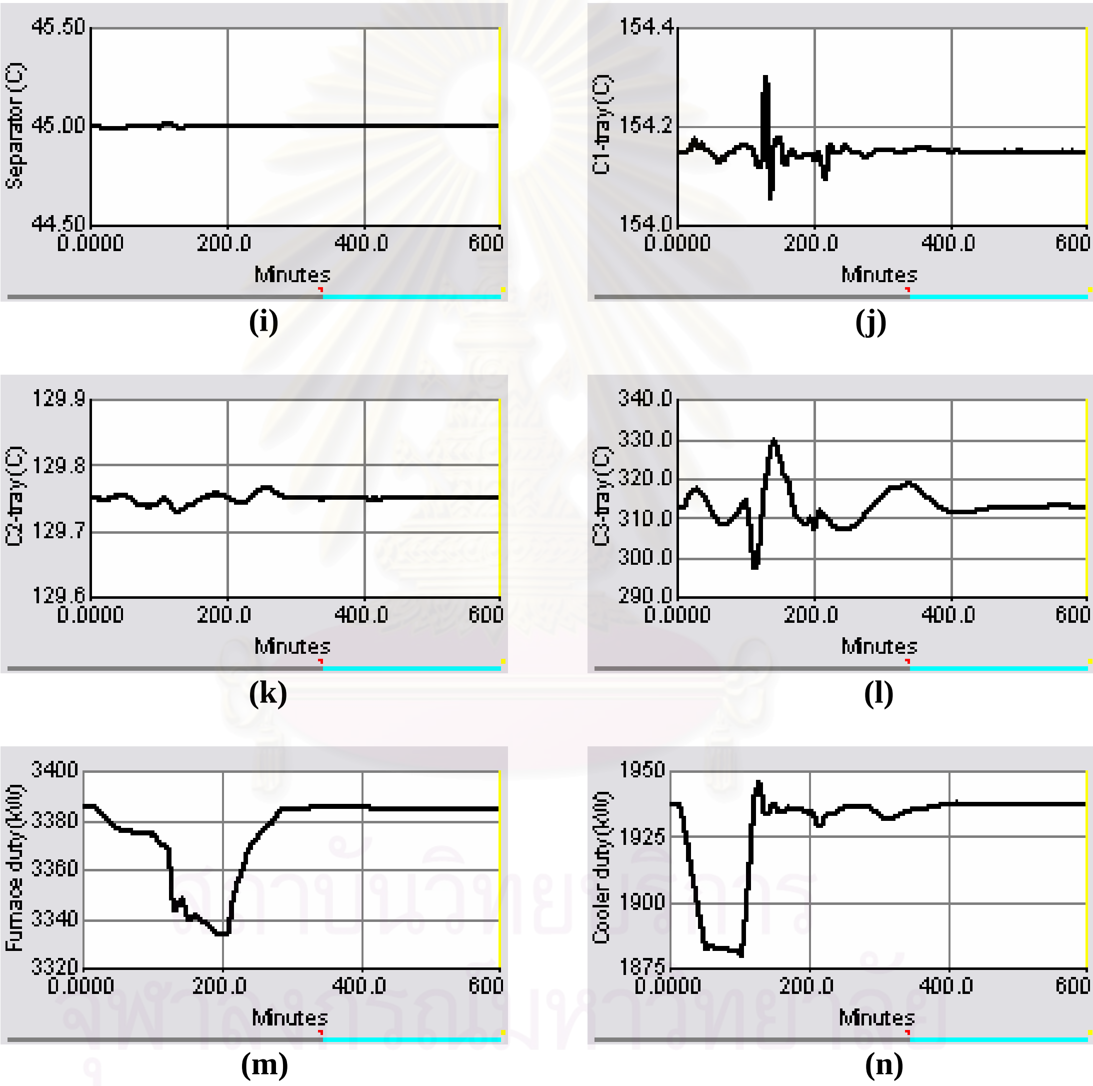


Figure 6.10 Dynamic responses of the HDA process alternative 4 with 2 LSSs to a change in the disturbance load of cold stream from the bottoms of product column C2; where, (a) C2-bottoms temperature, (b) FEHE2 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) FEHE2 hot outlet temperature, (e) R2 cold outlet temperature, (f) furnace inlet temperature, (g) cooler inlet temperature, (h) reactor inlet temperature, (i) separator temperature, (j) C1-tray temperature, (k) C2-tray temperature, (l) C3-tray temperature, (m) furnace duty, (n) cooler duty.



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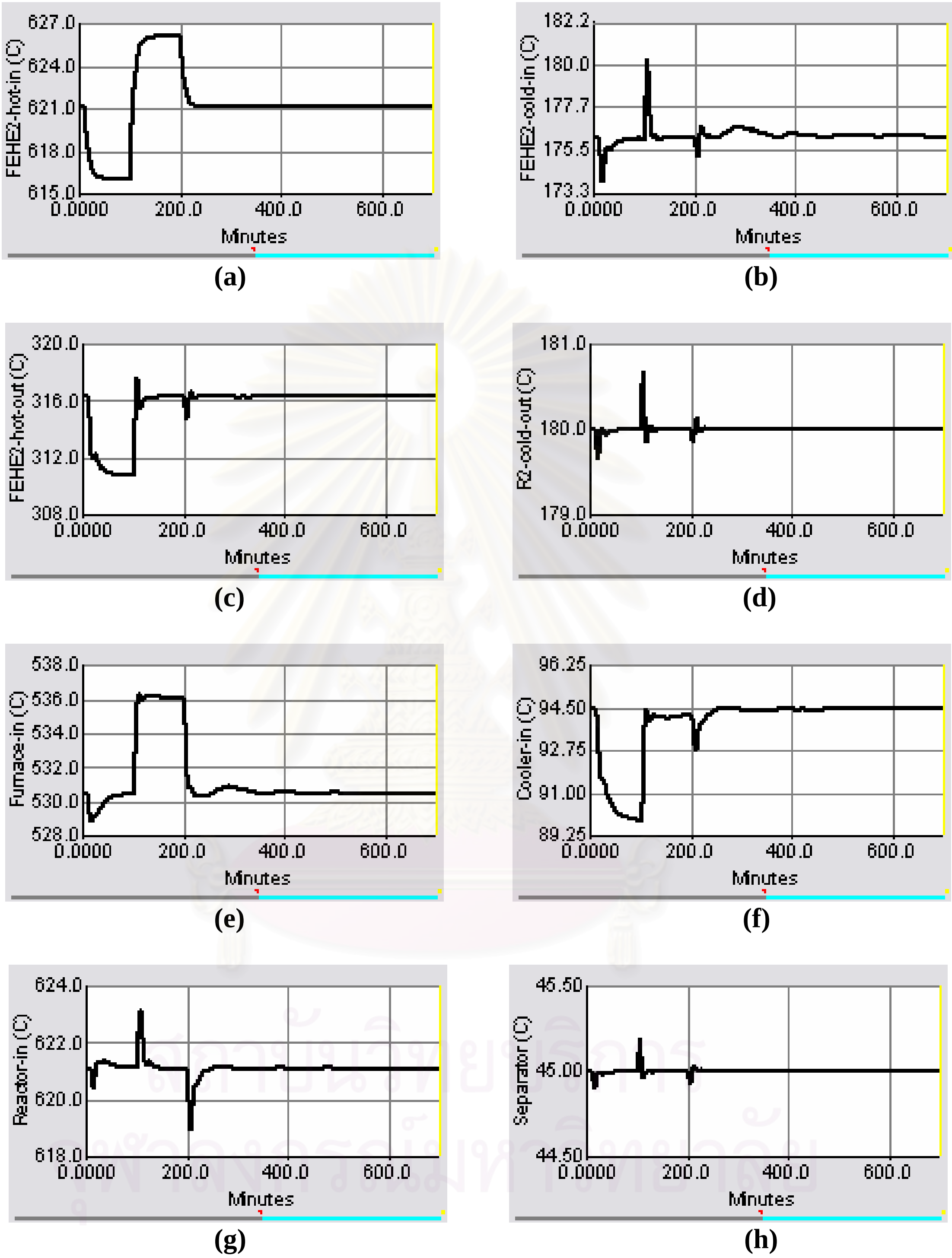
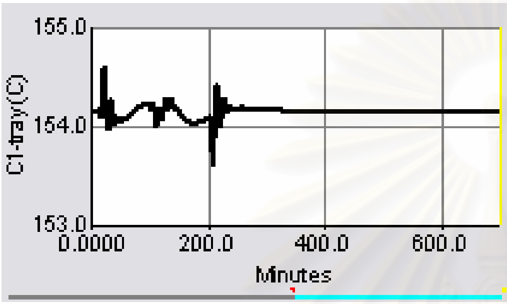


Figure 6.11 Dynamic responses of the HDA process alternative 4 with 2 LSSs to a change in the disturbance load of hot stream (reactor product stream); where, (a) FEHE2 hot inlet temperature, (b) FEHE2 cold inlet temperature, (c) FEHE2 hot outlet temperature, (d) R2 cold outlet temperature, (e) furnace inlet temperature, (f) cooler inlet temperature, (g) reactor inlet temperature, (h) separator temperature, (i) C1-tray temperature, (j) C2-tray temperature, (k) C3-tray temperature, (l) furnace duty, (m) cooler duty.



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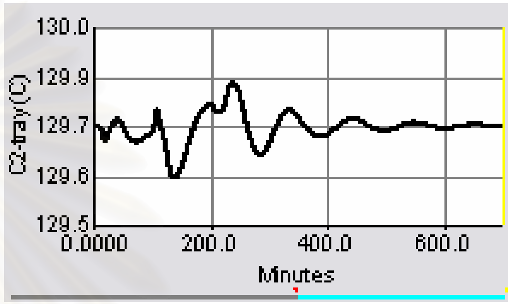

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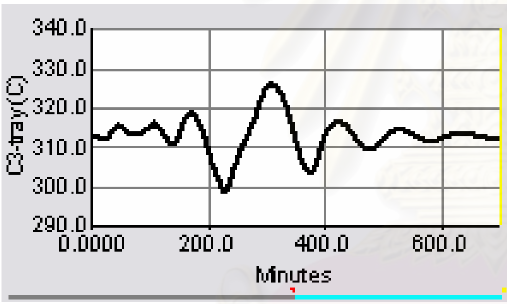

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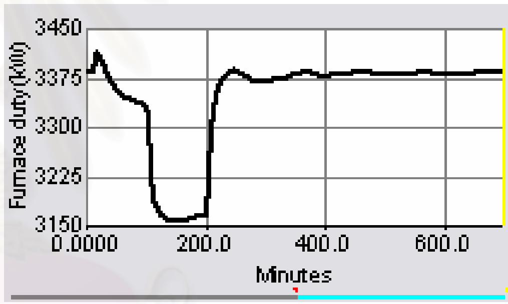

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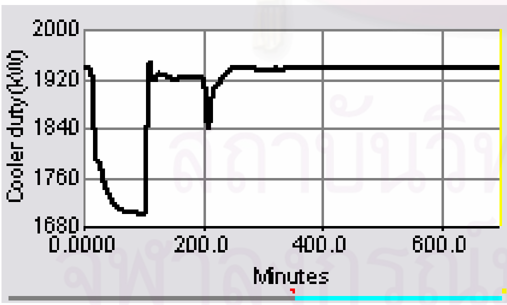


(m)

Figure 6.11 *Continued.*

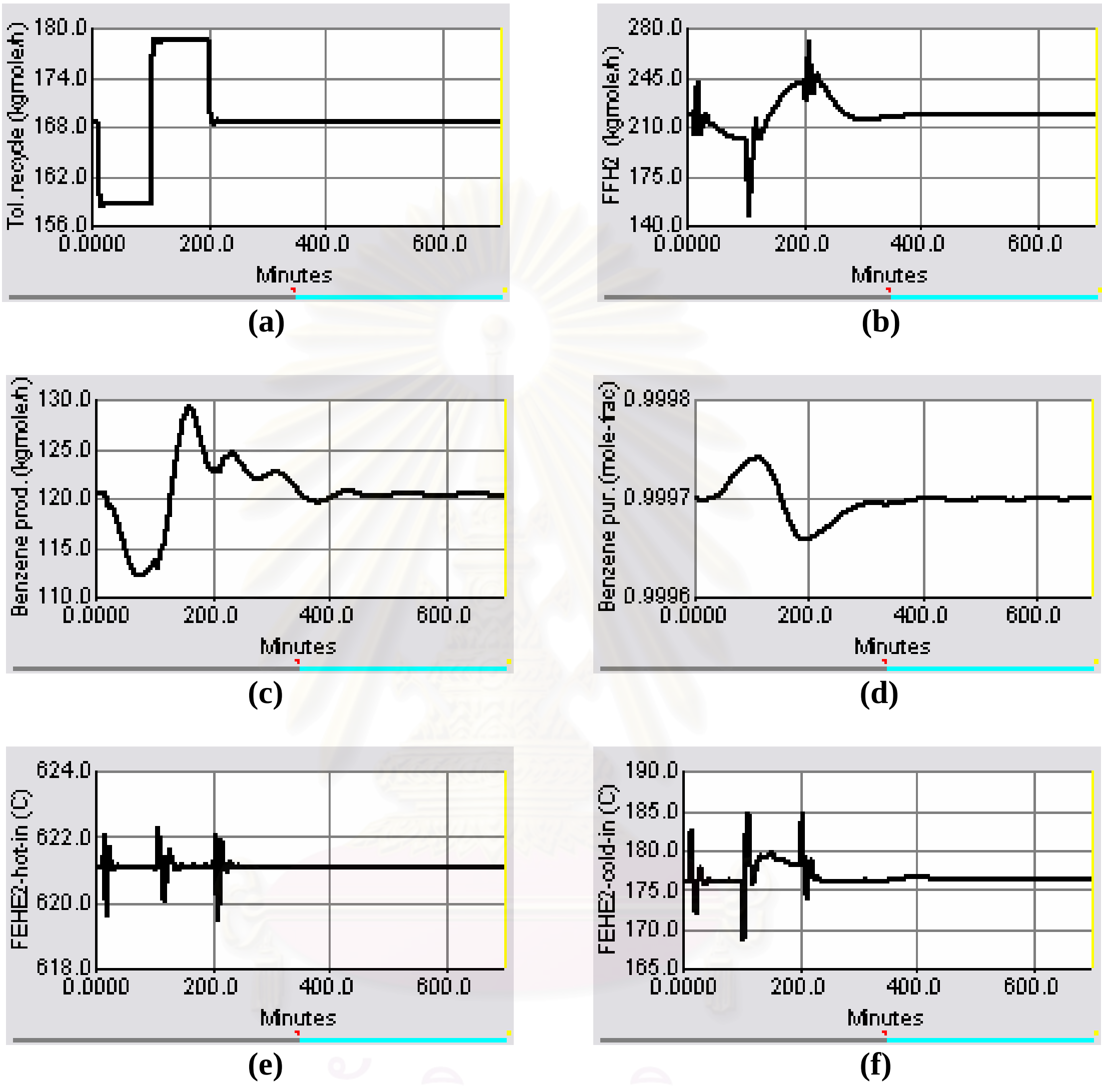


Figure 6.12 Dynamic responses of the HDA process alternative 4 with 2 LSSs to a change in the recycle toluene flowrates; where, (a) recycle toluene flowrates, (b) fresh feed hydrogen flowrates, (c) benzene product flowrates, (d) benzene purity in the product stream, (e) FEHE2 hot inlet temperature, (f) FEHE2 cold inlet temperature, (g) FEHE2 hot outlet temperature, (h) R2 cold outlet temperature, (i) furnace inlet temperature, (j) cooler inlet temperature, (k) reactor inlet temperature, (l) separator temperature, (m) C1-tray temperature, (n) C2-tray temperature, (o) C3-tray temperature, (p) furnace duty, (q) cooler duty.

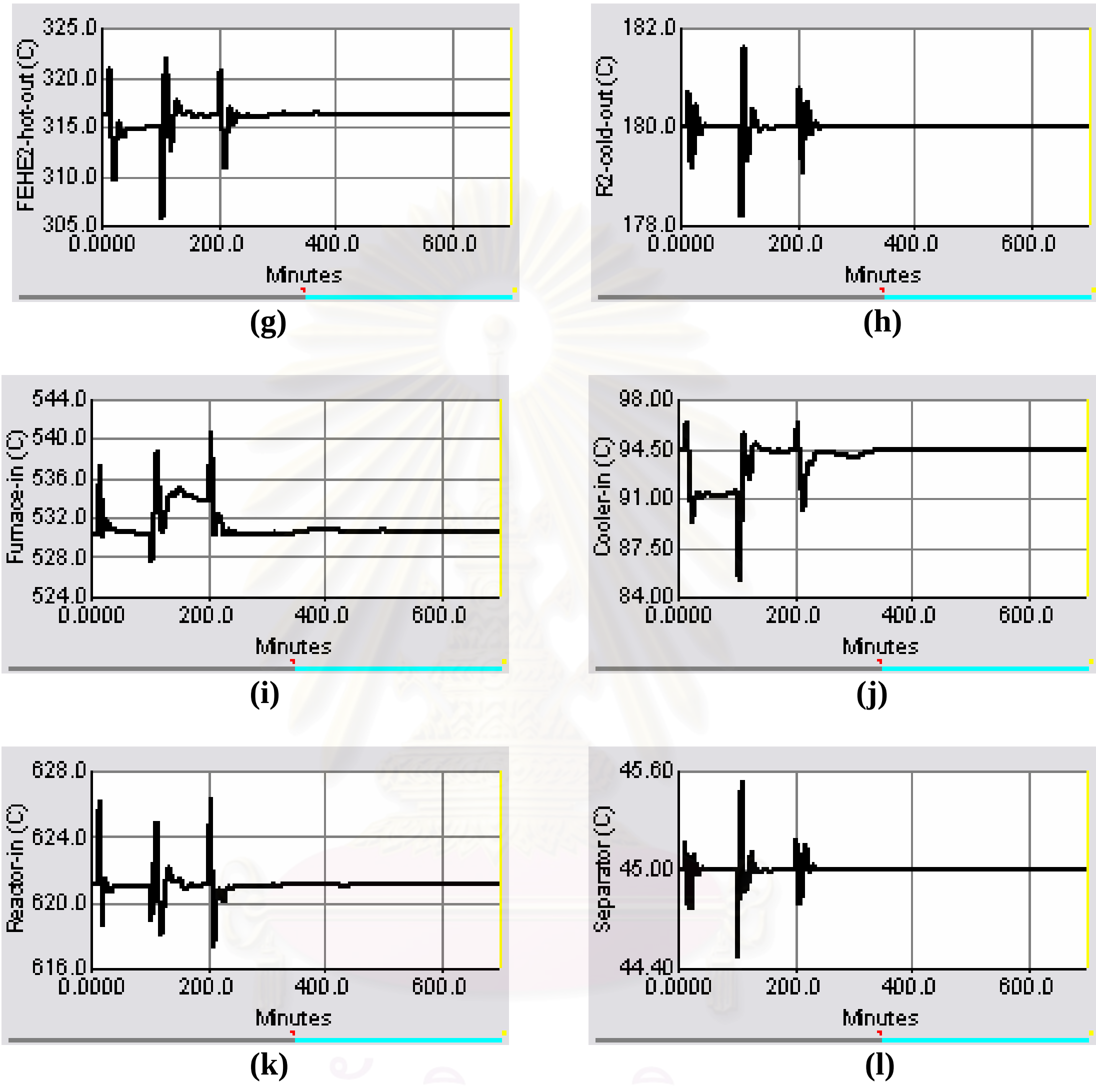
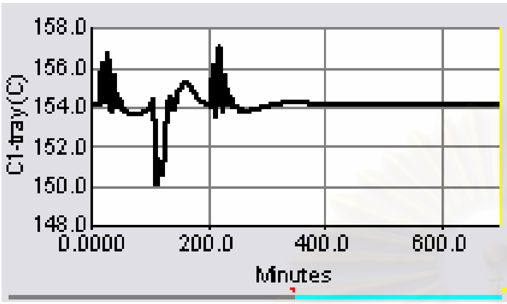


Figure 6.12 *Continued.*



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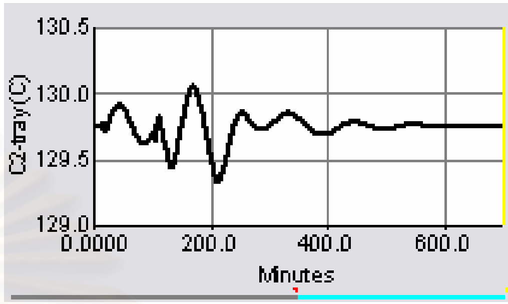

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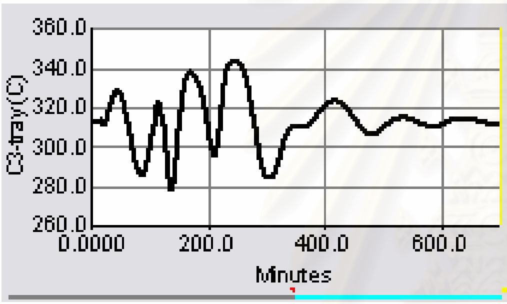

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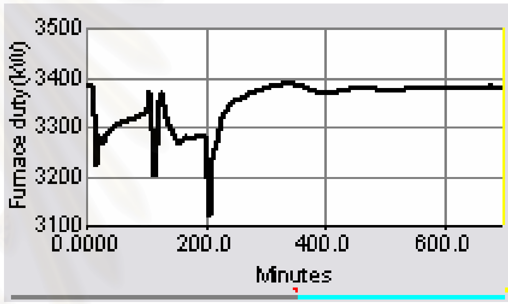


(p)

(q)

Figure 6.12 *Continued.*

6.6.1.1 Change in the heat load disturbance of cold stream

Figure 6.9 shows the dynamic responses of the control structure with 2 LSSs in the HDA process alternative 4 to a change in the heat load disturbance of cold stream (reactor feed stream). This disturbance is made as follows: first the fresh toluene feed temperature (stream FFtol in Figure 6.8) is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes (Figure 6.9.a).

