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นางสาวอมรรัตน์ ปานใย

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DESIGN OF HEAT INTEGRATED AND CONTROL STRUCTURES OF BUTANE ISOMERIZATION PLANT FOR REVERSIBLE REACTION CASE

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A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering
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อมรรัตน์ ปานใย : การออกแบบโครงสร้างการควบคุมและการเบ็ดเสร็จพลังงานของโรงงานบิวเทนไอโซเมอไรเซชันสำหรับกรณีปฏิกิริยาแบบผันกลับ. (DESIGN OF HEAT INTEGRATED AND CONTROL STRUCTURES OF BUTANE ISOMERIZATION PLANT FOR REVERSIBLE REACTION CASE) อ.ที่ปรึกษาวิทยานิพนธ์หลัก : ผศ.ดร. มนตรี วงศ์ศรี , 157 หน้า.

ในงานวิจัยนี้ได้ศึกษาการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ มาพัฒนาโครงสร้างการควบคุมโรงงานบิวเทนไอโซเมอไรเซชัน สำหรับปฏิกิริยาแบบผันกลับที่มีการเบ็ดเสร็จพลังงาน เพื่อให้เป็นไปตามวัตถุประสงค์ของการควบคุม โดยโรงงานบิวเทนไอโซเมอไรเซชันนั้น เป็นโรงงานที่มีความซับซ้อน ประกอบไปด้วยหน่วยปฏิบัติการหลายหน่วย โดยกระบวนการทำปฏิกิริยาจะทำการเปลี่ยนนอร์มอลบิวเทนไปเป็นไอโซบิวเทน ซึ่งไอโซบิวเทนที่ได้นั้นมีความสำคัญในอุตสาหกรรมปิโตรเคมี โดยในงานวิจัยนี้ได้ทำการจำลองข่ายงานเครื่องแลกเปลี่ยนความร้อนจำนวน 4 ทางเลือก ได้แก่ RHEN1-3 และกรณีฐานของ Luyben (1998) รวมทั้งโครงสร้างการควบคุมโรงงานบิวเทนไอโซเมอไรเซชัน สำหรับปฏิกิริยาแบบผันกลับ จำนวน 4 ทางเลือก ได้แก่ CS1-4 ซึ่ง CS1-3 ใช้หลักการออกแบบแพลนท์ไวด์ของ Luyben และ CS4 ใช้ทฤษฎี "Fixture point" ของวงศ์ศรี (2008) และสำหรับกระบวนการที่มีการเบ็ดเสร็จพลังงานใช้หลักการออกแบบ โดยวิธีส่งผ่านความแปรปรวนของ Wongsri เพื่อให้ได้มาซึ่งการนำกลับมวลสารเพื่อเข้ามาใช้ใหม่ในกระบวนการพลวัต จากนั้นทำการประเมินค่าประหยัดพลังงานของข่ายงานที่ 1-3 (RHEN1-3) เทียบกับกรณีฐานของ Luyben (1998) พบว่าสามารถประหยัดพลังงานได้ถึง 15.11-22.09 เปอร์เซนต์ และเนื่องจากกระบวนการที่มีการเบ็ดเสร็จพลังงานนั้น การควบคุมจะเป็นไปได้ยากมากขึ้น ดังนั้นโครงสร้างการควบคุมที่เหมาะสมจึงมีความจำเป็นต่อการดำเนินการของกระบวนการ และเมื่อนำโครงสร้างทั้งหมดนี้มาควบคุมกระบวนการที่มีการเบ็ดเสร็จพลังงานต่างๆ ในการประเมินสมรรถนะโครงสร้างการควบคุมโดยใช้ตัวรบกวนกระบวนการ 2 ชนิด ได้แก่ การรบกวนทางความร้อน และการรบกวนอัตราการไหลของสาร พบว่าโครงสร้าง CS2 และ CS3 เป็นโครงสร้างที่เหมาะสมเมื่อมีการรบกวนทางความร้อน และอัตราการไหล และข่ายงานเครื่องแลกเปลี่ยนความร้อนที่มีการเบ็ดเสร็จพลังงาน RHEN-1 ให้สมรรถนะในการควบคุมดีที่สุด โดยข่ายงานเครื่องแลกเปลี่ยนความร้อน และโครงสร้างการควบคุมที่ถูกออกแบบจะทำการประเมินสมรรถนะแบบจำลองโดยใช้โปรแกรมไฮซีส