Both the cold and hot outlet temperatures of FEHE1 decrease as the cold inlet temperature decreases, this is a desired condition for the hot stream, hence the LSS1 switches the control action from TCE1h to TCE1c to control the cold outlet temperature of FEHE1 at its minimum value of 176.1 ^{o}C (i.e. the cold inlet temperature of FEHE2 as shown in Figure 6.9.c). As a result, the hot outlet temperature of FEHE1 (i.e. the cooler inlet temperature) quickly drops to a new steady state value (Figure 6.9.g), and the cooler duty decreases (Figure 6.9.n).

When the cold inlet temperature of FEHE1 increases, first both the cold and hot outlet temperatures of FEHE1 increase, this is an MER choice, as expected the LSS1 switches the control action from TCE1c to TCE1h. As a result, the cooler inlet temperature drops to its nominal value (Figure 6.9.g). Therefore it is understandable that why the furnace duty decreases significantly (Figure 6.9.m), since the furnace inlet temperature increases (Figure 6.9.f).

The hot outlet temperature of FEHE2 (Figure 6.9.d), the cold outlet temperature of heat exchanger R2 (Figure 6.9.e) and the tray temperatures in the stabilizer and product columns (Figure 6.9.j and 14.k) are slightly well controlled. But the tray temperature in recycle column has the maximum deviation of about 4 ^{o}C and it takes over 600 minutes to return to its set point (Figure 6.9.l).

6.6.1.2 Change in the heat load disturbance of cold stream from the bottoms of product column

Figure 6.10 shows the dynamic responses of the control structure with 2 LSSs in the HDA process alternative 4 to a change in the heat load disturbance of cold stream from the bottoms of product column (C2). This disturbance is made as follows: first the set point of C2-bottom temperature controller (i.e. TCX2 in Figure 6.8) is decreased from 144.0 to 141.9 ^{o}C at time equals 10 minutes, the temperature is increased from 141.9 to 146.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 144.0 ^{o}C at time equals 200 minutes (Figure 6.10.a). As can be seen, the temperature response in the bottoms of product column is somewhat fast (Figure 6.10.a).

When C2-bottom temperature decreases (Figure 6.10.a), the hot inlet temperature of FEHE1 decreases, thus the LSS1 will take a control action to maintain the cold inlet temperature of FEHE2 (Figure 6.10.c), and allows the cooler inlet temperature to drop to a new steady state value (Figure 6.10.g). Thus, it will result in decrease of the cooler duty (Figure 6.10.n). On the other hand, when C2-bottom temperature increases (Figure 6.10.a), as expected the LSS1 switches the control action from TCE1c to TCE1h to maintain the cooler inlet temperature (Figure 6.10.g) at its nominal value. Therefore, the furnace duty decreases (Figure 6.10.m), since the furnace inlet temperature increases (Figure 6.10.f).

6.6.1.3 Change in the heat load disturbance of hot stream

Figure 6.11 shows the dynamic responses of the control structure with 2 LSSs in the HDA process alternative 4 to a change in the heat load disturbance of hot stream (the hot reactor product). This disturbance is made as follows: first the set point of FEHE2-hot-inlet temperature controller (i.e. TCX1 in Figure 6.8) is decreased from 621.1 to 616.1 ^{o}C at time equals 10 minutes, and the temperature is increased from 616.1 to 626.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 621.1 ^{o}C at time equals 200 minutes (Figure 6.11.a). As can be seen, this temperature response is very fast, the new steady state is reached quickly (Figure 6.11.a).

When the hot inlet temperature of FEHE2 decreases (Figure 6.11.a), it will result in decrease of the furnace inlet temperature. Thus, the LSS2 switches the control action from TCE2h to TCE2c to control the furnace inlet temperature at its minimum value of 530.4 ^{o}C (Figure 6.11.e) and allows the hot outlet temperature of

FEHE2 to drop to a new steady state value (Figure 6.11.c). As expected, the LSS1 will take the control action to maintain the cold inlet temperature of FEHE2 (Figure 6.11.b), and the cooler inlet temperature is allowed to drop to a new steady state value (Figure 6.11.f). Hence the cooler duty is significantly decreased (Figure 6.11.m).

When the hot inlet temperature of FEHE2 increases (Figure 6.11.a), the LSS2 switches the control action from TCE2c to TCE2h to control the hot outlet temperature of FEHE2 at its set point (Figure 6.11.c). The furnace inlet temperature will be further increased (Figure 6.11.e). Therefore, the furnace duty is significantly decreased (Figure 6.11.l).

6.6.1.4 Change in the recycle toluene flowrates

Figure 6.12 shows the dynamic responses of the control structure with 2 LSSs in the HDA process alternative 4 to a change in the recycle toluene flowrates from 168.6 to 158.6 kgmole/h at time equals 10 minutes, and the flowrates is increased from 158.6 to 178.6 kgmole/h at time equals 100 minutes, then its flowrates is returned to its nominal value of 168.6 at time equals 200 minutes (Figure 6.12.a). The recycle toluene flowrates response is very fast; the new steady state is reached very quickly.

As can be seen that the drop in toluene feed flowrates reduces the reaction rate, so the benzene product flowrates drops (Figure 6.12.c), and the benzene product quality increases (Figure 6.12.d) and vice versa. The tray temperature in the recycle column has a large deviation (Figure 6.12.o), and it takes over 600 minutes to slowly return to its nominal value of 313 ^{o}C. The furnace and cooler duties could be maintained below its nominal values (Figure 6.12.p and Figure 6.12.q).

6.6.2 Evaluation of the Dynamic Performances

As discussed in chapter 5, the Integral Absolute Error (IAE) is used for evaluation of the dynamic performances of the designed control structure. The IAE results of some temperature controllers for the control structures with one LSS and two LSSs in HDA alternative 4 are summarized in Tables 6.4 to 6.6.

In general, the implementation of two LSSs in HDA process alternative 4 makes the control configuration to be resilient i.e. the control system can handle any disturbance loads from the cold and hot streams. The control system with two LSSs is less effective than the control system with one LSS, since the values of IAE in the control system with two LSSs are larger than those in the control system with one LSS (see Tables 6.4 to 6.6). Nevertheless, the new control system with two LSSs is considered to be a resilient control configuration, since any disturbances from both the cold and hot streams can be managed which resulting in decrease of both the furnace and cooler utility duties.

Table 6.4 The IAE results of the control system in HDA process alternative 4 to a change in the disturbance load of cold stream (reactor feed stream)

Controller	Integral Absolute Error (IAE) in HDA process alternative 4	
	Control structure with one LSS	Control structure with two LSSs
TC1	6.3750	9.3162
TC2	1.6733	3.4558
TC3	182.9202	381.0301
TCE1c	15.1917	33.5507
TCE1h	67.3376	28.0869
TCE2c	-	21.9159
TCE2h	6.4417	17.2022
TCR2c	-	2.6282
TCQ	2.9611	3.7298
TCR	3.2800	20.9138
TCS	1.6626	1.7003
Total	287.8432	523.5299

Table 6.5 The IAE results of the control system in HDA process alternative 4 to a change in the disturbance load of hot stream (reactor product stream)

Controller	Integral Absolute Error (IAE) in HDA process alternative 4	
	Control structure with one LSS	Control structure with two LSSs
TC1	4.6492	22.6542
TC2	2.5758	17.687
TC3	265.9116	627.7638
TCE1c	16.1302	127.5529
TCE1h	34.6220	81.1439
TCE2c	-	127.2974
TCE2h	9.4564	45.3053
TCR2c	-	9.0711
TCQ	2.5347	8.8298
TCR	6.0488	71.4772
TCS	0.4252	2.8552
Total	342.3539	1141.6378

Table 6.6 The IAE results of the control system in HDA process alternative 4 to a change in the recycle toluene flowrates

Controller	Integral Absolute Error (IAE) in HDA process alternative 4	
	Control structure with one LSS	Control structure with two LSSs
TC1	196.0117	201.0637
TC2	17.3762	46.5757
TC3	5809.8166	6335.56
TCE1c	123.8851	230.8836
TCE1h	238.0049	162.8827
TCE2c	-	214.6227
TCE2h	58.8839	183.6644
TCR2c	-	36.8377
TCQ	47.6075	43.7532
TCR	24.3897	155.8172
TCS	5.5640	10.4255
Total	6521.5396	7622.0864

6.7 Application to Energy-Integrated HDA Process Alternative 6

The new plantwide control structure of HDA process alternative 6 with three LSSs is shown in Figure 6.13. The LSS1, LSS2, and LSS3 are employed in FEHE1, FEHE2, and FEHE3, respectively. Auxiliary reboilers are installed in the stabilizer and product columns at both steady state and dynamic condition in order to handle any imbalance in reboiling heat duties (AR1 and AR2). The duties of AR1 and AR2 are manipulated to control the tray temperatures in the stabilizer and product columns, respectively (TC1 and TC2). The cold outlet temperatures of heat exchangers R1 and R2 are controlled by manipulating valves on the bypass lines (TCR1c and TCR2c). In the recycle column, the cold stream of condenser/reboiler (CR) is bypassed and manipulated to control its pressure column.

In order to make the disturbance loads of the hot stream (i.e. stream H_1 in Figure 6.7) and of the cold streams from the bottoms of the three columns (i.e. streams C_2, C_3, and C_4 in Figure 6.7), four heat exchangers are artificially installed (see exchangers X1, X2, X3, and X4 in Figure 6.13). Note that, these exchangers are not used in the real plant. The temperature controllers TCX1, TCX2, TCX3, and TCX4 are set to be “off” whenever these are not used to make the disturbances. The initial values of all the controlled and manipulated variables are listed in Table 6.7. The control structure and controller parameters are given in Table 6.8. P controllers are employed for the level loops, and PI controllers for the remaining loops.

Three LSSs are employed in FEHE1, FEHE2 and FEHE3

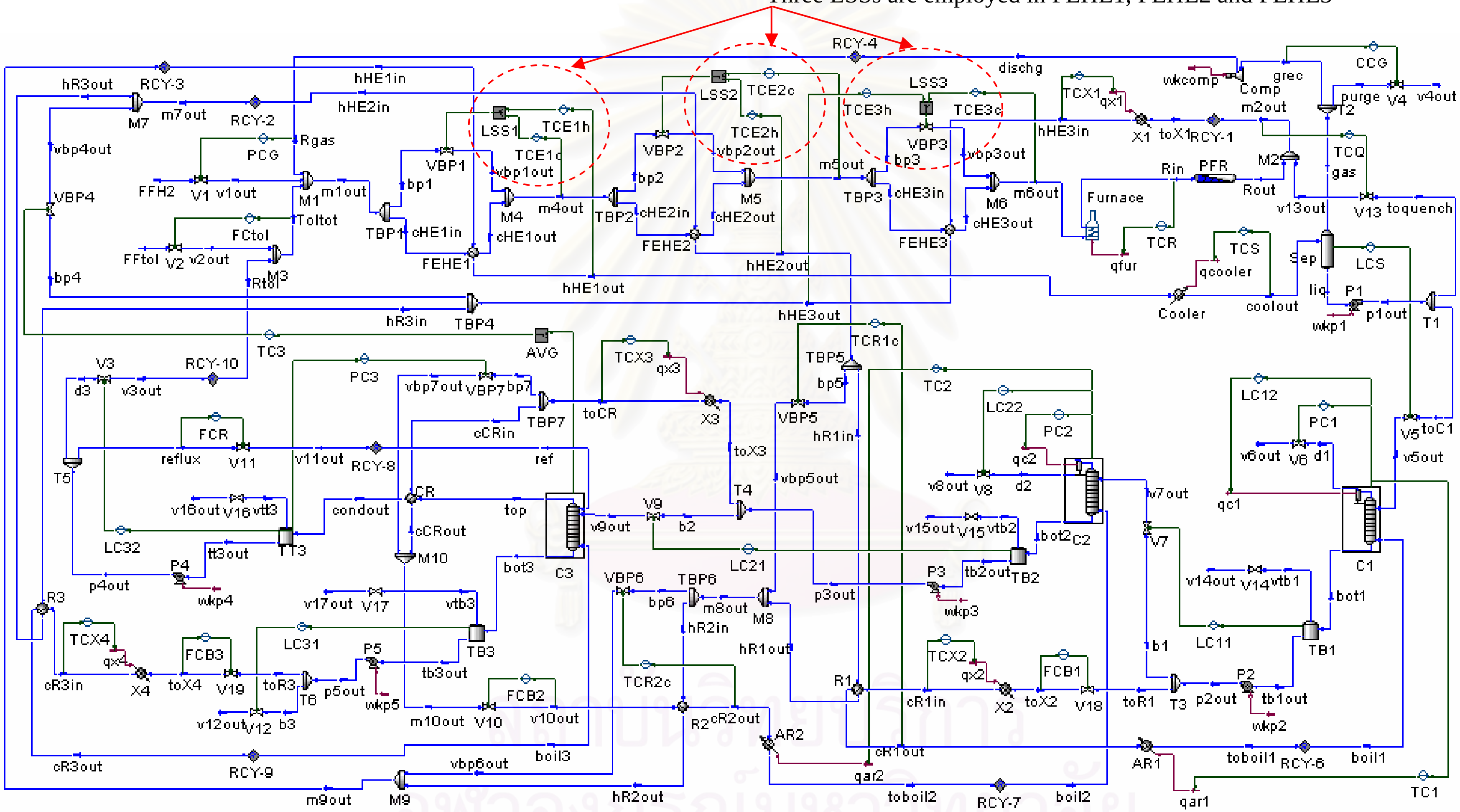


Figure 6.13 Plantwide control structure of the HDA process alternative 6 with 3 LSSs

Table 6.7 The initial values of controlled and manipulated variables for HDA process alternative 6 with 3 LSSs

controlled variable		manipulated variable	
process variable	initial value	process variable	initial value
total toluene flow rate	168.4 kgmole/hr	fresh toluene feed flow rate	129 kgmole/hr
gas recycle stream pressure	4171 kPa	fresh hydrogen feed flow rate	220 kgmole/hr
methane in gas recycle	0.5876 mole-frac	purge flow rate	217.4 kgmole/hr
quenched temperature	621.1 ^oC	quench flow rate	49 kgmole/hr
reactor inlet temperature	621.1 ^oC	furnace duty (qfur)	4585 kW
separator temperature	45 ^oC	cooler duty (qcooler)	1483 kW
FEHE2 cold inlet temperature	165 ^oC	FEHE1 bypass flow rate	117.3 kgmole/hr
cooler inlet temperature	84.4 ^oC	FEHE1 bypass flow rate	117.3 kgmole/hr
FEHE3 cold inlet temperature	295.5 ^oC	FEHE2 bypass flow rate	203.2 kgmole/hr
FEHE2 hot outlet temperature	327 ^oC	FEHE2 bypass flow rate	203.2 kgmole/hr
furnace inlet temperature	496.6 ^oC	FEHE3 bypass flow rate	138.0 kgmole/hr
FEHE3 hot outlet temperature	450 ^oC	FEHE3 bypass flow rate	109.8 kgmole/hr
R1 cold outlet temperature	200 ^oC	R1 bypass flow rate	561.0 kgmole/hr
R2 cold outlet temperature	180 ^oC	R2 bypass flow rate	139.7 kgmole/hr
separator liquid level	50 %-level	column C1 feed flow rate	171.4 kgmole/hr
column C1 pressure	1034 kPa	column C1 gas flow rate	8.7 kgmole/hr
column C1 tray-6 temperature	166.5 ^oC	auxiliary reboiler AR1 duty (qar1)	278.3 kW
column C1 base level	50 %-level	column C2 feed flow rate	162.7 kgmole/hr
column C1 reflux drum level	50 %-level	column C1 condenser duty (qc1)	368.8 kW
column C1 boil up flowrate	183 kgmole/hr	cold-inlet flow rate of R1	183 kgmole/hr
column C2 pressure	206.8 kPa	column C2 condenser duty (qc2)	4986 kW
column C2 tray-12 temperature	129.65 ^oC	auxiliary reboiler AR2 duty (qar2)	649.2 kW
column C2 base level	50 %-level	column C3 feed flow rate	42.2 kgmole/hr
column C2 reflux drum level	50 %-level	column C2 product flow rate	120.4 kgmole/hr
column C2 boil up flowrate	385 kgmole/hr	R2 cold-inlet flow rate	385 kgmole/hr
column C3 pressure	526.2 kPa	CR bypass flow rate	35.02 kgmole/hr
avg. C3-tray 1, 2, 3, and 4 temp.	326.7 ^oC	R3 bypass flow rate	135.4 kgmole/hr
column C3 base level	50 %-level	column C3 bottom flow rate	2.64 kgmole/hr
column C3 reflux drum level	50 %-level	toluene recycle flow rate	39.6 kgmole/hr
column C3 boil up flowrate	47.26 kgmole/hr	R3 cold-inlet flow rate	47.26 kgmole/hr
column C3 reflux flow rate	9.94 kgmole/hr	column C3 reflux flow rate	9.94 kgmole/hr

Table 6.8 Control structure and controller parameters for HDA process alternative 6 with 3 LSSs

controller	controlled variable	manipulated variable	type	K_C	τ_I [min]	controlled variable Range
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	PI	0.01	0.1	0 - 300 kgmole/hr
PCG	gas recycle stream pressure	fresh feed hydrogen valve (V1)	PI	1.2	0.1	3792.1 – 4481.6 kPa
CCG	methane in gas recycle	purge valve (V4)	PI	0.2	15	0.4 - 0.7 mole-fraction
TCQ	quenched temperature	quench valve (V13)	PI	0.15	0.5	593.33 - 648.89 ^oC
TCR	reactor inlet temperature	furnace duty (qfur)	PI	0.0887	0.1	593.33 - 648.89 ^oC
TCS	separator temperature	cooler duty (qcooler)	PI	0.154	0.1	30 - 100 ^oC
TCE1c	FEHE2 cold inlet temperature	FEHE1 bypass valve (VBP1)	PI	1	1	100 – 200 ^oC
TCE1h	cooler inlet temperature	FEHE1 bypass valve (VBP1)	PI	1	2	30 - 130 ^oC
LSS1	output of TCE1c and TCE1h	FEHE1 bypass valve (VBP1)	Min	-	-	-

Table 6.8*Continued*.

controller	controlled variable	manipulated variable	type	K_C	τ_I	range
TCE2c	FEHE3 cold inlet temperature	FEHE2 bypass valve (VBP2)	PI	1	1	250 – 350 ^oC
TCE2h	FEHE2 hot-outlet temperature	FEHE2 bypass valve (VBP2)	PI	1	2	275 - 375 ^oC
LSS2	output of TCE2c and TCE2h	FEHE2 bypass valve (VBP2)	Min	-	-	-
TCE3c	furnace inlet tepmerature	FEHE3 bypass valve (VBP3)	PI	1	1	450 - 550 ^oC
TCE3h	FEHE3 hot-outlet temperature	FEHE3 bypass valve (VBP3)	PI	1	2	400 - 500 ^oC
LSS3	output of TCE3c and TCE3h	FEHE3 bypass valve (VBP3)	Min	-	-	-
TCR1c	R1 cold outlet temperarure	R1 bypass valve (VBP5)	PI	15	1	150 – 250 ^oC
TCR2c	R2 cold outlet temperature	R2 bypass valve (VBP6)	PI	15	1	130 – 230 ^oC
LCS	separator liquid level	column C1 feed valve (V5)	P	2	-	0 - 100 %-level
PC1	column C1 pressure	column C1 gas valve (V6)	PI	0.1	10	689.48 - 1378.95 kPa
TC1	column C1 tray-6 temperature	AR1 duty (qar1)	PI	1	10	100 - 200 ^oC
LC11	column C1 base level	column C2 feed valve (V7)	P	2	-	0 - 100 %-level
LC12	column C1 reflux drum level	column C1 condenser duty (qc1)	P	1	-	0 - 100 %-level
FCB1	column C1 boil up flowrate	cold-inlet valve of R1 (V18)	PI	0.2	0.1	130 - 230 kgmole/hr
PC2	column C2 pressure	column C2 condenser duty (qc2)	PI	1	10	137.89 - 275.79 kPa
TC2	column C2 tray-12 temperature	AR2 duty (qar2)	PI	2	8	93.33 - 148.89 ^oC
LC21	column C2 base level	column C2 feed valve (V9)	P	2	-	0 - 100 %-level
LC22	column C2 reflux drum level	column C2 product valve (V8)	P	2	-	0 - 100 %-level
FCB2	column C2 boil up flowrate	R2 cold-inlet valve (V10)	PI	0.2	0.1	300 - 400 kgmole/hr
PC3	column C3 pressure	CR bypass valve (VBP7)	PI	10	20	344.74 - 689.48 kPa
AVG	avg. temp. of C3-tray 1, 2, 3, and 4	-	Avg	-	-	-
TC3	output of AVG	R3 bypass valve (VBP4)	PI	1	2	275 - 375 ^oC
LC31	column C3 base level	column C3 bottom valve (V12)	P	2	-	0 - 100 %-level
LC32	column C3 reflux drum level	toluene recycle valve (V3)	P	2	-	0 - 100 %-level
FCB3	column C3 boil up flowrate	R3 cold-inlet valve (V19)	PI	0.2	0.1	20 - 80 kgmole/hr
FCR	column C3 reflux flow rate	column C3 reflux valve (V11)	PI	0.2	0.1	0 - 20 kgmole/hr
TCX1	FEHE1 hot inlet temperature	exchanger X1 duty (qx1)	PI	0.08	0.3	600 – 650 ^oC
TCX2	column C1 bottoms temperature	exchanger X2 duty (qx2)	PI	0.08	1.0	165 – 215 ^oC
TCX3	column C2 bottoms temperature	exchanger X3 duty (qx3)	PI	0.05	1.2	125 – 175 ^oC
TCX4	column C3 bottoms temperature	exchanger X4 duty (qx4)	PI	0.01	2.0	325 – 375 ^oC

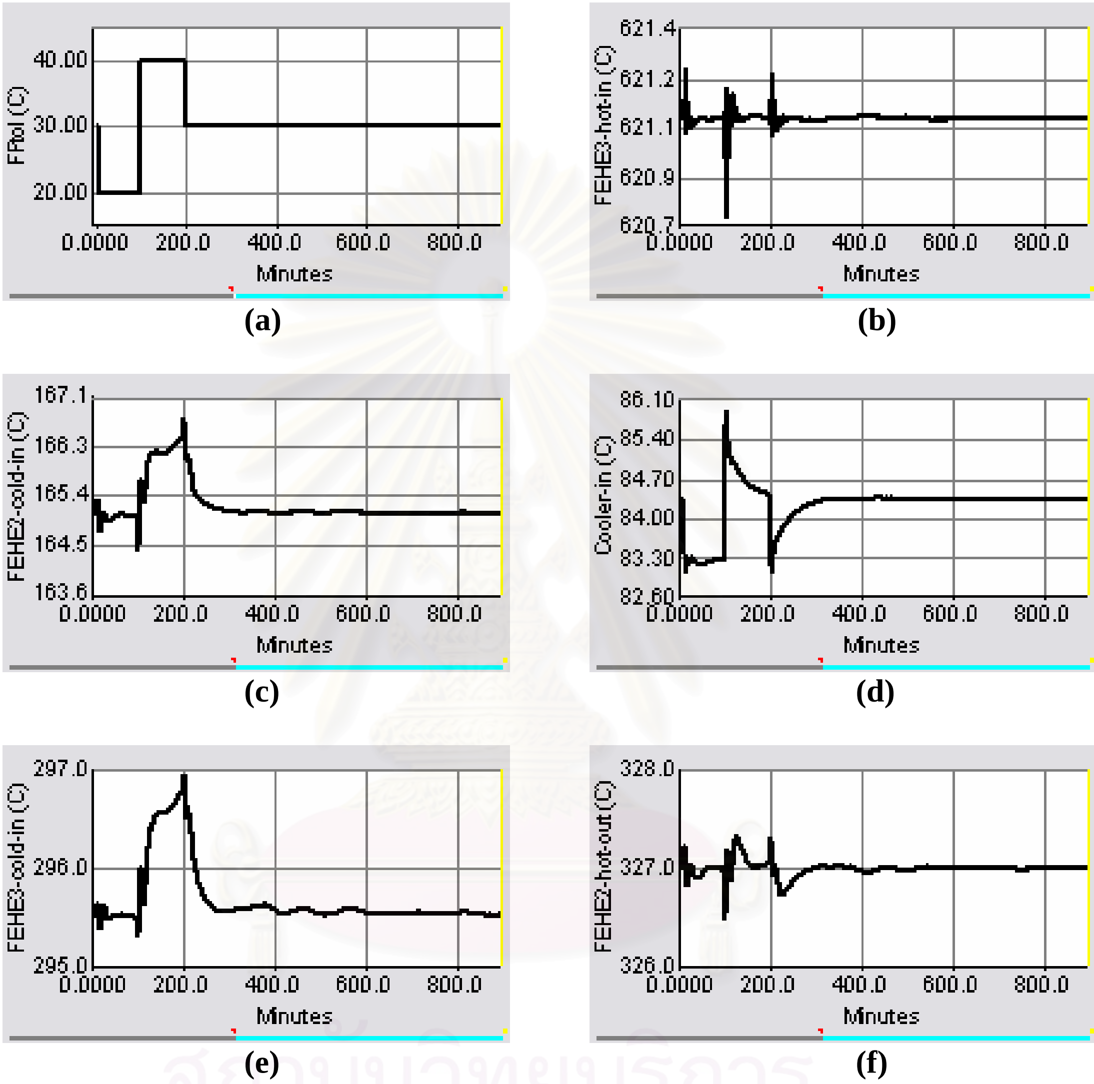
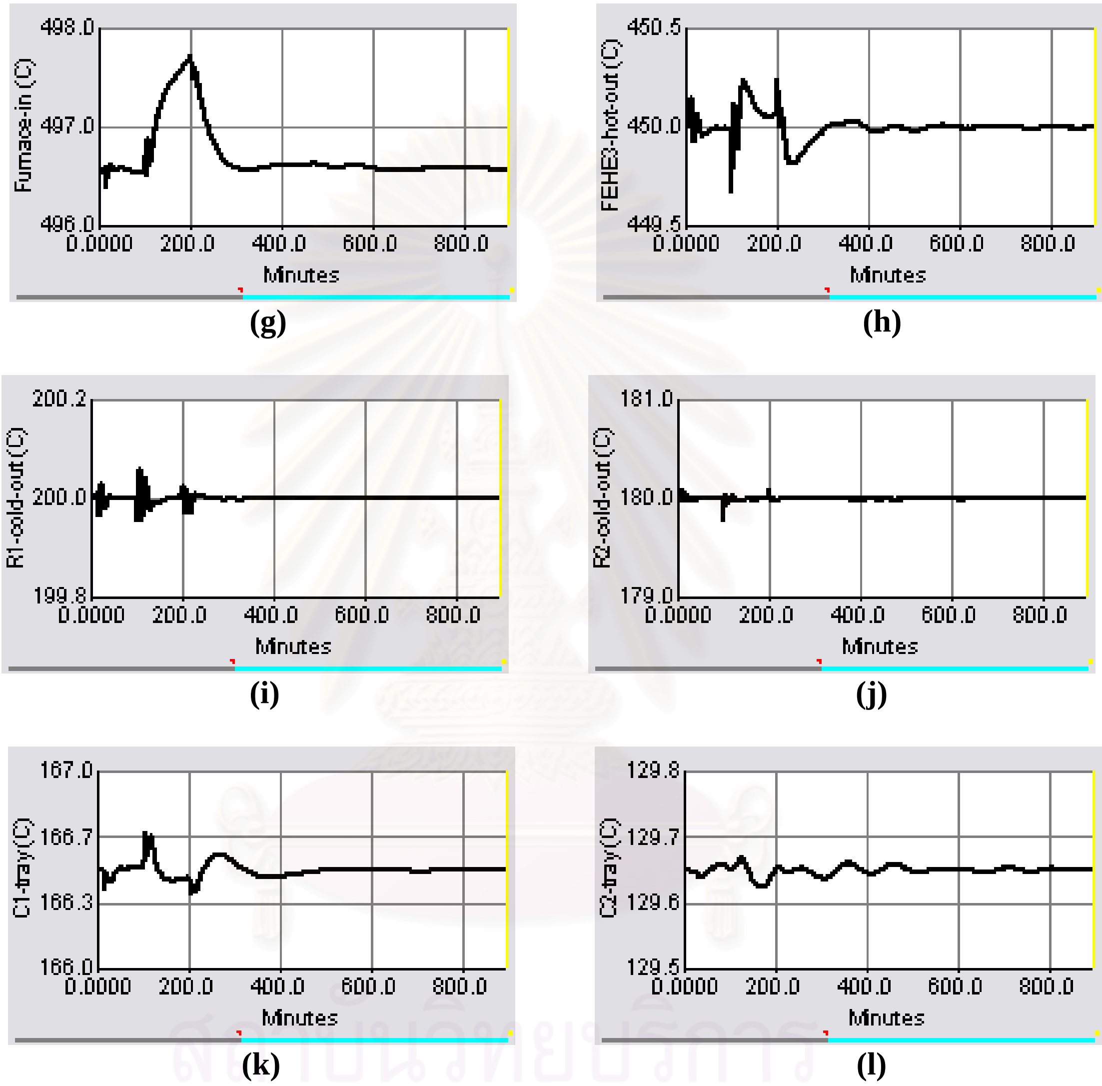


Figure 6.14 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the disturbance load of cold stream (reactor feed stream), where: (a) fresh feed toluene temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) cooler inlet temperature, (e) FEHE3 cold inlet temperature, (f) FEHE2 hot outlet temperature, (g) furnace inlet temperature, (h) FEHE3 hot outlet temperature, (i) R1 cold outlet temperature, (j) R2 cold outlet temperature, (k) C1-tray temperature, (l) C2-tray temperature, (m) C3-tray temperature, (n) reactor inlet temperature, (o) separator temperature, (p) furnace duty, (q) cooler duty.



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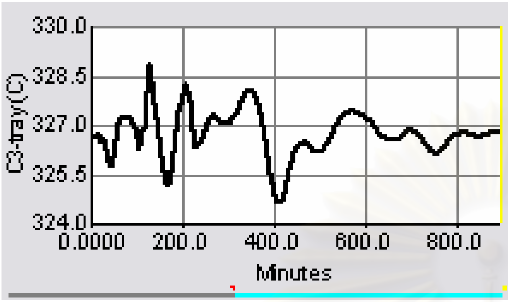

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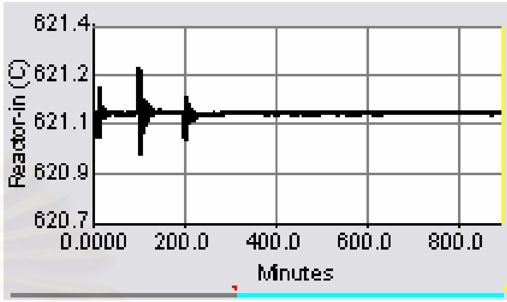

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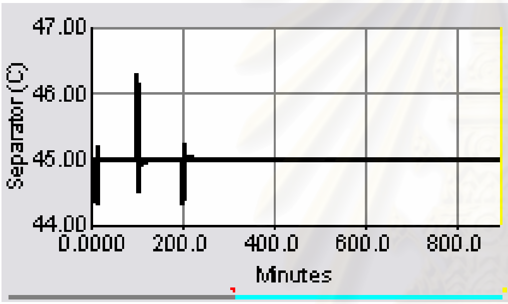

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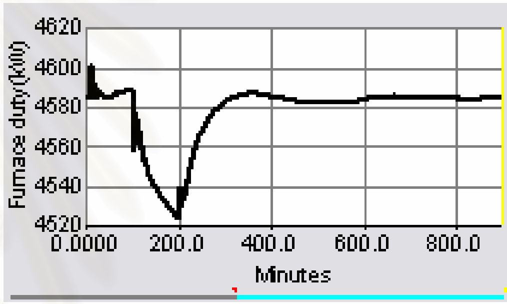

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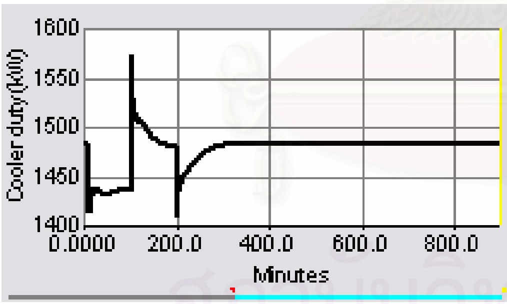

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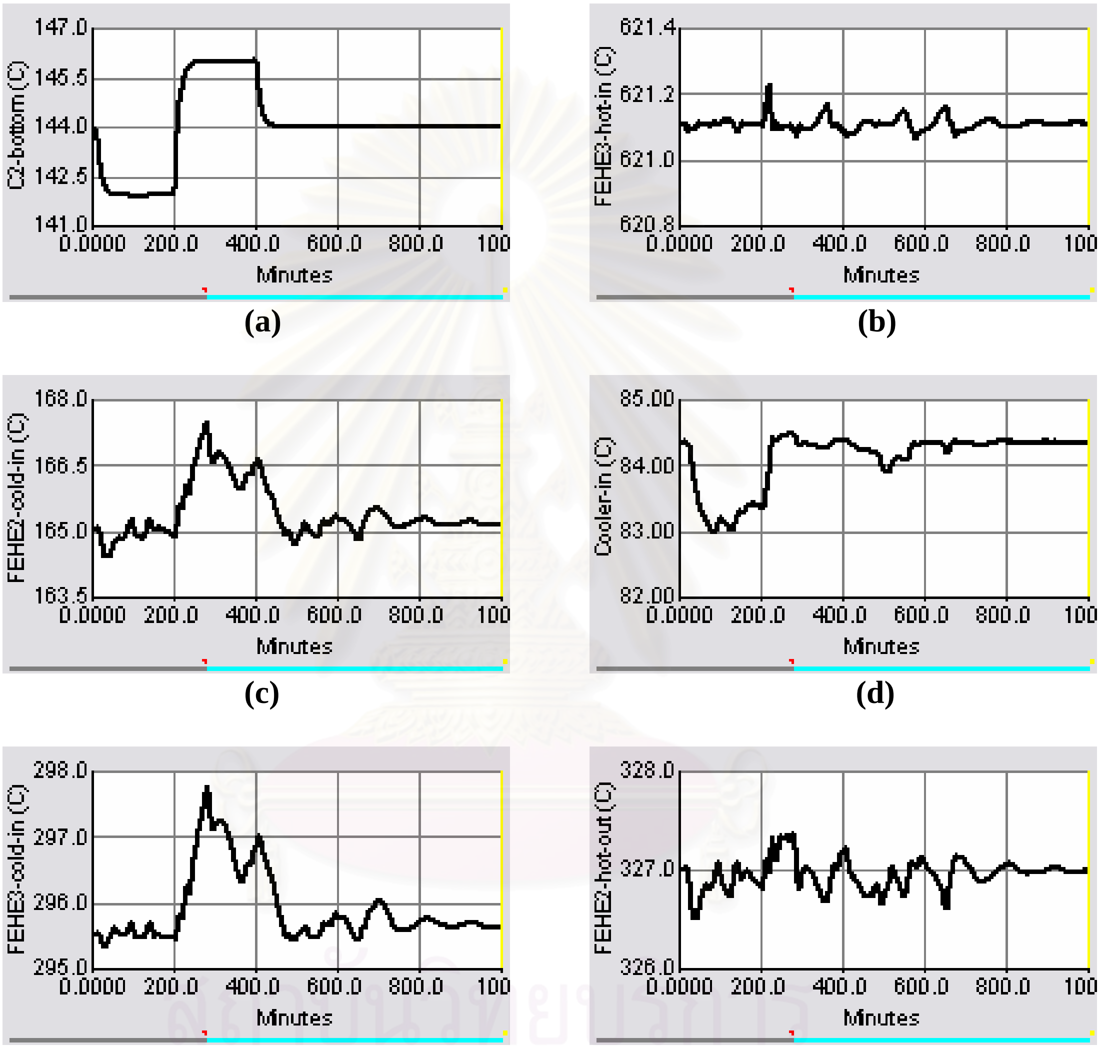
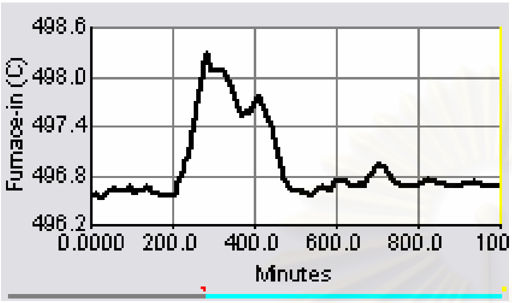


Figure 6.15 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the disturbance load of cold stream from the bottoms of product column (C2), where: (a) C2-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) cooler inlet temperature, (e) FEHE3 cold inlet temperature, (f) FEHE2 hot outlet temperature, (g) furnace inlet temperature, (h) FEHE3 hot outlet temperature, (i) R1 cold outlet temperature, (j) R2 cold outlet temperature, (k) C1-tray temperature, (l) C2-tray temperature, (m) C3-tray temperature, (n) reactor inlet temperature, (o) separator temperature, (p) furnace duty, (q) cooler duty.