ภาควิชา........วิศวกรรมเคมี........ ลายมือชื่อนิสิต.......อมรรัตน์ ปานใย.......................
สาขาวิชา.......วิศวกรรมเคมี........ ลายมือชื่ออ.ที่ปรึกษาวิทยานิพนธ์หลัก.........................
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AMORNRAT PANYAI : DESIGN OF HEAT INTEGRATED AND CONTROL STRUCTURES OF BUTANE ISOMERIZATION PLANT FOR REVERSIBLE REACTION CASE. ADVISOR: ASST. PROF. MONTREE WONGSRI, D.Sc., 157 pp.

This study is to use plantwide control strategies to develop the control structures for the butane isomerization plant for reversible reaction case with energy integration schemes that are designed to achieve the control objective. The butane isomerization process is a complex plant consisting of many unit operations converting normal butane (nC_4) into isobutane (iC_4). In this work presents 4 alternatives of heat integrated (RHEN1-3 and Base case) with 4 alternatives of the control structure (CS1-4) for butane isomerization plant for reversible reaction are simulated using Luyben's heuristics method and Fixture point theorem (Wongsri, 2008). Various heat pathways throughout the network designed using Wongsri's disturbance propagation method to achieve dynamic maximum energy recovery. They are evaluated energy saving compared to Base case (Luyben, 1998), the energy saved is 15.11-22.09 %. Because of control difficulties associated with heat integration, the suitable control structure is necessary to process operation. We found that CS2 and CS3 are proper control structures with heat-integrated process when change in thermal disturbance and change in material flow disturbance and RHEN-1 have a performance control better than RHEN-2 and RHEN-3. The performances of the plants using software HYSYS for heat exchanger networks and control structures.

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Student's Signature:...Amornrat Panyai....
Advisor's Signature:........................

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LIST OF ABBREVIATIONS

Alt1	Alternative 1
Alt2	Alternative 2
Alt3	Alternative 3
C_3	Propane
Ci	Cold stream
CS1	Reference control structure I
CS2	Reference control structure II
CS3	Design of control structure I
CS4	Design of control structure II
D	Disturbance
DMER	Dynamic maximum energy recovery
Hi	Hot stream
HEN	Heat exchanger network
HPH	Heat pathway heuristics
IAE	Integral absolute error
iC_4	isobutane
k_F	Forward rate constant
k_R	Reverse rate constant
MER	Maximum energy recovery
nC_4	normal butane
P	Pressure, psia
R	Reaction rate of isomerization reaction
RHEN	Resilient heat exchanger network
T	Temperature, ^oF
V_R	Reactor volume
W	The heat capacity flowrate units of Btu/hr-^oF

CHAPTER I

INTRODUCTION

This chapter consists of importance and reasons for research, objectives of research, scopes of research, contributions of research, procedure plan and research contents.

1.1 Importance and Reasons for Research

At present, the energy demands and fuel cost are increasing in every year. Therefore energy saving, conserving energy and minimizing losses are the most important and the best way in the petrochemical industry, the importance of developing process to use heat exchanger network (HEN) because it determines to large extent the net energy consumption of the process.

In general, most industrial processes contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. The economic can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. They also interconnect separate unit operations and create a path for disturbance propagation. Therefore, strategies for plantwide control are required to operate an entire plant safely and achieve its design objectives. Essentially, the plantwide control problem is how to develop the control loops needed to operate an entire process and achieves its design objectives.

The butane isomerization process is a complex plant consisting of many unit operations. Process to convert normal butane (nC_4) into isobutane (iC_4), this process is quite important in the petroleum industry because isobutene is usually more valuable as a chemical feedstock than normal butane. The typical amount of iC_4 contain in crude oil and produce in refinery operations such as catalytic cracking is sometimes not enough to satisfy the demand.

This study is to use plantwide control strategies to develop the new control structures for the butane isomerization process for reversible reaction case with energy integration schemes that are designed to achieve the control object. In this work, the performances of the heat exchanger network (HEN) are designed and their control structures are evaluated via commercial software HYSYS to carry out both steady state and dynamic simulations.