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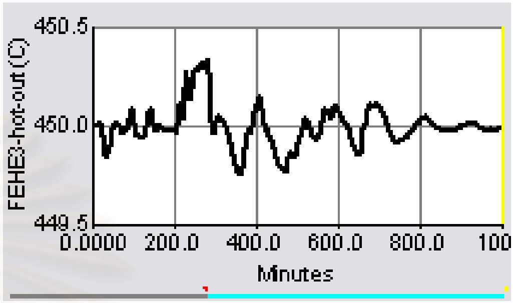

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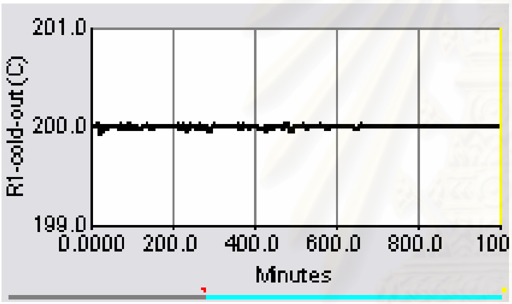

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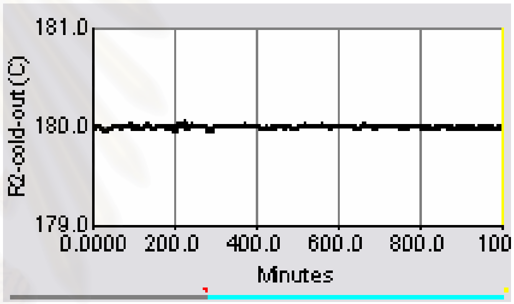

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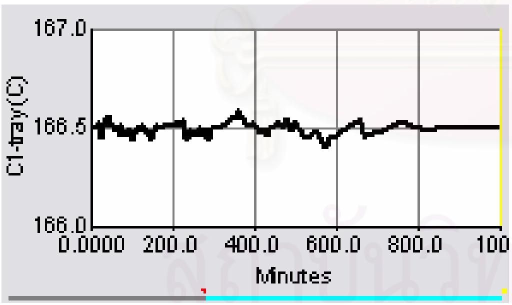

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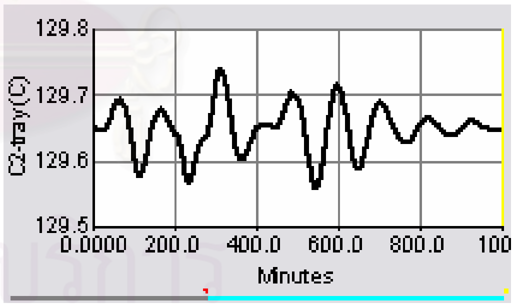

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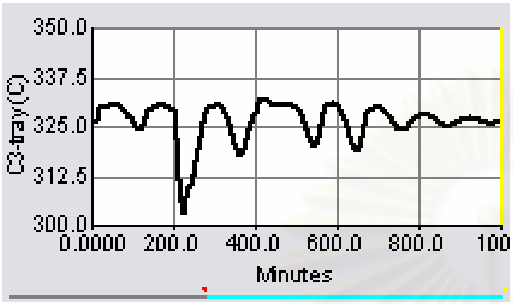

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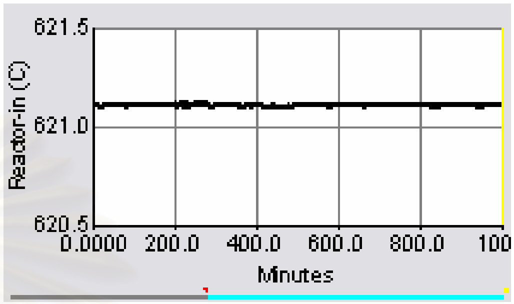

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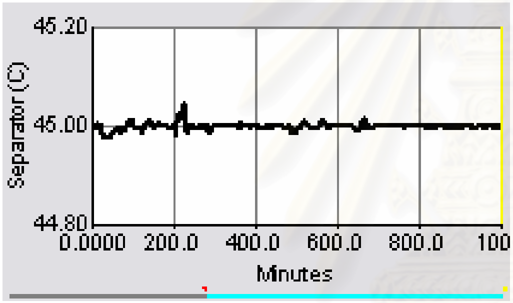

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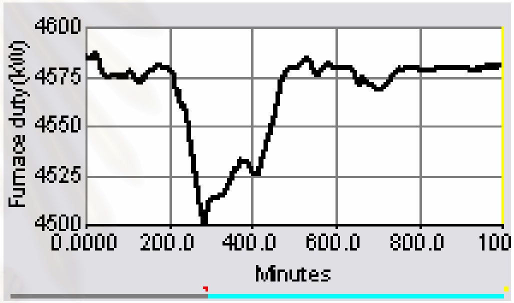

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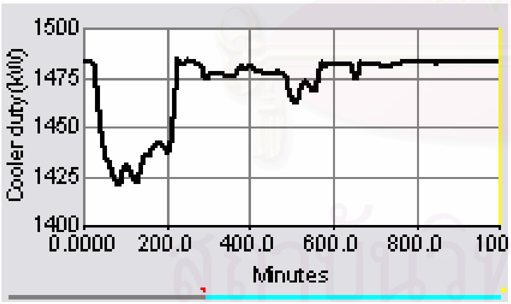

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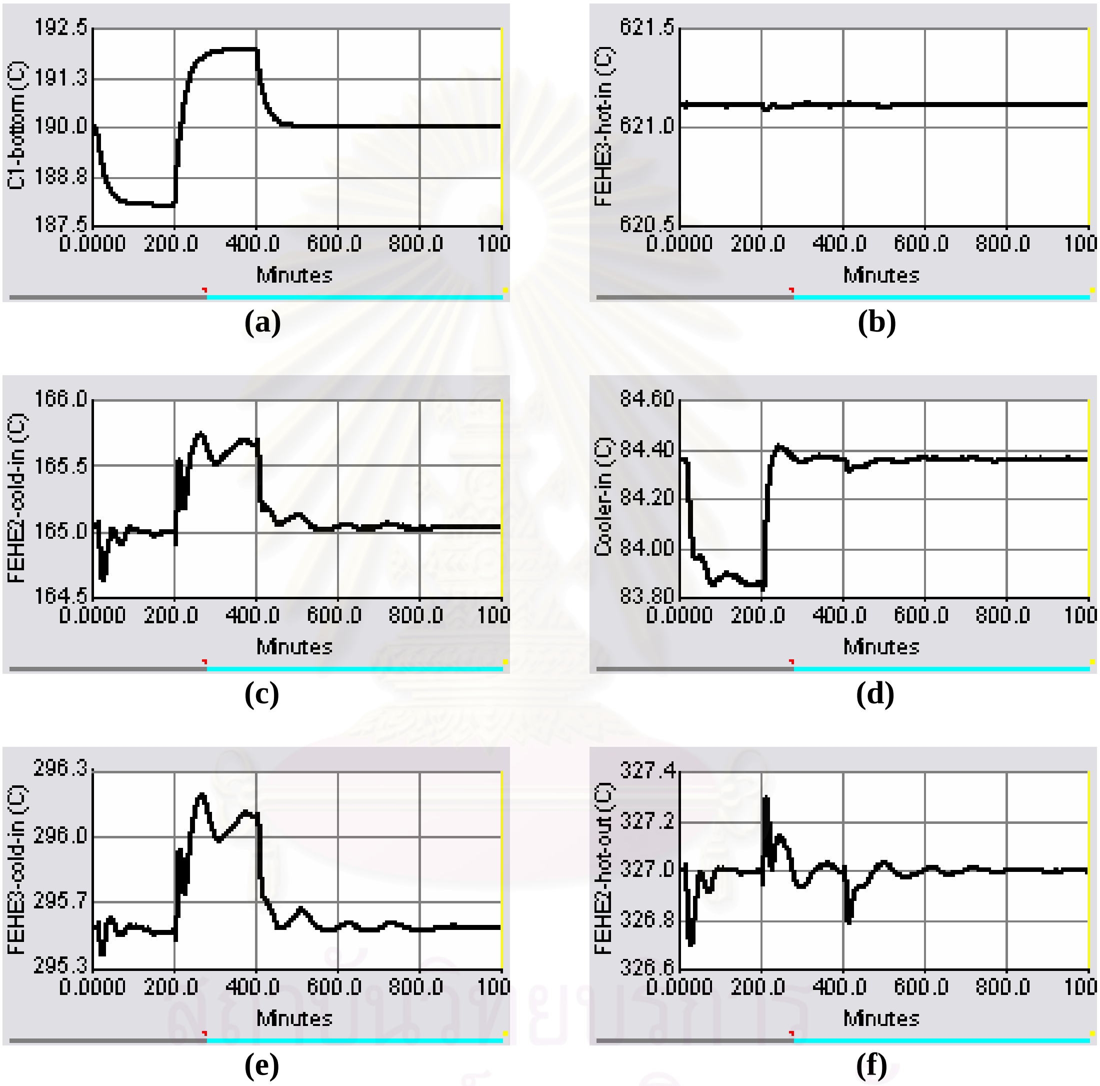
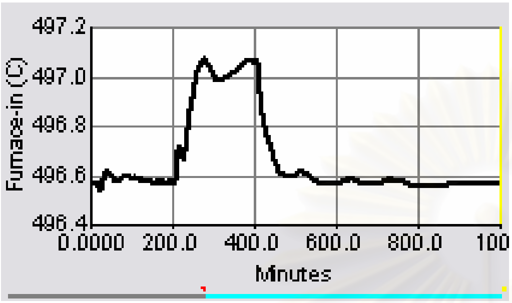


Figure 6.16 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the disturbance load of cold stream from the bottoms of stabilizer column (C1), where: (a) C1-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) cooler inlet temperature, (e) FEHE3 cold inlet temperature, (f) FEHE2 hot outlet temperature, (g) furnace inlet temperature, (h) FEHE3 hot outlet temperature, (i) R1 cold outlet temperature, (j) R2 cold outlet temperature, (k) C1-tray temperature, (l) C2-tray temperature, (m) C3-tray temperature, (n) reactor inlet temperature, (o) separator temperature, (p) furnace duty, (q) cooler duty.



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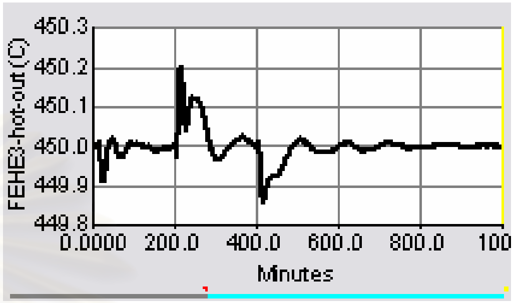

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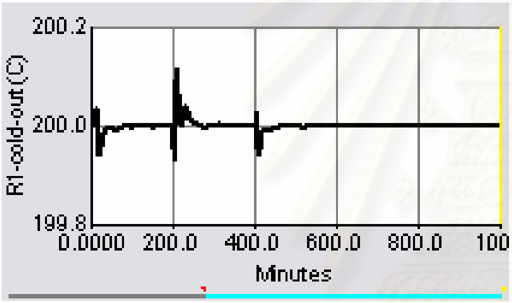

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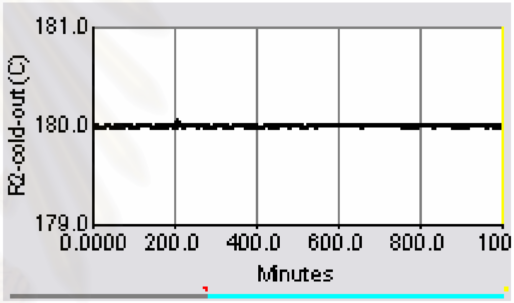

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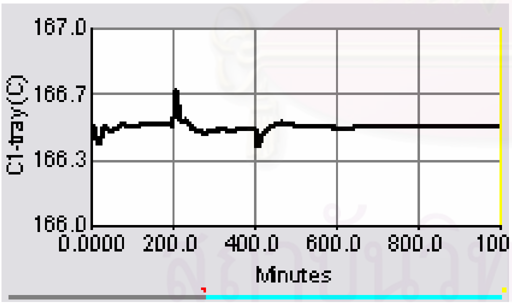

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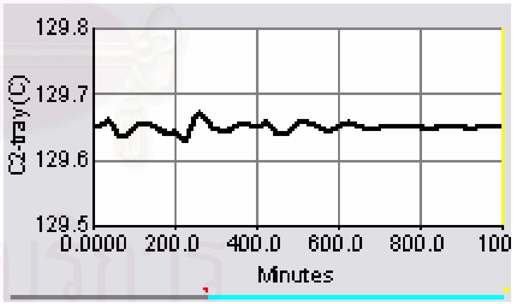

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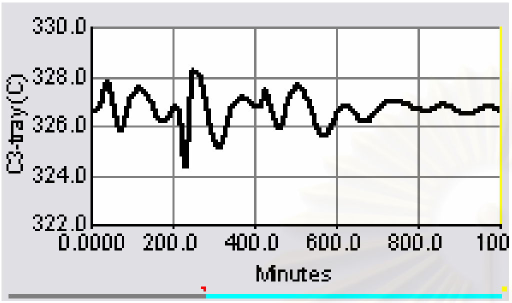

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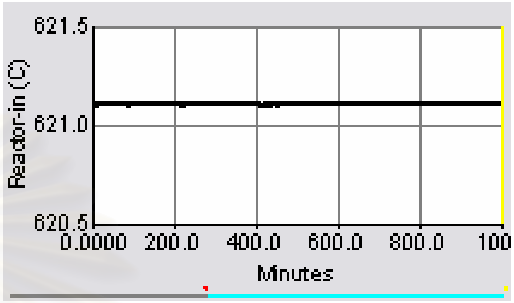

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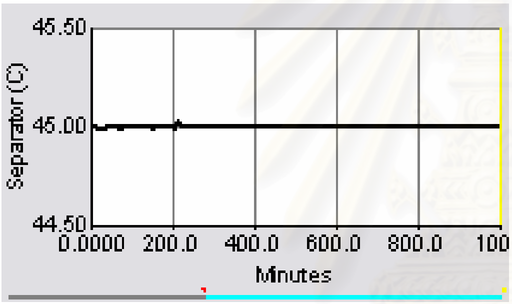

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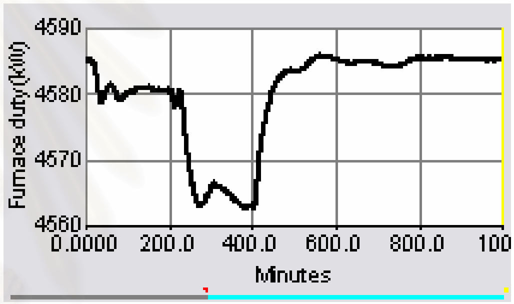

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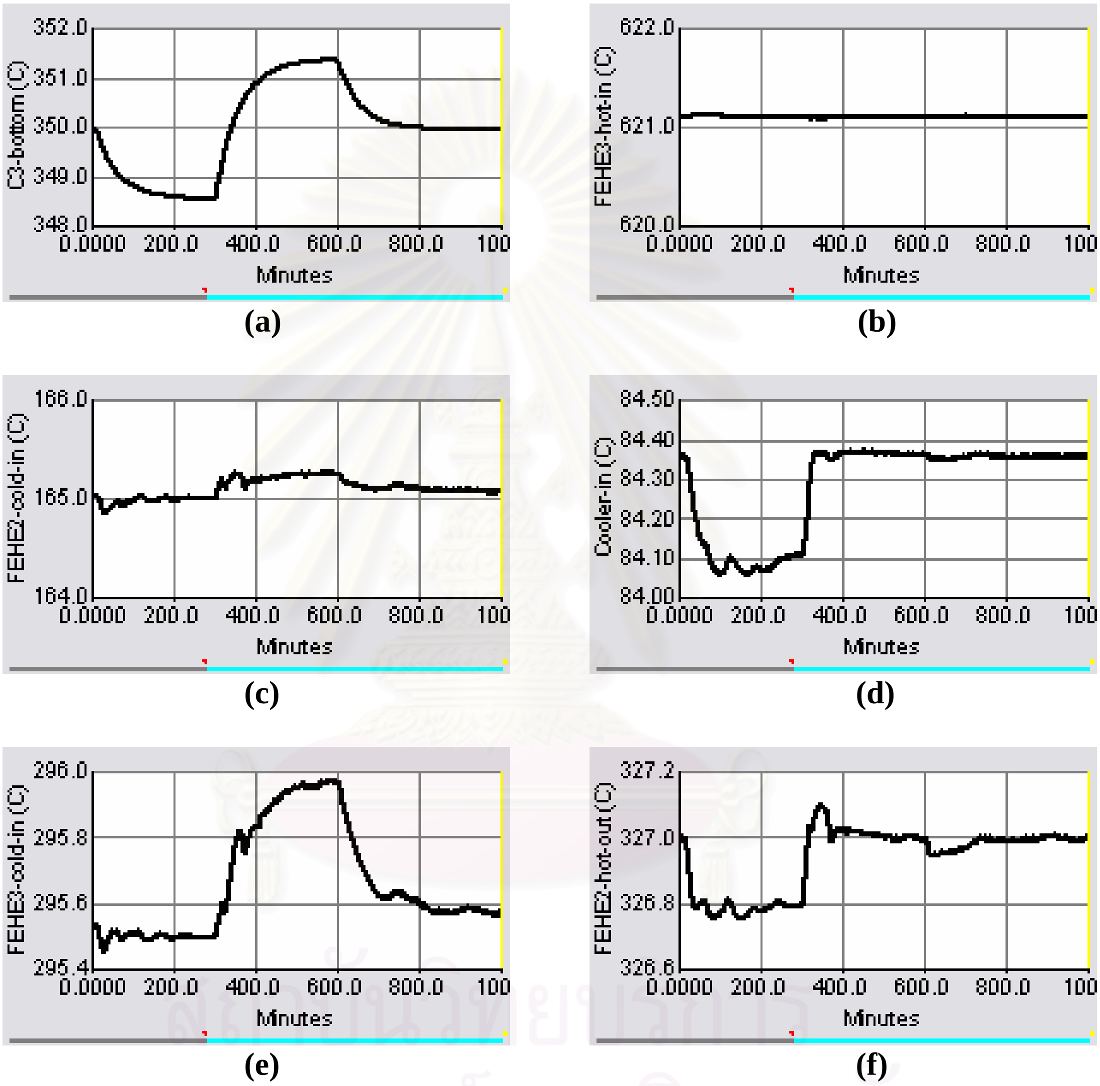
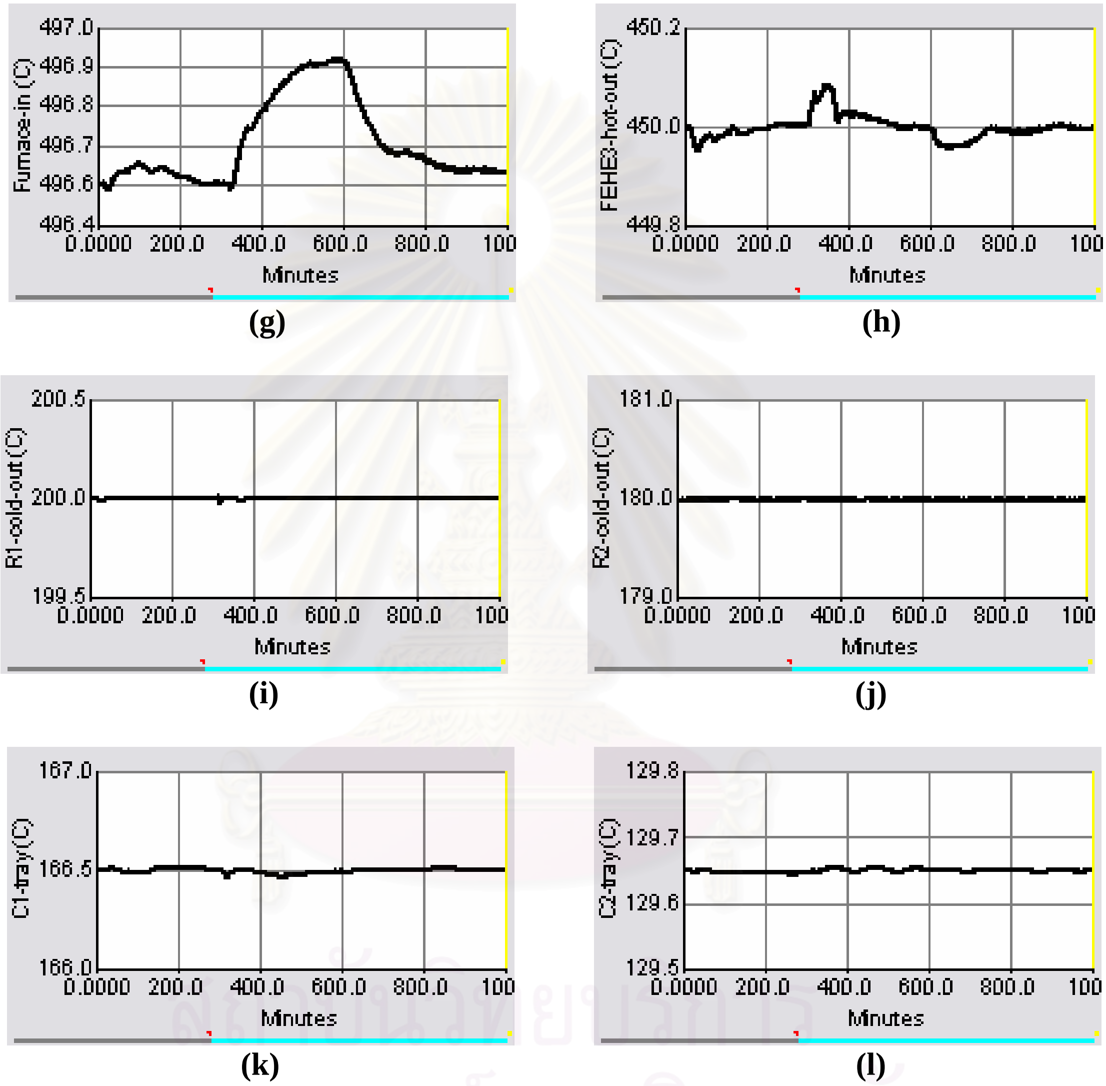


Figure 6.17 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the disturbance load of cold stream from the bottoms of recycle column (C3), where: (a) C3-bottoms temperature, (b) FEHE3 hot inlet temperature, (c) FEHE2 cold inlet temperature, (d) cooler inlet temperature, (e) FEHE3 cold inlet temperature, (f) FEHE2 hot outlet temperature, (g) furnace inlet temperature, (h) FEHE3 hot outlet temperature, (i) R1 cold outlet temperature, (j) R2 cold outlet temperature, (k) C1-tray temperature, (l) C2-tray temperature, (m) C3-tray temperature, (n) reactor inlet temperature, (o) separator temperature, (p) furnace duty, (q) cooler duty.



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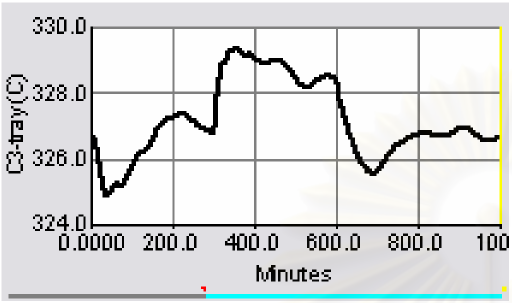

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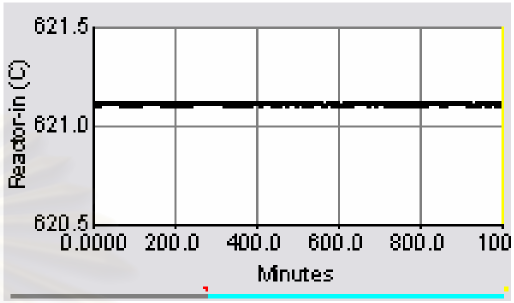

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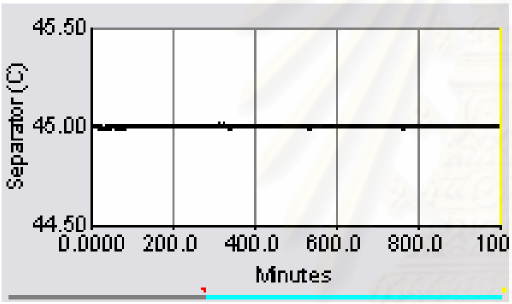

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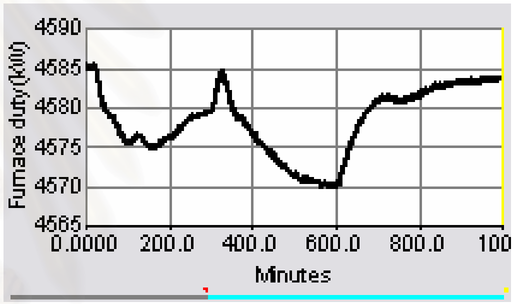

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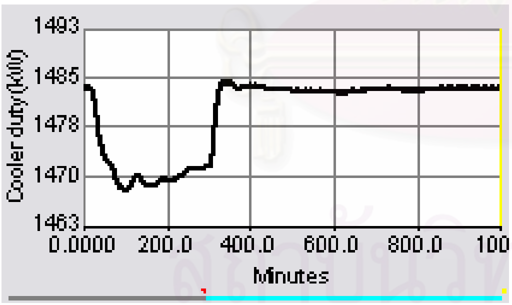

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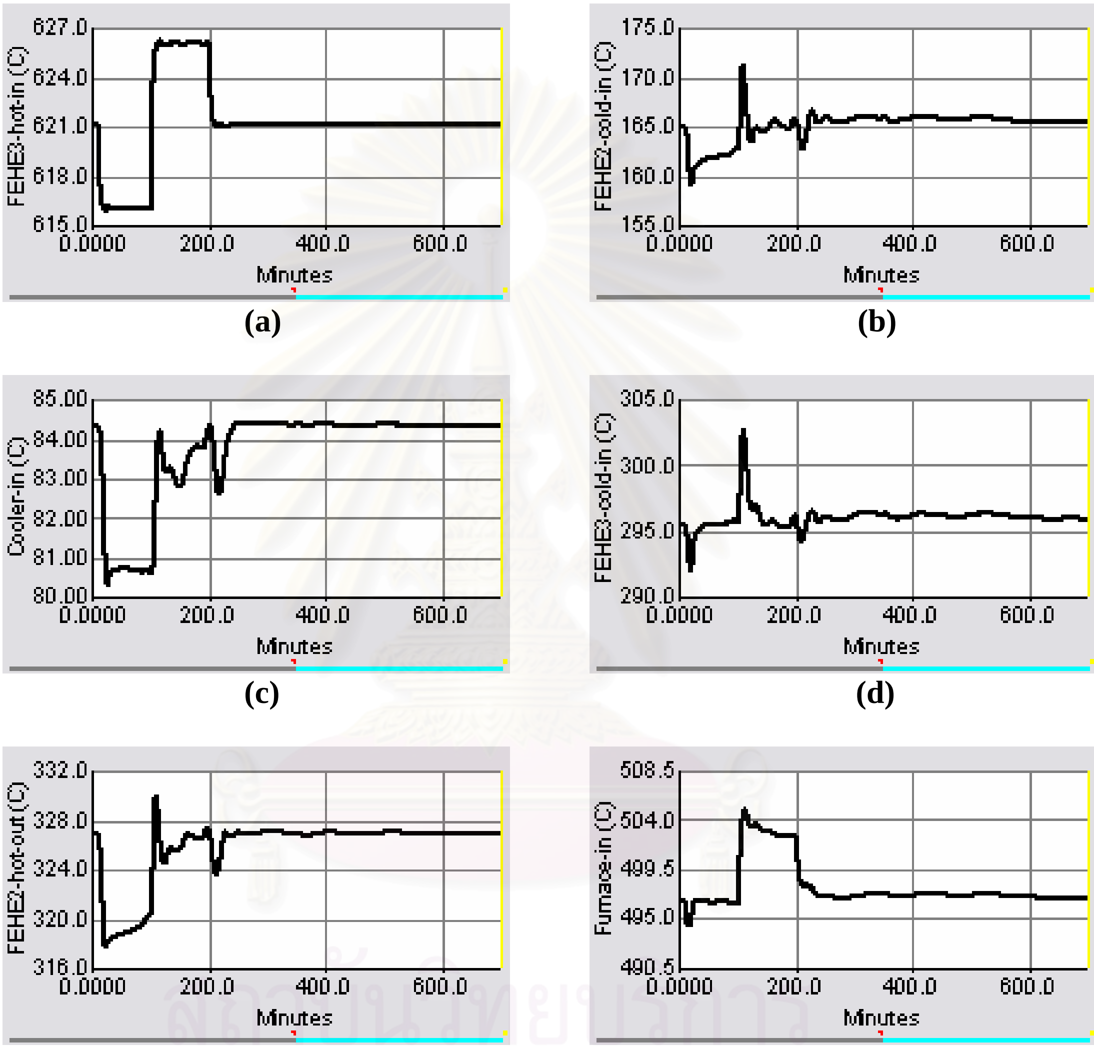
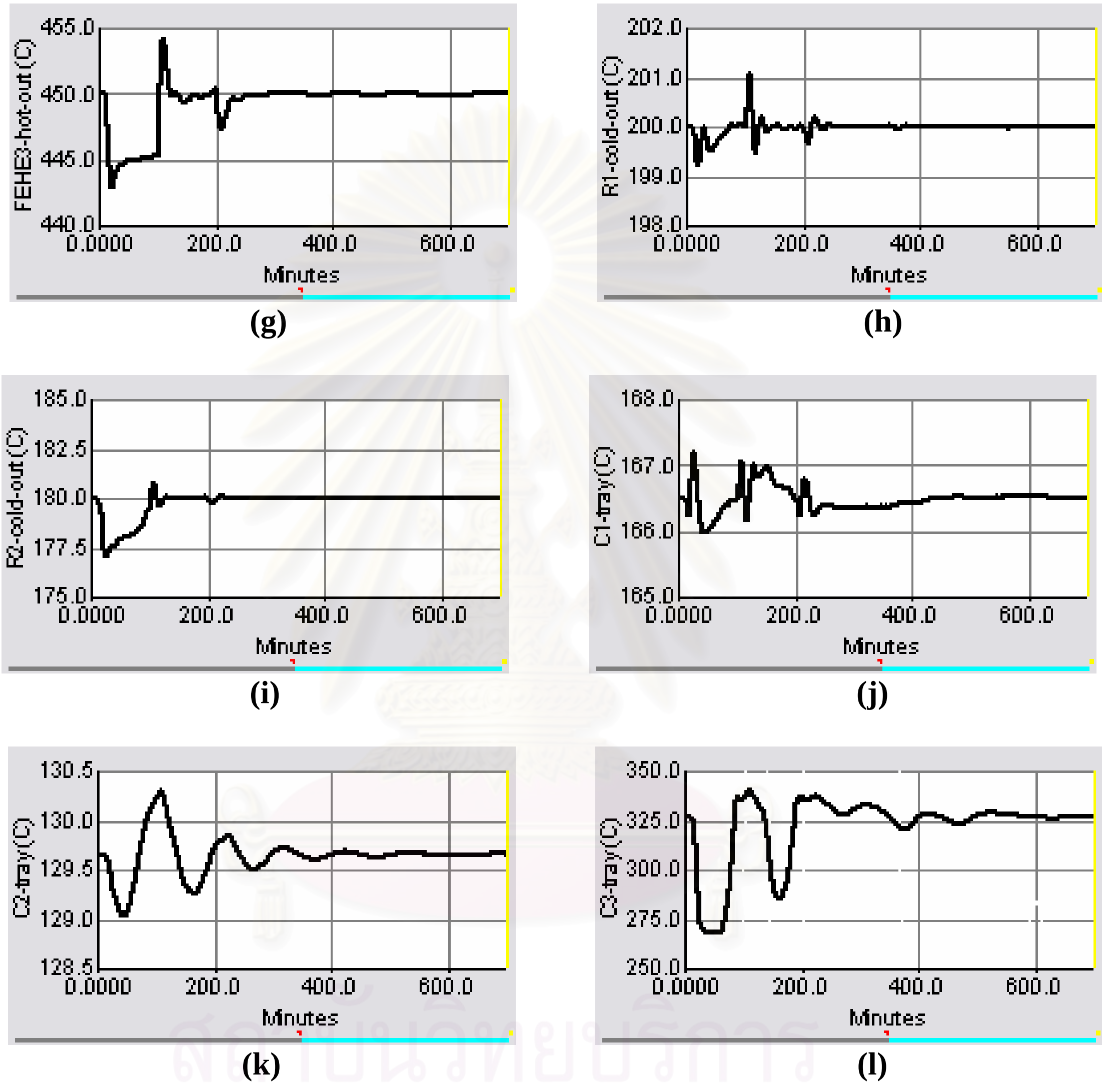


(a) (b) (c) (d) (e) (f)

Figure 6.18 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the disturbance load of hot stream (reactor product stream), where: (a) FEHE3 hot inlet temperature, (b) FEHE2 cold inlet temperature, (c) cooler inlet temperature, (d) FEHE3 cold inlet temperature, (e) FEHE2 hot outlet temperature, (f) furnace inlet temperature, (g) FEHE3 hot outlet temperature, (h) R1 cold outlet temperature, (i) R2 cold outlet temperature, (j) C1-tray temperature, (k) C2-tray temperature, (l) C3-tray temperature, (m) reactor inlet temperature, (n) separator temperature, (o) furnace duty, (p) cooler duty.



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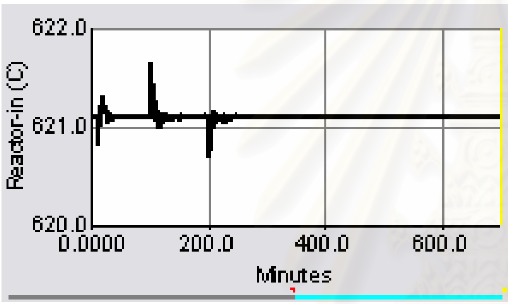

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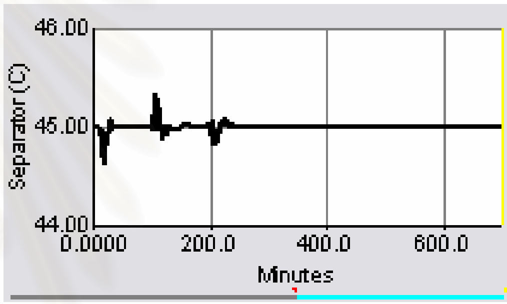

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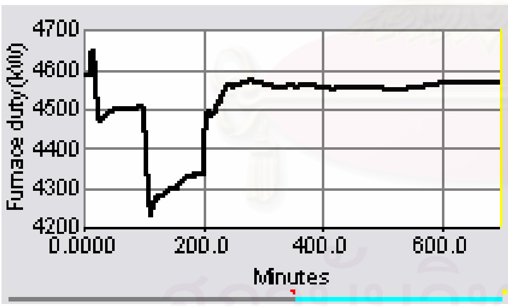

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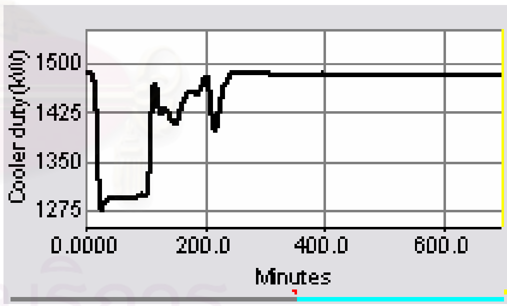

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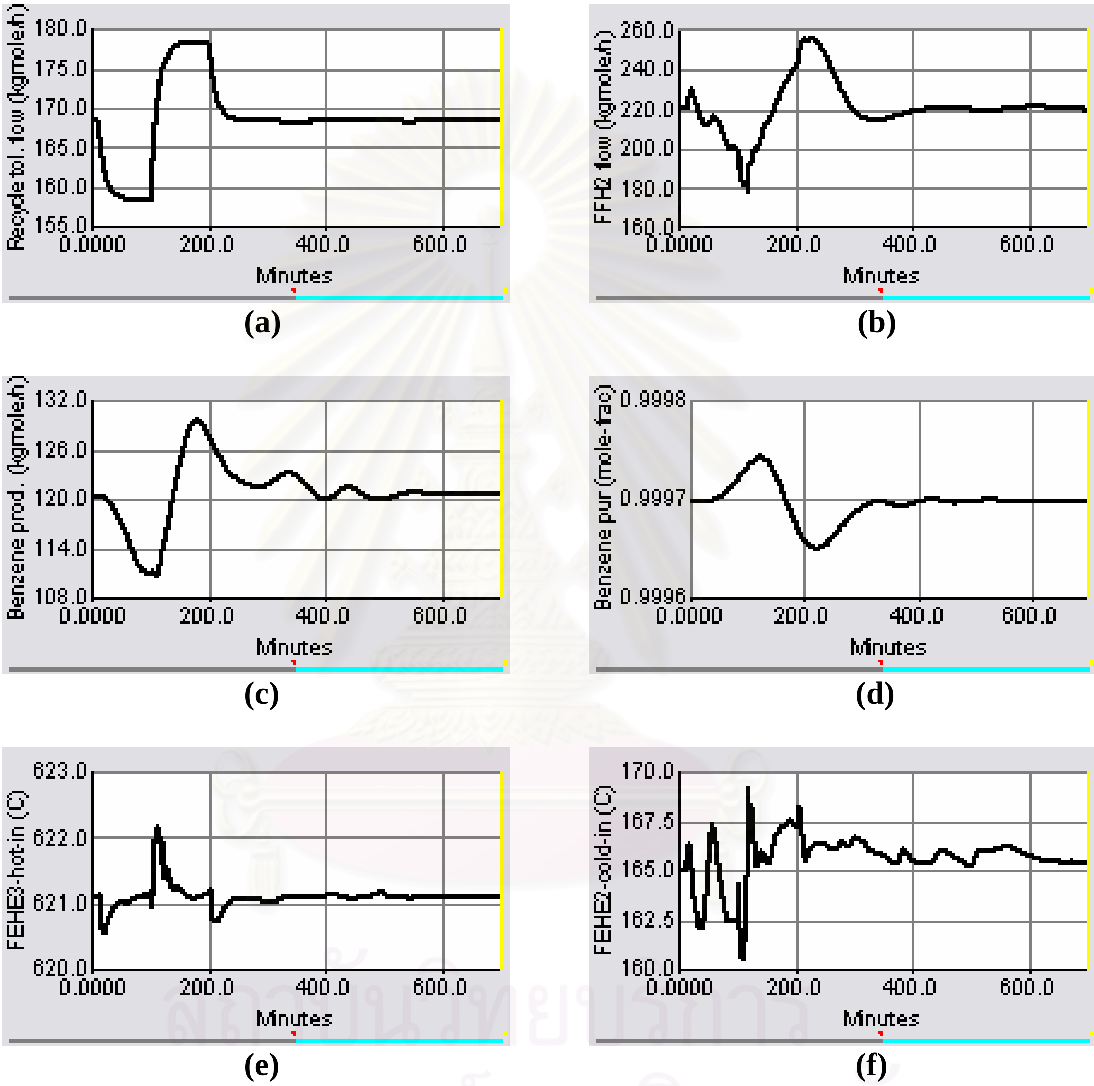
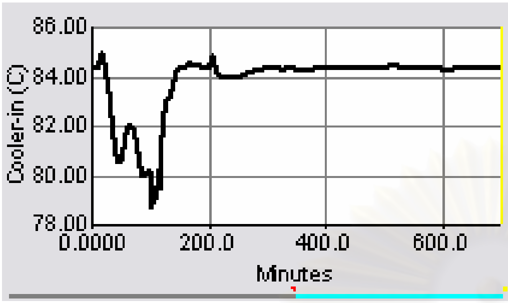


Figure 6.19 Dynamic responses of the HDA process alternative 6 with 3 LSSs to a change in the recycle toluene flowrates, where: (a) recycle toluene flowrates, (b) fresh feed hydrogen flowrates, (c) benzene product flowrates, (d) benzene purity, (e) FEHE3 hot inlet temperature, (f) FEHE2 cold inlet temperature, (g) cooler inlet temperature, (h) FEHE3 cold inlet temperature, (i) FEHE2 hot outlet temperature, (j) furnace inlet temperature, (k) FEHE3 hot outlet temperature, (l) R1 cold outlet temperature, (m) R2 cold outlet temperature, (n) C1-tray temperature, (o) C2-tray temperature, (p) C3-tray temperature, (q) reactor inlet temperature, (r) separator temperature, (s) furnace duty, (t) cooler duty.



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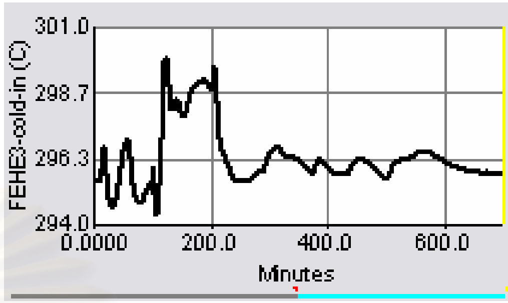

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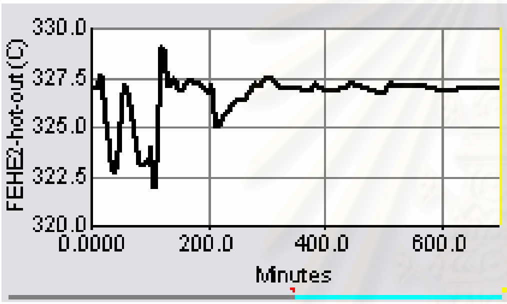
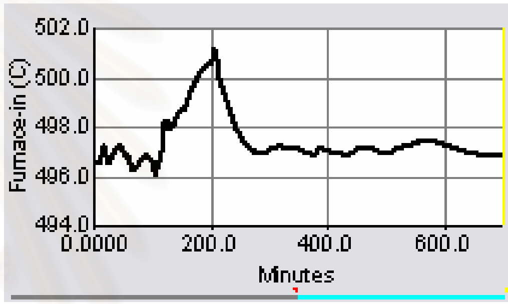
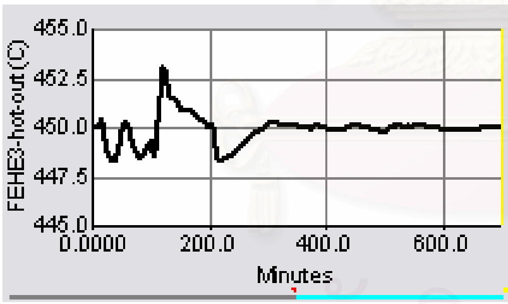


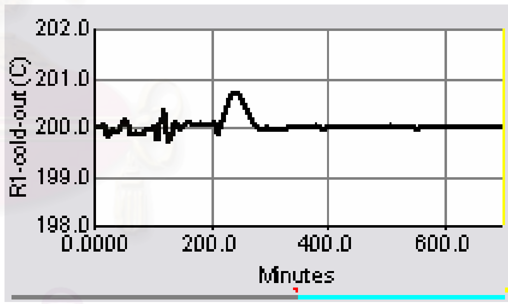
(i)



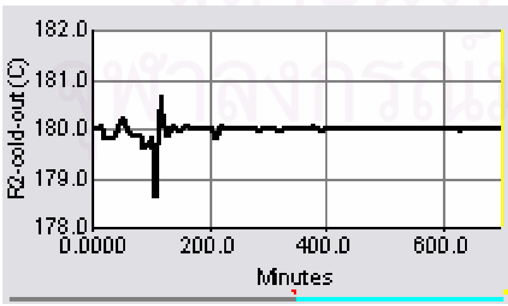
(j)



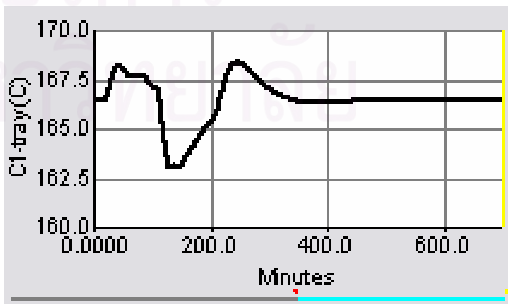
(k)



(l)

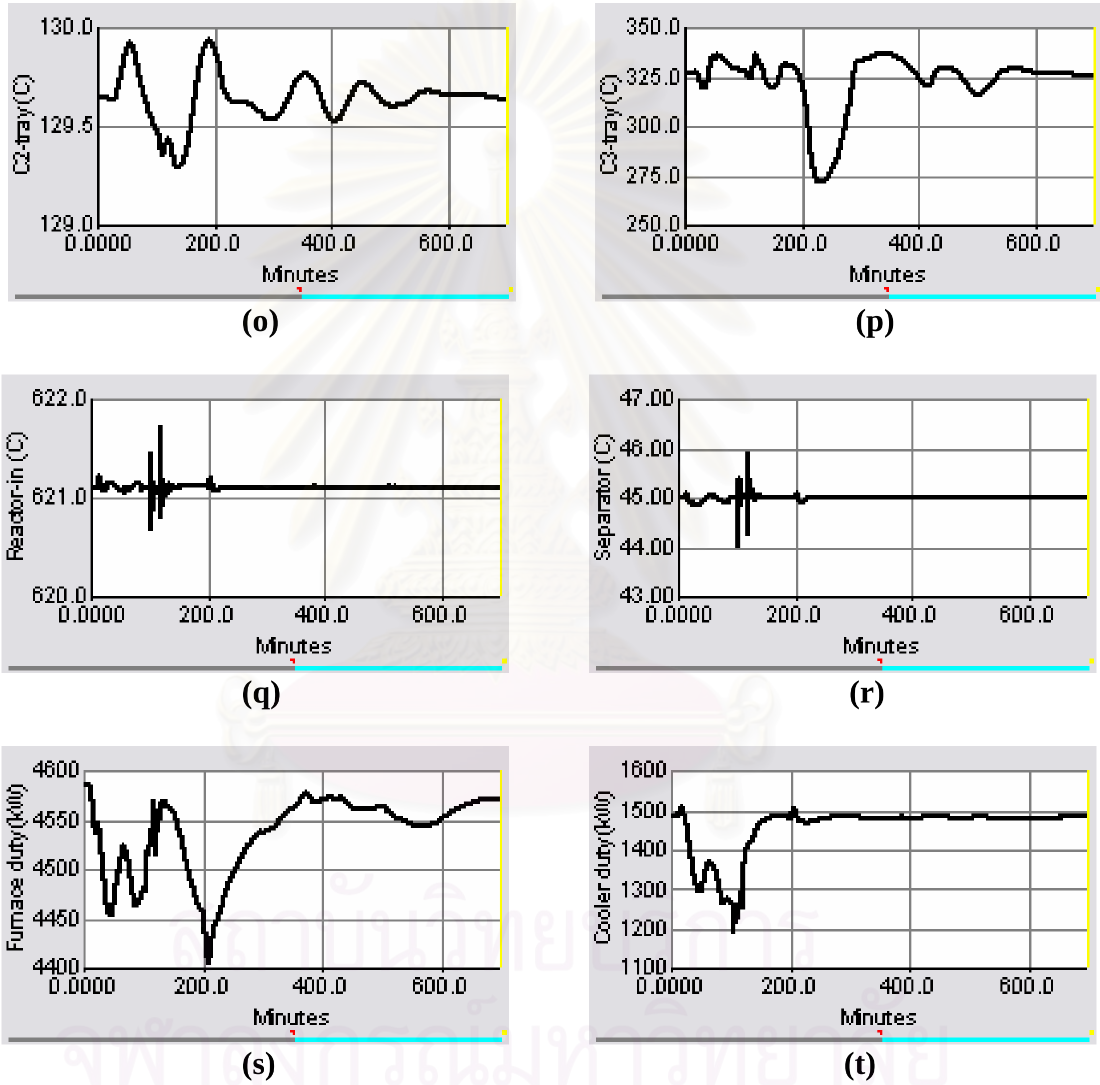


(m)



(n)

Figure 6.19 *Continued.*



(o) (p) (q) (r) (s) (t)

Figure 6.19 *Continued.*

6.7.1 Dynamic Simulation Results

In order to illustrate the dynamic behaviors of the new control structure with 3 LSSs in HDA process alternative 6, several disturbance loads were made. Figures 6.14 to 6.19 show the dynamic responses of the control structure with 2 LSSs for the HDA process alternative 4. Results for individual disturbance load changes are as follows:

6.7.1.1 Change in the heat load disturbance of cold stream

Figure 6.14 shows the dynamic responses of the control system with 3 LSSs in HDA process alternative 6 to a change in the heat load disturbance of cold stream (reactor feed stream). This disturbance is made as follows: first the fresh toluene feed temperature (stream FFtol in Figure 6.13) is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes (Figure 6.14.a).

Both the cold and hot outlet temperatures of FEHE1 decrease as the cold inlet temperature decreases, this is a desired condition for the hot stream, hence the LSS1 switches the control action from TCE1h to TCE1c to control the cold outlet temperature of FEHE1 at its minimum value of 165 ^{o}C (i.e. the cold inlet temperature of FEHE2 as shown in Figure 6.14.c). As a result, the hot outlet temperature of FEHE1 (i.e. the cooler inlet temperature) quickly drops to a new steady state value (Figure 6.14.d), and the cooler duty decreases (Figure 6.14.q).

When the cold inlet temperature of FEHE1 increases, first both the cold and hot outlet temperatures of FEHE1 increase, this is an MER choice, as expected the LSS1 switches the control action from TCE1c to TCE1h. As a result, the cooler inlet temperature drops to its nominal value (Figure 6.14.d). Therefore it is understandable that why the furnace duty decreases (Figure 6.14.p), since the furnace inlet temperature increases (Figure 6.14.g).

The tray temperatures in the stabilizer and product columns (Figure 6.14.k and 10.l) are slightly well controlled. But the tray temperature in recycle column has the maximum deviation of about 2 ^{o}C and it takes over 800 minutes to return to its set point (Figure 6.14.m).

6.7.1.2 Change in the heat load disturbance of cold stream from the bottoms of product column

Figure 6.15 shows the dynamic responses of the control system with 3 LSSs in HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of product column (C2). This disturbance is made as follows: first the set point of C2-bottom temperature controller (i.e. TCX3 in Figure 6.13) is decreased from 144.18 to 142.18 ^{o}C at time equals 10 minutes, the temperature is increased from 142.18 to 146.18 ^{o}C at time equals 200 minutes, then its temperature is returned to its nominal value of 144.18 ^{o}C at time equals 400 minutes (Figure 6.15.a). As can be seen, the temperature response in the bottoms of product column is somewhat fast (Figure 6.15.a).

When the cold inlet temperature of reboiler R2 (i.e. C2-bottom temperature as shown in Figure 6.15.a) decreases, the hot inlet temperature of FEHE1 decreases, thus the LSS1 switches the control action from TCE1h to TCE1c to maintain the cold inlet temperature of FEHE2 (Figure 6.15.c) and allows the cooler inlet temperature to drop to a new steady state value (Figure 6.15.d). Thus, it will result in decrease of the cooler duty (Figure 6.15.q). On the other hand, when C2-bottom temperature increases (Figure 6.15.a), as expected the LSS1 switches the control action from TCE1c to TCE1h to maintain the cooler inlet temperature (Figure 6.15.d) at its nominal value. Therefore, the furnace duty decreases (Figure 6.15.p), since the furnace inlet temperature increases (Figure 6.15.g).

6.7.1.3 Change in the heat load disturbance of cold stream from the bottoms of stabilizer column

Figure 6.16 shows the dynamic responses of the control system with 3 LSSs in HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of stabilizer column (C1). This disturbance is made as follows: first the set point of C1-bottom temperature controller (i.e. TCX2 in Figure 6.13) is decreased from 190 to 188 ^{o}C at time equals 10 minutes, and the temperature is increased from 188 to 192 ^oC at time equals 200 minutes, then its temperature is returned to its nominal value of 190 ^oC at time equals 400 minutes (Figure 6.16.a). As can be seen, the temperature response in the bottoms of stabilizer column is slower than that in the bottoms of product column.

Principally, shifting of both the positive and negative disturbance loads from the bottoms of stabilizer column are the same as those from the bottoms of product column. When the cold inlet temperature of reboiler R1 (i.e. C1-bottom temperature as shown in Figure 6.16.a) decreases, it will result in decrease of the hot inlet temperature of FEHE1. The LSS1 will take an action to control the cold inlet temperature of FEHE2 (Figure 6.16.c). Therefore, the cooler duty decreases (Figure 6.16.q). When C1-bottom temperature increases (Figure 6.16.a), it will result in increase of the hot inlet temperature of FEHE1. As expected, the LSS1 switches the control action from TCE1c to TCE1h to maintain the cooler inlet temperature (Figure 6.16.d) at its nominal value. As a result, the furnace duty decreases (Figure 6.16.p).

6.7.1.4 Change in the heat load disturbance of cold stream from the bottoms of recycle column

Figure 6.17 shows the dynamic responses of the control system with 3 LSSs in HDA process alternative 6 to a change in the heat load disturbance of cold stream from the bottoms of recycle column (C3). This disturbance is made as follows: first the set point of C3-bottom temperature controller (i.e. TCX4 in Figure 6.13) is decreased from 349.9 to 348.5 ^oC at time equals 10 minutes, and the temperature is increased from 348.5 to 351.3 ^oC at time equals 300 minutes, then its temperature is returned to its nominal value of 349.9 ^oC at time equals 600 minutes (Figure 6.17.a). As can be seen, this set point change is sluggish (Figure 6.17.a).

When the cold inlet temperature of reboiler R3 (C3-bottom temperature as shown in Figure 6.17.a) decreases, the hot inlet temperature of FEHE2 decreases. The LSS2 takes the control action to maintain the cold inlet temperature of FEHE3 at its set point (Figure 6.17.e) and allows the hot outlet temperature of FEHE2 to drop (Figure 6.17.f). The disturbance load is directed to reach its destination in the cooler utility. Thus, the cooler duty decreases (Figure 6.17.q). Consider the case when C3-bottom temperature increases (Figure 6.17.a), the hot inlet temperature of FEHE2 increases. The LSS2 switches the control action from TCE2c to TCE2h to maintain the hot outlet temperature of FEHE2 at its set point (Figure 6.17.f). The disturbance load is now directed to reach its destination in the furnace utility. Thus, the furnace duty decreases (Figure 6.17.p).

6.7.1.5 Change in the heat load disturbance of hot stream

Figure 6.18 shows the dynamic responses to a change in the heat load disturbance of hot stream (the hot reactor product). This disturbance is made as follows: first the set point of FEHE3-hot-inlet temperature controller (i.e. TCX1 in Figure 6.13) is decreased from 621.1 to 616.1 ^{o}C at time equals 10 minutes, and the temperature is increased from 616.1 to 626.1 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 621.1 ^{o}C at time equals 200 minutes (Figure 6.18.a). As can be seen, this temperature response is very fast (Figure 6.18.a), the new steady state is reached quickly (Figure 6.18.a).

In this particular case, the LSS3 plays a significant role in selecting proper pathway. When the hot inlet temperature of FEHE3 decreases (Figure 6.18.a), it will result in decrease of the furnace inlet temperature (Figure 6.18.f), so the LSS3 will take an action to control the furnace inlet temperature at its set point (Figure 6.18.f) and allows the hot outlet temperature of FEHE3 to drop to a new steady state value (Figure 6.18.g). The disturbance load is directed throughout the down stream units to reach its destination in the cooler utility. Thus, the cooler duty is significantly decreased (Figure 6.18.p). On the other hand, when the hot inlet temperature of FEHE3 increases (Figure 6.18.a), the LSS3 switches the control action from TCE3c to TCE3h to control the hot outlet temperature of FEHE3 (Figure 6.18.g) and lets the furnace inlet temperature to further increase (Figure 6.18.f). Therefore, the furnace duty is significantly decreased (Figure 6.18.o).

6.7.1.6 Change in the recycle toluene flowrates

On the other case, a disturbance in the production rate is also made for this study. Figure 6.19 shows the dynamic responses to a disturbance in the recycle toluene flowrates from 168.4 to 158.4 kgmole/h at time equals 10 minutes, and the flowrates is increased from 158.4 to 178.4 kgmole/h at time equals 100 minutes, then its flowrates is returned to its nominal value of 168.4 kgmole/h at time equals 200 minutes (Figure 6.19.a). The recycle toluene flowrates response is sluggish; the new steady state is reached slowly (Figure 6.19.a).

As can be seen that the drop in toluene feed flowrates reduces the reaction rate, so the benzene product flowrates drops (Figure 6.19.c), and the benzene product quality increases (Figure 6.19.d) and vice versa. The tray temperature in the recycle column has a large deviation (Figure 6.19.p), and it takes over 600 minutes to slowly return to its nominal value of 326.7 ^{o}C. The furnace and cooler duties could be maintained below its nominal values (Figure 6.19.s and Figure 6.19.t).

6.7.2 Evaluation of the Dynamic Performances

The IAE results of some temperature controllers for the control structures with one LSS and three LSSs in HDA alternative 6 are summarized in Tables 6.9 to 6.11. The implementation of three LSSs in HDA process alternative 6 makes the control configuration to be resilient i.e. the control system can handle any disturbance loads from the cold and hot streams. The control system with three LSSs is less effective than the control system with one LSS, since the values of IAE in the control system

Table 6.9 The IAE results of the control system in HDA process alternative 6 to a change in the disturbance load of cold stream (reactor feed stream)

Controller	Integral Absolute Error (IAE) in HDA process alternative 6	
	Control structure with one LSS	Control structure with three LSSs
TC1	11.3125	19.3678
TC2	1.2637	4.0640
TC3	215.5248	457.4748
TCE1c	19.6066	82.2323
TCE1h	82.5746	78.1100
TCE2c	-	75.0966
TCE2h	8.4007	25.9050
TCE3c	-	76.9973
TCE3h	5.7239	25.4723
TCQ	5.2978	5.7640
TCR	3.1052	3.1992
TCS	4.9324	6.3232
TCR1c	-	2.6326
TCR2c	-	4.2791
Total	357.7422	866.9182

Table 6.10 The IAE results of the control system in HDA process alternative 6 to a change in the disturbance load of hot stream (reactor product stream)

Controller	Integral Absolute Error (IAE) in HDA process alternative 6	
	Control structure with one LSS	Control structure with three LSSs
TC1	39.7498	82.5833
TC2	9.3419	79.0402
TC3	491.9192	4539.8481
TCE1c	47.2940	684.1117
TCE1h	63.9595	142.7182
TCE2c	-	369.9596
TCE2h	67.1568	180.9003
TCE3c	-	360.7418
TCE3h	59.4044	136.3212
TCQ	17.3824	16.7078
TCR	8.7348	8.0273
TCS	3.2174	9.1573
TCR1c	-	40.4407
TCR2c	-	169.5819
Total	808.1602	6820.1394

Table 6.11 The IAE results of the control system in HDA process alternative 4 to a change in the recycle toluene flowrates

Controller	Integral Absolute Error (IAE) in HDA process alternative 6	
	Control structure with one LSS	Control structure with three LSSs
TC1	383.1165	461.8289
TC2	7.3873	56.5834
TC3	1779.9686	5653.8529
TCE1c	162.9453	603.3928
TCE1h	70.3792	165.0919
TCE2c		404.2374
TCE2h	60.2920	210.3200
TCE3c		422.1800
TCE3h	37.1340	222.0633
TCQ	29.4596	49.9664
TCR	10.4217	7.5412
TCS	8.2798	12.0240
TCR1c		50.4454
TCR2c		34.7892
Total	2549.3840	8354.3168

with three LSSs are larger than those in the control system with one LSS (see Tables 6.9 to 6.11). Nevertheless, the new control system with three LSS is considered to be a resilient control configuration, since any disturbances from both the cold and hot streams can be managed which resulting in decrease of both the furnace and cooler utility duties.

6.8 Conclusions

General heuristic design procedure for heat exchanger networks control configuration and operation is proposed. This procedure gives the simple but effective ways to design the control configuration for resilient HEN. Several typical HEN examples are considered to describe the implementation of the design procedure for HEN control configuration and operation. A selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway to carry the associated load to a utility unit. In particular case, multiple LSSs (i.e. more than one LSS) are required in order to direct the associated load to the utility unit. The number of LSS can be easily determined based on the proposed design procedure.

The proposed heuristic design procedure is used in conjunction with Luyben's plantwide control procedure to design plantwide control structure of energy integrated HDA process. Two and three LSSs are employed in the HDA process alternatives 4 and 6, respectively in order for the HEN to be resilient, i.e. any disturbances from both the cold and hot streams can be managed which resulting in decrease of both the cooler and heater utility duties. The new designed control structure is evaluated based on the rigorous dynamic simulation using HYSYS simulator. This 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 DMER can be achieved.

CHAPTER VII
SUMMARY AND CONCLUSIONS

The proposed heat pathway heuristics (HPH) was used in conjunction with Luyben's plantwide control procedure to model heat pathway management systems and the control configuration of energy-integrated hydrodealkylation of toluene (HDA) process. In chapter 4, design of heat pathways for dynamic maximum energy recovery (DMER) was introduced and applied to the HDA process based on steady state considerations. The dynamic simulation of the new designed plantwide control structures in the HDA process was presented in chapter 5 in order to illustrate the effective principles of the use of HPH for plantwide control. The extended heuristic design procedure for heat exchanger networks control configuration and operation was summarized in chapter 6. In this chapter, the main points of this dissertation are discussed.

7.1 Design of Heat Pathways for Dynamic MER in HDA Process

In this dissertation, the HDA process with energy integration schemes (i.e. alternatives 1, 4, and 6) were chosen for a case study, since it consists of many recycle streams and energy integrations. The commercial software HYSYS was utilized to carry out both the steady state and dynamic simulations.

7.1.1 Steady State Simulation Results of HDA Process

The steady state simulation results are found to be consistent with those in Luyben et al. (1999). However, there are some differences: for example, in the current study the flowrates of the reflux streams in the product and the recycle columns are larger and the reactor effluent temperature is lower than those in Luyben's work.

The possible reasons for these differences may be that in Luyben et al. (1999), vapor-liquid equilibrium behavior was assumed to be ideal and the stabilizer column was modeled as a component splitter and tank whereas the current study is based on the Peng-Robinson equation of state and the stabilizer column is modeled rigorously. The operating pressure for this column is chosen to be 1034 kPa according to the design information in Douglas (1988), whereas in Luyben's work is assumed to be 3310 kPa. Consequently, the pressures for the streams around the stabilizer column are different. In our simulation, the heats of reaction are directly calculated by HYSYS. The heats of reaction in the current study are –41,867 Joule/mole for the first reaction and 8,141 Joule/mole for the second reaction, whereas in Luyben et al. (1999) they are –50,008 Joule/mole and 0 Joule/mole for the first and second reaction, respectively. Therefore, it is understandable that the reactor effluent temperature in the current work is lower than that obtained in Luyben's work, since the absolute value of the heat of reaction for the first reaction is smaller, and also, the second reaction is slightly endothermic.

The steady state simulation results of HDA process alternative 1 have been compared with the earlier study (Luyben et al., 1999). The results were found consistent with those in Luyben et al. (1999). Then, considering the consistency of the simulation results of the HDA process alternative 1 with respect to the previous work, the other alternatives considered in this work, i.e. alternatives 4 and 6 were also developed in the HYSYS software environment.

7.1.2 Heat Pathways Management of HDA Process

For the purpose of plantwide energy management, various heat pathways through the heat exchanger network alternatives of HDA process have been systematically investigated. In this case, the disturbance loads are shifted to the process streams that are serviced by the furnace or cooler utility exchanger. Therefore, both furnace and cooler utility duties decrease according to the input heat load disturbance. The heat pathways management for HDA process to achieve DMER can be summarized bellow:

1. HDA process alternative 1 is the simplest one, since it includes only one FEHE and all reboilers in the three distillation columns are serviced by utility exchangers. In this HEN, D^+ of cold stream and D^- of hot stream are shifted to the cooler utility by controlling the cold outlet temperature of FEHE, so that its

duty can be decreased. Whereas D^- of cold stream and D^+ of hot stream are shifted to the furnace utility by controlling the hot outlet temperature of FEHE, so that its duty can be decreased. Hence, DMER can be achieved.

2. HDA process alternative 4 is more complex than alternative 1. In alternative 4, two FEHEs are required and the reboiler in the product column is driven by the hot reactor products. Heat-integrated system was used for both the product and recycle columns. In order to prevent the propagation of thermal disturbance to the column, the hot temperature at the entrance of reboiler is maintained constant. Thus, all the disturbance loads that are coming with the hot stream (i.e. reactor product stream) are shifted to the furnace utility. Consequently, D^- of the hot stream will result in increase of the furnace duty. And D^+ of the hot stream will result in decrease of the furnace duty.
3. HDA process alternative 6 is the most complex one compared with the others, since it includes three FEHEs and all reboilers in the three distillation columns are driven by the hot reactor products. With the same strategy as applied to alternative 4, the hot temperatures at the entrance of reboilers are kept constant to prevent the propagation of thermal disturbance to the columns. As a result, when D^- is coming with the hot stream, this will result in increase of the furnace duty. But, when D^+ is coming with the hot stream, as expected, this will result in decrease of the furnace duty.
4. In the particular complex HENs (HDA alternatives 4 and 6), several disturbance loads are transferred across the pinch temperature in order to achieve DMER, for instance: D^- of cold stream should be transferred across the pinch to the heater utility and D^- of hot stream should be transferred across the pinch to the cooler utility. Otherwise, we don't get the true MER.

Therefore, this steady state study reveals that by selecting an appropriate heat pathway to carry the associated load to a utility unit, its duty can be decreased; hence DMER can be achieved.

7.2 The New Heuristic Design Procedure for Heat Exchanger Network Control Configuration and Operation

The new heuristic design procedure for HEN control configuration and operation to achieve DMER is proposed as follows:

1. The HEN for a particular processing plant should be designed as a resilient HEN following the match pattern proposed by Wongsri (1990) (see Appendix C)
   1.1. Design the match pattern in HEN as Class A or Class B so that they are considered to be potential resilient match pattern.
   1.2. If there is the match pattern in HEN as Class C or Class D, they are considered as non-resilient match pattern. For the remedy, any Class C or Class D in the match pattern should be redesigned so that its residual stream must be connected to either Class A or Class B. Hence the only two classes of interests are Class A and Class B.
2. From the economic point of view, we strongly suggest to:
   2.1. shift D^+ of the cold stream or D^- of the hot stream to the cooler utility unit, thus its duty will be decreased.
   2.2. shift D^- of the cold stream or D^+ of the hot stream to the heater utility unit, thus its duty will be decreased.
3. A selective controller with low selector switch (LSS) should be employed to select an appropriate heat pathway through the network to carry the associated load to a utility unit.
4. The number of LSS to be used in a particular case can be determined as follows:
   4.1. Identify the heat link in HEN that can be used for the propagation of disturbance load, note that the propagation is co-current with the process stream (see Figure 6.5).
   4.2. If there is only one heat link (see Fig. 6.5.a), the only one LSS is employed and placed on the last heat exchanger (see Fig. 6.6.a).
   4.3. If there are more than one heat link (see Figures 6.5.b and 6.5.c):
      4.3.1. Design the heat links so that all of them will end up at the same heat exchanger unit in order to reduce the number of LSS.

4.3.2. If all heat links end up at the different heat exchanger units, so the number of LSS is equal to the number of heat link (see Fig. 6.5.b) or the number of the last heat exchangers. For instance, based on the HEN model 2 (see Fig. 6.5.b), there are 2 heat links, which end up at the different heat exchangers (HE1 and HE4). Thus, the number of LSS is equal to 2 (see Fig. 6.6.b).

4.3.3. If there are some heat links, which end up at the same heat exchanger unit (see Fig. 6.5.c), the number of LSS is equal to the number of the last heat exchangers. For instance, based on the HEN model 3 (see Fig. 6.5.c); There are three heat links (links 1, 2, and 3). Two of the three heat links (i.e. links 1 and 3) end up at the same heat exchanger unit (i.e. HE1). And HE4 is used for link 2. Therefore, there are two the last heat exchangers (i.e. HE1 and HE4) for all heat links. Hence, two LSS are required and placed on HE1 and HE4 (see Fig. 6.6.c).

7.3 Dynamic Simulation and Control of HDA Process

Based on the steady state study of heat pathways management for HDA process, strategies for plantwide control are generated to operate the entire process. Furthermore, the designed control strategy should be able to handle all disturbance loads entering the process in such a way that MER can be achieved.

7.3.1 Design of Plantwide Control Structures

Plantwide control structures of HDA process with energy integration schemes (i.e. alternatives 1, 4, and 6) are designed based on the heuristic design procedure given by Luyben e. al. (1999) and the heat pathway heuristics (HPH) with the objective of selecting what path should be used to carry the associated load to the utility unit, so that MER can be achieved.

A selective controller with low selector switch (LSS) is used for the HDA process in order to manage the disturbance load entering the process. The LSS that consists of one manipulated variable and two controlled variables is employed to prevent a process variable (i.e. the furnace inlet temperature) from exceeding a lower limit, so that the furnace duty is kept at a good level. Design of plantwide control structures for HDA process alternatives 1, 4 and 6 are summarized bellow:

7.3.1.1 Design of plantwide control structure for HDA process alternative 1

In HDA process alternative 1, its major control loops are the same as those used in Luyben et al. (1999), except for the temperature control in the FEHE. In the current work, the LSS is employed and placed on FEHE1 to direct and manage the disturbance load. This new control system is compared with the previous control system given by Luyben et al. (1999). In Luyben et al. (1999), a single controller was used to control the furnace inlet temperature.

Since the temperature profile in the recycle column is very sharp because of the large difference in boiling point between toluene and diphenyl, this produces large temperature changes from tray to tray, which mean that the process gain is very large when a single tray temperature is controlled. The standard solution for this problem is to use an average (AVG) temperature of several trays instead of a single tray.

7.3.1.2 Design of plantwide control structure for HDA process alternative 4

In HDA process alternative 4, its major control loops are the same as those used in the HDA process alternative 1, except for the tray temperature control in the product distillation columns and the pressure control in the recycle column.

Since the hot reactor product is used to drive the reboiler in the product distillation column, part of this stream in process-to-process exchanger (R2) is bypassed and manipulated to control the tray temperature in the product column (TC2). The hot outlet temperature of FEHE2 (the temperature at the entrance of the reboilers R2) is controlled by manipulating the valve on the bypass stream to prevent the propagation of thermal disturbance to the separation section.

Since heat-integrated distillation system was used for both the product and recycle columns, the pressure in the two columns should be adjusted so that there is a reasonable differential temperature driving force for heat transfer in the heat exchangers. In this case, the pressure required in the recycle column is 540 kPa to provide a reasonable temperature differential in Condenser/Reboiler (CR). In the recycle column, the cold inlet stream of CR is bypassed and manipulated to control its pressure column (PC3). The averaging tray temperature control (AVG) in the recycle column is used instead of a single tray temperature control (TC3). But its set point increases due to the effect of pressure shifting in the recycle column.

7.3.1.3 Design of plantwide control structure for HDA process alternative 6

In HDA process alternative 6, its major control loops are the same as those used in HDA process alternative 1, except for the tray temperature control in the three distillation columns (TC1, TC2, and TC3) and the pressure control in the recycle column (PC3).

Since the hot reactor product is used to drive all reboilers in the three distillation columns, part of this stream in process-to-process exchanger is bypassed and manipulated to control all the tray temperatures in the three columns. The hot outlet temperatures of FEHE2 and FEHE3 (the temperatures at the entrance of the reboilers R2 and R3) are controlled by manipulating the valve on the bypass stream to prevent the propagation of thermal disturbance to the separation section.

Following the same strategy as HDA alternative 4, the cold inlet stream of CR is bypassed and manipulated to control pressure of the recycle column (PC3). The averaging tray temperature control (AVG) in the recycle column is used instead of a single tray temperature control (TC3).

7.3.1.4 Design of multiple LSSs for HDA process alternatives 4 and 6

In order for the resilient HEN, two LSSs and three LSSs are employed in HDA process alternatives 4 and 6, respectively (see Figures 6.8 and 613). Auxiliary reboilers are installed at both steady state and dynamic simulations in order to handle any imbalance in reboiling heat duties in the stabilizer and product columns.

7.3.2 Dynamic Simulation Results of HDA Process

In order to evaluate the dynamic behaviors of the control systems of HDA process, several disturbances were made as follows:

1. $D^{\pm}$ of the cold stream (reactor feed stream)
2. $D^{\pm}$ of the cold stream from the bottoms of the stabilizer column
3. $D^{\pm}$ of the cold stream from the bottoms of the product column
4. $D^{\pm}$ of the cold stream from the bottoms of the recycle column
5. $D^{\pm}$ of the hot stream (reactor products stream)
6. Decrease and increase in the recycle toluene flowrates

In general better responses of the furnace and cooler utility consumptions are achieved in this study compared to the Luyben's control system. Both furnace and cooler duties could be decreased according to the input heat load disturbance, since the HPH is applied in the current work. Therefore, the proposed HPH is very useful in terms of heat load or disturbance management to achieve DMER.

The integral absolute error (IAE) method was used to evaluate the effectiveness of the designed control systems. The IAE results show that the HDA process alternative 1 is the most effective one compared with the others (i.e. alternatives 4 and 6). Therefore, those results indicate that the implementation of complex energy integration alters dynamic performance of the process.

The control systems with multiple LSSs are less effective than the control systems with one LSS, since the values of IAE are larger. Nevertheless, the control systems with multiple LSSs are considered to be a resilient control configuration, since any disturbances from both the cold and hot streams can be managed which resulting in decrease of both the furnace and cooler utility duties.

7.4 Recommendations for Future Work

1. Implementation of auxiliary reboilers to control the tray temperatures in the distillation columns for the other HEN alternatives of HDA process, in order to face some control difficulties in energy-integrated process.
2. Application of the new heuristic design procedure to other process systems associated with energy integration (e.g. feed-effluent-heat-exchanger reactor systems, heat exchanger network systems) to achieve the DMER.

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APPENDICES

APPENDIX A

PROCESS STREAM DATA OF HDA PROCESS

Table A.1 Process stream data of HDA process alternative 4

	Fresh toluene	Fresh hydrogen	Purge gas	Stabilizer gas	Benzene product	Diphenyl product
Stream name	FFtol	FFH2	purge	d1	d2	b3
Temperature [C]	30.00	30.00	45	51.05	105.55	349.74
Pressure [kPa]	4378.17	4378.17	3211.58	1034.21	206.84	550.00
Molar Flow [kgmole/hr]	130.00	222.72	219.62	8.75	121.77	2.80
H_2, mole fraction	0	0.97	0.3980	0.0890	0	0
CH_4	0	0.03	0.5906	0.8686	0	0
C_6H_6	0	0	0.0102	0.0420	0.9997	0
C_7H_8	1	0	0.0012	0.0003	0.0003	0.00026
$C_{12}H_{10}$	0	0	0	0	0	0.99974

Table A.1 *Continued*

	Gas recycle	Toluene recycle	FEHE1 cold in	FEHE2 cold in	Furnace inlet	Reactor inlet
Stream name	dischg	d3	cHE1in	cHE1out	cHE2out	Rin
Temperature [C]	72.83	183.85	67.91	145.10	513.20	621.11
Pressure [kPa]	4171.33	4378.17	4171.33	3881.75	3605.96	3468.06
Molar Flow [kgmole/hr]	1596.30	38.72	1987.62	1987.62	1987.62	1987.62
H_2, mole fraction	0.3980	0	0.4280	0.4280	0.4280	0.4280
CH_4	0.5906	0	0.4781	0.4781	0.4781	0.4781
C_6H_6	0.0102	0.00027	0.0082	0.0082	0.0082	0.0082
C_7H_8	0.0012	0.99917	0.0858	0.0858	0.0858	0.0858
$C_{12}H_{10}$	0	0.00056	0	0	0	0

Table A.1 *Continued*

	Reactor outlet	Quench	FEHE2 hot in	FEHE2 hot out	FEHE1 hot in	FEHE2 hot out
Stream name	Rout	quench	hHE2in	hHE2out	hR2out	hHE1out
Temperature [C]	665.61	45.43	621.00	307.60	176.00	94.22
Pressure [kPa]	3350.85	3350.85	3350.85	3309.48	3275.01	3233.64
Molar Flow [kgmole/hr]	1987.62	49.00	2036.62	2036.62	2036.62	2036.94
H_2, mole fraction	0.3642	0.0045	0.3555	0.3555	0.3555	0.3553
CH_4	0.5432	0.0442	0.5312	0.5312	0.5312	0.5313
C_6H_6	0.0706	0.7098	0.0860	0.0860	0.0860	0.0861
C_7H_8	0.0206	0.2252	0.0255	0.0255	0.0255	0.0255
$C_{12}H_{10}$	0.0014	0.0163	0.0018	0.0018	0.0018	0.0018

Table A.1 *Continued*

	Separator inlet	Separator gas out	Stabilizer feed	Stabilizer bottoms	Product bottoms
Stream name	coolout	gas	toC1	b1	b2
Temperature [C]	45.00	45.00	45.25	189.77	145.10
Pressure [kPa]	3211.58	3211.58	3727.31	1041.11	907.53
Molar Flow [kgmole/hr]	2036.94	1815.92	172.03	163.28	41.52
H_2, mole fraction	0.3553	0.3980	0.0045	0	0
CH_4	0.5313	0.5906	0.0442	0	0
C_6H_6	0.0861	0.0102	0.7098	0.7456	0.0003
C_7H_8	0.0255	0.0012	0.2252	0.2372	0.9319
$C_{12}H_{10}$	0.0018	0	0.0163	0.0172	0.0678

Table A.1 *Continued*

	Con/Reb cold in	Reb2 cold in	Reb2 cold out	Con/Reb hot in	Con/Reb hot out
Stream name	cCRin	cCRout	cR2out	top	condout
Temperature [C]	145.10	162.52	193.00	182.78	180.80
Pressure [kPa]	907.53	400.68	228.32	540.00	526.21
Molar Flow [kgmole/hr]	385.00	385.00	385.00	48.66	48.66
H_2, mole fraction	0	0	0	0	0
CH_4	0	0	0	0	0
C_6H_6	0.0003	0.0003	0.0003	0.0003	0.0003
C_7H_8	0.9319	0.9319	0.9319	0.9992	0.9992
$C_{12}H_{10}$	0.0678	0.0678	0.0678	0.0006	0.0006

Table A.1 *Continued*

	Column reflux			Column boilup		
	C1	C2	C3	C1	C2	C3
Temperature [C]	51.05	105.55	184.00	189.77	193.00	349.74
Pressure [kPa]	1034.21	206.84	570.00	1041.11	228.32	550.00
Molar Flow [kgmole/hr]	14.92	490.95	9.94	180.22	385.00	47.52
H_2, mole fraction	0.0003	0	0	0	0	0
CH_4	0.0214	0	0	0	0	0
C_6H_6	0.9574	0.9997	0.00027	0.8412	0.0003	0
C_7H_8	0.0208	0.0003	0.99918	0.1581	0.9319	0.0018
$C_{12}H_{10}$	0	0	0.00055	0.0007	0.0678	0.9982

Table A.2 Process stream data of HDA process alternative 6

	Fresh toluene	Fresh hydrogen	Purge gas	Stabilizer gas	Benzene product	Diphenyl product
Stream name	FFtol	FFH2	purge	d1	d2	b3
Temperature [C]	30.00	30.00	45.00	51.08	105.47	349.63
Pressure [kPa]	4378.17	4378.17	3115.05	1034.00	206.84	798.21
Molar Flow [kgmole/hr]	130.00	222.72	219.96	8.40	121.51	2.76
$H_{2,}$ mole fraction	0	0.97	0.4007	0.0897	0	0
CH_4	0	0.03	0.5876	0.8679	0	0
C_6H_6	0	0	0.0104	0.0420	0.9997	0
C_7H_8	1	0	0.0012	0.0004	0.0003	0.00076
$C_{12}H_{10}$	0	0	0	0	0	0.99924

Table A.2 *Continued*

	Gas recycle	Toluene recycle	FEHE1 cold in	FEHE1 cold out	FEHE2 cold out	FEHE3 cold out
Stream name	dischg	d3	cHE1in	cHE1out	cHE2out	cHE3out
Temperature [C]	76.16	183.83	69.67	145.20	246.14	454.79
Pressure [kPa]	4171.33	4378.17	4171.33	3950.70	3743.85	3537.01
Molar Flow [kgmole/h]	1596.30	38.22	1987.26	1987.26	1987.26	1987.26
$H_{2,}$ mole fraction	0.4007	0	0.4304	0.4304	0.4304	0.4304
CH_4	0.5876	0	0.4756	0.4756	0.4756	0.4756
C_6H_6	0.0104	0.00026	0.0084	0.0084	0.0084	0.0084
C_7H_8	0.0012	0.99714	0.0856	0.0856	0.0856	0.0856
$C_{12}H_{10}$	0.0000	0.00260	0	0	0	0

Table A.2 *Continued*

	Reactor inlet	Reactor outlet	Quench	FEHE3 hot in	FEHE3 hot out	Reb3 hot out
Stream name	Rin	Rout	quench	hHE3in	hHE3out	hR3out
Temperature [C]	621.11	665.68	45.38	621.02	450.00	434.88
Pressure [kPa]	3468.06	3350.85	3350.85	3350.85	3309.48	3275.01
Molar Flow [kgmole/h]	1987.26	1987.26	49.00	2036.16	2036.16	2036.16
$H_{2,}$ mole fraction	0.4304	0.3666	0.0044	0.3579	0.3579	0.3579
CH_4	0.4756	0.5408	0.0427	0.5288	0.5288	0.5288
C_6H_6	0.0084	0.0708	0.7123	0.0862	0.0862	0.0862
C_7H_8	0.0856	0.0204	0.2240	0.0253	0.0253	0.0253
$C_{12}H_{10}$	0	0.0014	0.0166	0.0018	0.0018	0.0018

Table A.2 *Continued*

	FEHE2 hot out	Reb1 hot out	Reb2 hot out	FEHE1 hot out	Separator inlet	Separator gas outlet
Stream name	hHE2out	hR1out	hR2out	hHE1out	coolout	gas
Temperature [C]	352.00	307.64	175.69	95.18	45.00	45.00
Pressure [kPa]	3233.64	3212.96	3178.48	3137.12	3115.05	3115.05
Molar Flow [kgmole/h]	2036.16	2036.16	2036.16	2036.16	2036.16	1816.26
H_2, mole fraction	0.3579	0.3579	0.3579	0.3579	0.3579	0.4007
CH_4	0.5288	0.5288	0.5288	0.5288	0.5288	0.5876
C_6H_6	0.0862	0.0862	0.0862	0.0862	0.0862	0.0104
C_7H_8	0.0253	0.0253	0.0253	0.0253	0.0253	0.0012
$C_{12}H_{10}$	0.0018	0.0018	0.0018	0.0018	0.0018	0

Table A.2 *Continued*

	Stabilizer feed	Stabilizer bottoms	Product bottoms	Reb1 cold in	Reb1 cold out	Con/Reb cold in
Stream name	toC1	b1	b2	cR1in	cR1out	cCRin
Temperature [C]	45.25	189.95	145.19	189.92	215.00	145.26
Pressure [kPa]	3630.78	1297.95	907.53	1091.11	1051.11	607.53
Molar Flow [kgmole/h]	170.90	162.49	40.99	183.00	183.00	385.00
H_2, mole fraction	0.0044	0	0	0	0	0
CH_4	0.0427	0	0	0	0	0
C_6H_6	0.7122	0.7476	0.0002	0.7476	0.7476	0.0002
C_7H_8	0.2241	0.2349	0.9300	0.2349	0.2349	0.9300
$C_{12}H_{10}$	0.0166	0.0175	0.0698	0.0175	0.0175	0.0698

Table A.2 *Continued*

	Con/Reb cold out	Reb2 cold out	Reb3 cold in	Reb3 cold out	Con/Reb hot in	Con/Reb hot out
Stream name	cCRout	cR2out	cR3in	cR3out	top	condout
Temperature [C]	162.64	193.00	349.63	350.70	185.07	180.80
Pressure [kPa]	400.68	228.32	591.37	556.89	540.00	526.21
Molar Flow [kgmole/h]	385.00	385.00	47.26	47.26	48.16	48.16
H_2, mole fraction	0	0	0	0	0	0
CH_4	0	0	0	0	0	0
C_6H_6	0.00025	0.00025	0	0	0.00026	0.00026
C_7H_8	0.92996	0.92996	0.00076	0.00076	0.99714	0.99714
$C_{12}H_{10}$	0.06979	0.06979	0.99924	0.99924	0.00260	0.00260

Table A.2 *Continued*

	Column reflux			Column boilup		
	C1	C2	C3	C1	C2	C3
Temperature [C]	51.08	105.47	183.99	215.00	193.00	350.70
Pressure [kPa]	1034.00	206.84	570.00	1051.11	228.32	556.89
Molar Flow [kgmole/hr]	32.73	491.50	9.94	183.00	385	47.26
H_2, mole fraction	0.0003	0	0	0	0	0
CH_4	0.0214	0	0	0	0	0
C_6H_6	0.9564	0.9997	0.00027	0.7476	0.0002	0
C_7H_8	0.0218	0.0003	0.99722	0.2349	0.9300	0.00076
$C_{12}H_{10}$	0	0	0.00251	0.0175	0.0698	0.99924

APPENDIX B
EQUIPMENT AND DATA SPECIFICATION OF HDA PROCESS

Table B.1 Equipment data and specifications of HDA process

Equipments	Specifications	Altenative		
		1	4	6
Reactor	Diameter (m) Length (m) Number of tube	17.374 2.905 1	17.374 2.905 1	17.374 2.905 1
Furnace	Tube volume (m^3)	8.5	8.5	8.5
Cooler	Tube volume (m^3)	8.5	8.5	8.5
Separator	Liquid volume (m^3)	1.13	1.13	1.13
FEHE1*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	14.16 14.16 1.20×10^7	14.16 14.16 2.44×10^6	14.16 14.16 2.37×10^6
FEHE2*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	14.16 14.16 1.68×10^6	14.16 14.16 5.10×10^4
FEHE3*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	- - -	14.16 14.16 1.775×10^5
Reboiler1 (R1)*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	- - -	14.16 14.16 4.01×10^4
Reboiler2 (R2)*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	14.6 14.6 1.60×10^6	14.16 14.16 1.565×10^6
Reboiler3 (R3)*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	- - -	14.16 14.16 2.18×10^4
Condensor/Reboiler (CR)*	Shell volume (m^3) Tube volume (m^3) UA (kJ/C-h)	- - -	14.6 14.6 5.27×10^4	14.16 14.16 5.15×10^4
Tank Bottom C1 (TB1)**	Vesel volume (m^3)	-	-	7.08
Tank Bottom C2 (TB2)**	Vesel volume (m^3)	-	9.06	9.06
Tank Bottom C3 (TB3)**	Vesel volume (m^3)	-	-	2.83
Tank Top C3 (TT3)***	Vesel volume (m^3)	-	4.25	4.25

* simulated by heat exchanger
** simulated by drum to accumulate liquid from the bottom of the three columns
*** simulated by drum to accumulate condensate from the top of column C3

Tabel B.2 Column Specifications of HDA process alternative 1

	Stabilizer Column	Product Column	Recycle Column
Column model	Distillation Column	Distillation Column	Distillation Column
Number of theoretical tray	6	27	7
Feed tray	3	15	5
Pressure (kPa)	1034.25	206.85	206.85
Diameter (m)	1.067	1.829	0.762
Weir length (m)	0.8842	1.265	0.5181
Weir height (m)	0.0508	0.0508	0.0508
Tray spacing (m)	0.6096	0.6096	0.6096
Tray type	Sieve	Sieve	Sieve
Reboiler vol. (m^3)	7.079	9.061	1.416
Condenser vol. (m^3)	0.283	8.495	2.832
Specification 1	Benzene mole fraction in overhead = 0.042	Toluene mole fraction in overhead = 0.0003	Diphenyl mole fraction in overhead = 0.00002
Specification 2	Methane mole fraction in bottoms = 0.000001	Benzene mole fraction in bottoms = 0.0006	Toluene mole fraction in bottoms = 0.00026

Table B.3 Column Specifications of HDA process alternative 4

	Stabilizer Column	Product Column	Recycle Column
Column model	Distillation Column	Refluxed Absorber	Reboiled Absorber
Number of theoretical tray	6	27	7
Feed tray	3	15	5
Pressure (kPa)	1034.25	206.85	540.00
Diameter (m)	1.067	1.981	0.762
Weir length (m)	0.8842	1.405	0.5563
Weir height (m)	0.0508	0.0508	0.0508
Tray spacing (m)	0.6096	0.6096	0.6096
Tray type	Sieve	Sieve	Sieve
Reboiler vol. (m^3)	7.079	-	2.832
Condenser vol. (m^3)	0.510	10.370	-
Specification 1	Benzene mole fraction in overhead = 0.042	Toluene mole fraction in overhead = 0.0003	-
Specification 2	Methane mole fraction in bottoms = 0.000001	-	Toluene mole fraction in bottoms = 0.00026

Table B.4 Column Specifications of HDA process alternative 6

	Stabilizer Column	Product Column	Recycle Column
Model	Refluxed Absorber	Refluxed Absorber	Absorber
Number of theoretical tray	6	27	7
Feed tray	3	15	5
Pressure (kPa)	1034.25	206.85	540.00
Diameter (m)	1.067	1.981	0.6096
Weir length (m)	0.8842	1.405	0.4544
Weir height (m)	0.0508	0.0508	0.0508
Tray spacing (m)	0.6096	0.6096	0.6096
Tray type	Sieve	Sieve	Sieve
Reboiler vol. (m^3)	-	-	-
Condenser vol. (m^3)	0.510	10.37	-
Specification 1	Benzene mole fraction in overhead = 0.042	Toluene mole fraction in overhead = 0.0003	-
Specification 2	-	-	-

APPENDIX C
MATCH PATTERN

A heuristic approach to design or synthesize a resilient HEN has been presented by Wongsri (1990). A resilient network is defined as a network that provides a down path for variable process streams so that their specified input heat load disturbances can be shifted to the heaters or coolers in their network without violation in the specified target temperatures and MER. HEN synthesis is usually considered as a combinatorial matching problem. Match patterns are the descriptions of the match configuration of two, and possibly more, process streams and their properties that are thermally connected with the heat exchangers.

C.1 Classes of Match Paterns

There are four match patterns for a pair of hot and cold streams according to the match position and the length (heat load) of stream. The four match patterns are considered to be the basic match pattern classes and simply called A, B, C, and D as shown in Figures C.1 to C.4. Any eligible match must belong to one of the four match pattern classes.

C.1.1 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 (Figure C.1).

C.1.2 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 (Figure C.2).

C.1.3 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 (Figure C.3).

C.1.4. 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 (Figure C.4).

C.2 Resilient Match Patterns

When the residual heat load in a match pattern is matched to a utility stream, it is a 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 requirements (depend on the types of the problems and the match pattern) then the chances that the match pattern will be matched to a utility stream is high. So, we give a match pattern which its residual less than the minimum heating or cooling requirement a high priority in match selection.

Resiliency of a match pattern can be achieved if the disturbances in input conditions of the hot and cold streams can be transferred to the active stream (a residual portion). For Class A and Class B (Figures C.1 and C.2), the disturbance of a member stream can be transferred to the residual. So, they are considered to be potential resilient match pattern.

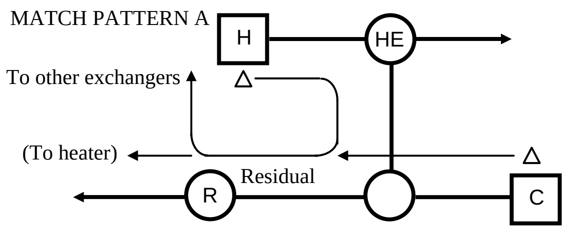


Figure C.1 Class A Match Pattern

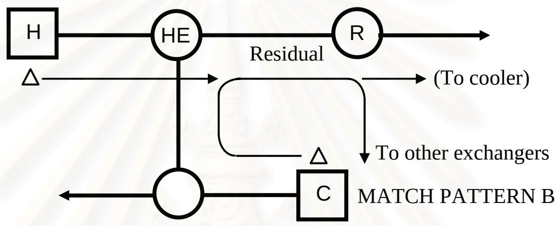


Figure C.2 Class B Match Pattern

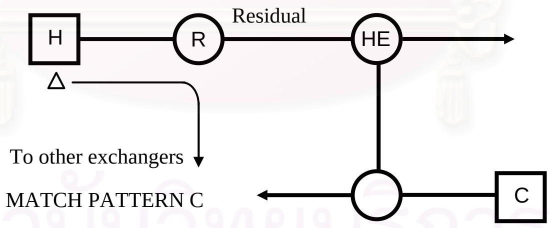


Figure C.3 Class C Match Pattern

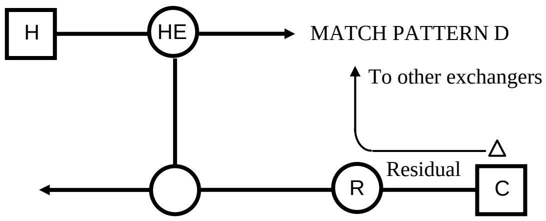


Figure C.4 Class D Match Pattern

For Class C and Class D (Figures C.3 and C.4), we can see that only the disturbances of a hot stream in Class C and of a cold stream in Class D can be managed but neither a cold stream in Class C nor a hot stream in Class D. Since these two classes cannot handle disturbance of one of their streams, they are considered non-resilient match pattern. Class C and Class D match patterns can be taken into account only when the non-resilient streams in these classes are not subjected to the variations. If the other streams in Class C and Class D must be resilient, its residual stream must be connected to either Class A or Class B match patterns. Hence the only two classes of interests are Class A and Class B.

APPENDIX D
DISTURBANCE PROPAGATION DESIGN

Wongsri (1990) developed the disturbance propagation design (DPD) based on the shift approach. 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.

D.1 Design Conditions

There several design conditions, and usually, these are spesified at extreme operating conditions as follows:

1. *Nominal operating condition*

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

2. *Maximum heat load condition.*

   This is a condition where all process streams at their maximum heat loads. For example, input temperatures of hot streams are the highest and of cold streams are the lowest. This is also known as the largest maximum energy recovery condition.

3. *Minimum heat load condition*

   This is a condition where all process streams at their minimum heat loads. For example, input temperatures of hot streams are the lowest and of cold streams are the higest. This is also known as the lowest maximum energy recovery condition.

D.2 Shift Approach

The variations of temperature and heat capacity flowrate can be viewed as a heat packet that can be shifted through the streams and heat exchangers to dissipate in heat sinks (coolers) or heat sources (heater) of a network.

In this approach, there are two cases to be considered as follows:

1. The disturbance load is shifted to a utility exchanger within its network, where it does not across the pinch temperature.

2. The disturbance load is shifted across the pinch temperature to a utility exchanger within its network.

Wongsri (1990) focused on the first case to develop synthesis procedure for a resilient heat exchanger network.

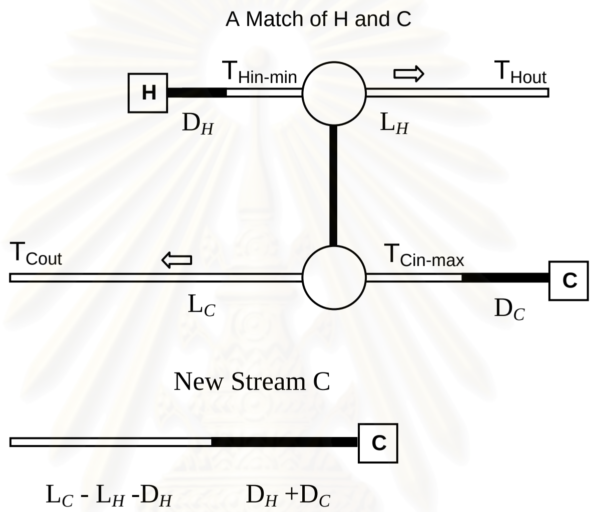
D.3 Disturbance Propagation Design (DPD)

The principles of the DPD can be summarized as follows:

1. The disturbance load of a smaller stream will be shifted to a larger stream. The propagated disturbance of a process stream is the disturbance caused by a variation in heat load of process stream 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 D.1).

2. The design condition was selected to be the minimum heat load condition. This is a condition where all process streams are at their minimum heat loads. For example the input temperatures of hot streams are the lowest and those of cold stream are the highest.

3. Then only the positive disturbance loads of process streams were considered. Thus, the positive disturbance load originating from the hot stream is shifted to heater, and the positive disturbance load originating from the cold stream is shifted to the cooler.



Notes:

D_H : The original disturbance of hot stream

D_C : The original disturbance of cold stream

L_H : The Load of hot stream

L_H : The Load of cold stream

$T_{Hin\text{-}min}$: the inlet temperature of hot stream at the lowest

$T_{Cin\text{-}max}$: the inlet temperature of cold stream at the highest

Design condition was selected to be the minimum heat load condition. Thus, only positive disturbances were considered.

Figure D.1 A concept of propagated disturbance

APPENDIX E
PINCH TEMPERATURE FOR HEN OF HDA PROCESS

The pinch design method (Linnhoff and Hindmarsh, 1983) is used to determine the pinch temperature for heat exchanger network (HEN) of the HDA process. The pinch location for HEN problem, together with the minimum utility requirement can be calculated using the problem table algorithm for a specified value of ΔT_{min}.

E.1 HEN Problem of HDA Process Alternative 4

The stream data for the HDA process alternative 4 are given in Table E.1. Note that the data is based on constant heat capacity flowrate (CP). The results of the problem table algorithm for the HDA process alternative 4 with a ΔT_{min} of 10 ^oC are shown in Table E.2.

Based on Table E.2, for the HDA process alternative 4, in the table stream data are shown on the left, divided into six temperature intervals, corresponding to sub-networks and therefore called SN1 – SN6. For example, SN2 is defined by the target temperature of stream C2 and the supply temperature of stream H2. Note that to ensure the feasibility of complete heat exchange hot and cold streams are separated by ΔT_{min}. For example, the upper boundary of SN2 is defined by cold stream C2 at 193 ^oC while the hot stream at this point is 203 ^oC.

Table E.1 Stream data for HEN of HDA process alternative 4

Stream	Type	Heat Capacity Flowrate, CP (kW/^{o}C)	Temperature (^{o}C) Supply	Target
C1	COLD	32.240	68	621
C2	COLD	91.300	145	193
H1	HOT	32.985	621	45
H2	HOT	196.700	183	181

Table E.2 The problem table for HEN of HDA process alternative 4

Sub-					1	2	3	4	5
Network	Streams and Temperatures				Deficit	Accumulated		Heat Flow	
SN	C1 C2	^{o}C	^{o}C	H1 H2	kW	input	output	input	output
		621	621						
SN1		193	203		10.99	0.00	-10.99	3964.23	3953.24
SN2		173	183		1811.10	-10.99	-1822.09	3953.24	2142.14
SN3		171	181		-212.29	-1822.09	-1609.80	2142.14	2354.43
SN4		145	155		2354.43	-1609.80	-3964.23	2354.43	0.00
SN5		68	78		-57.36	-3964.23	-3906.87	0.00	57.36
SN6			45		-1088.51	-3906.87	-2818.36	57.36	1145.87

The feasibility of complete heat exchange between all hot and cold streams is an important feature of the problem table algorithm. It means that for each sub-network there will either be a net deficit or surplus but never both. These deficit or surplus figures are shown in column 1 of Table E.2. The sign convention is such that a surplus is negative and a deficit is positive.

Another important feature of the problem table algorithm is the feasibility of heat transfer from higher to lower sub-networks (cascading). In other words, heat surplus from higher temperature sub-network can be used to satisfy heat deficit of lower temperature sub-networks. The calculation of the amount of heat which can be passed on this manner is performed in column 2 and column 3 of Table E.2. It is initially assumed that the heat input from external utilities is zero. This is represented by a zero input for SN1 (see column 2 of Table E.2). Having made this assumption, it is easy to calculate the output (column 3 of Table E.2) from SN1 by simply adding the surplus to the input. Then, this forms the input to SN2. The procedure is repeated for al sub-networks.

To be feasible, the flow of heat from high temperature sub-networks to low temperature sub-networks must not be negative. Thus if negative values are generated in columns 2 and 3 of Table E.2 the heat input to SN1 must be increased. The minimum increase is that which guarantees that all heat flows are positive or negative (see columns 4 and 5 of Table E.2). The minimum hot utility usage for HDA process alternative 4 is then given by the input heat to SN1, i.e. its value is 3964.23

kW (column 4 of Table E.2). The minimum cold utility usage is given by the heat flow out of SN6, i.e. its value is 1145.87 kW (column 5 of Table E.2).

Notice that the heat flow from SN4 to SN5 is zero. All other flows are positive. The point of zero heat flow represents the pinch. Therefore, the pinch temperature for HEN of HDA process alternative 4 is 150 ^{o}C.

E.2 HEN Problem of HDA Process Alternative 6

The stream data for the HDA process alternative 6 are given in Table E.3. Note that the data is based on constant heat capacity flowrate (CP). The results of the problem table algorithm for the HDA process alternative 6 with a ΔT_{min} of 10 ^{o}C are shown in Table E.4.

Based on Table E.4, for the HDA process alternative 6, in the table stream data are shown on the left, divided into ten temperature intervals, corresponding to sub-networks and therefore called SN1 – SN10. For example, SN2 is defined by the target temperature of stream C4 and the supply temperature of stream C4. Note that to ensure the feasibility of complete heat exchange hot and cold streams are separated by ΔT_{min}. For example, the upper boundary of SN2 is defined by cold stream C4 at 350.7 ^{o}C while the hot stream at this point is 360.7 ^{o}C.

Table E.3 Stream data for HEN of HDA process alternative 6

Stream	Type	Heat Capacity Flowrate, CP (kW/^{o}C)	Temperature (^{o}C) Supply	Target
C1	COLD	32.240	69	621
C2	COLD	91.300	145	193
C3	COLD	58.5	190	215
C4	COLD	422.3	349.4	350.7
H1	HOT	32.985	621	45
H2	HOT	99.5	185	181

Table E.4 The problem table for HEN of HDA process alternative 6

Sub-									1	2	3	4	5
network	Streams and Temperatures								Deficit	Accumulated		Heat Flow	
SN	C1	C2	C3	C4	^oC	^oC	H1	H2	kW	input	output	input	output
					621	621							
SN1					350.7	360.7			128.48	0.00	-128.48	5971.13	5842.66
SN2					349.4	359.4			548.03	-128.48	-676.51	5842.66	5294.62
SN3					215	225			-100.13	-676.51	-576.38	5294.62	5394.75
SN4					193	203			1270.61	-576.38	-1846.99	5394.75	4124.14
SN5					190	200			447.17	-1846.99	-2294.16	4124.14	3676.98
SN6					175	185			1358.33	-2294.16	-3652.48	3676.98	2318.65
SN7					171	181			-35.78	-3652.48	-3616.70	2318.65	2354.43
SN8					145	155			2354.43	-3616.70	-5971.13	2354.43	0.00
SN9					69	79			-56.62	-5971.13	-5914.51	0.00	56.62
SN10						45			-1121.49	-5914.51	-4793.02	56.62	1178.11

By using the same procedure with that used in HDA process alternative 4, the minimum hot utility usage for HDA process alternative 6 is given by the input heat to SN1, i.e. its value is 5971.13 kW (column 4 of Table E.4). The minimum cold utility usage is given by the heat flow out of SN10, i.e. its value is 1178.11 kW (column 5 of Table E.4). Notice that the heat flow from SN8 to SN9 is zero. All other flows are positive. The point of zero heat flow represents the pinch. Therefore, the pinch temperature for HEN of HDA process alternative 6 is 150 ^oC.

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