1.2 Research Objectives

1. To design heat exchanger networks of the butane isomerization plant for reversible reaction by using disturbance load propagation method (Wongsri, 1990).
2. To design control structures for heat exchanger network in butane isomerization plant for reversible reaction.
3. To evaluate performance of the designed control structures for heat exchanger network compared to the structures of Luyben (1998) and Wilailak (2007).

1.3 Scopes of research

1. The heat exchanger networks with control structures of the butane isomerization plant for reversible reaction are programmed using HYSYS for control structure performance tests.
2. Description and data of the heat exchanger network in butane isomerization plant are obtained from Luyben, Tyreus, and Luyben (1998).
3. The design control structures for energy-integrated butane isomerization plant for reversible reaction are designed using Luyben's heuristics method and Fixture point theorem.

4. The number of design heat exchanger networks in the butane isomerization plant are 3 alternatives (not include Luyben).
5. The number of control structures are 4 alternatives include Luyben's 1 alternative, Wilailak's 1 alternative and new design 2 alternatives which are designed heat exchanger network.

1.4 Contributions of research

1. The new control structures of the butane isomerization plant for reversible reaction with heat integration are designed and compared with the earlier work given by Luyben with no energy recovery
2. New energy integrated designs of the butane isomerization plant for reversible reaction.

1.5 Procedure Plan

1. Study of plantwide process control theory, the butane isomerization plant for reversible reaction and concerned information.
2. Study and design heat exchanger networks of the butane isomerization plant for reversible reaction by using HEN heuristics.
3. Steady state modeling and simulation of heat exchanger networks of the butane isomerization plant for reversible reaction.
4. Study of dynamic modeling and simulation of the heat exchanger network in butane isomerization plant for reversible reaction with no energy integration.
5. Design of control structures for heat exchanger network in butane isomerization plant for reversible reaction

6. Dynamic Simulation for the energy-integrated butane isomerization plant for reversible reaction with control structures design.
7. Assessment of the dynamic performance of the control structure.
8. Analysis of the design and simulation results.
9. Conclusion of the thesis.

1.6 Research Contents

This thesis is divided into six chapters.

Chapter I is an introduction to this research. This chapter consists of research objectives, scope of research, contribution of research, and procedure plan.

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

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

Chapter IV describes the process description and the design of heat exchanger networks for the butane isomerization plant.

Chapter V describes the design of plantwide control structures and dynamic simulation results and compare with control structures of Luyben and Wilailak.

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

This is follow by:

References

Appendix A: Process and Equipment Data.

Appendix B: Parameter Tuning of Control Structures.

Appendix C: Dynamic Responses.

Appendix D: Fixture Point Theorem Data.

CHAPTER II

LITERATURE REVIEW

2.1 Heat Exchanger Networks (HENs)

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

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

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 with no more units than 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 problem 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, 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, Dunford and Smith (1983) studied heat integration of distillation columns into overall process. This study reveals that good integration between distillation and the overall process can result in column operating at effectively zero utility cost. Generally, the good integration is when the integration as column not crossing heat recovery pinches of the process and either the reboiler or the condenser being integrated with the process. If these criteria can be met, energy cost for distillation can effectively be zero.

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

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

Saboo and Morari (1984) proposed the corner point theorem which states that for temperature variation only, if a network allows MER without violating ?Tmin at M corner points, then the network is structurally resilient or flexible. This is the case where the constraint is convex, so examining the vertices of the polyhedron is sufficient. This procedure again can only apply to restricted classes of HEN problem. Their design procedure is similar to Marselle et al. (1982), but using two extreme cases to develop the network structure. The strategy for both procedures is finding similar optional network structures for the extreme cases and the base case design in order that they may be easily merged and not have too many units. Two extreme cases are:

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

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

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

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

Wongsri (1990) presented a resilient HEN design. 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 ability of a HEN to tolerate unwanted changes is called resiliency. A resilient HEN synthesis procedure was developed based on the match pattern design and a physical understanding of the disturbances propagation concept.

2.2 Design and Control of Energy-Integrated Process

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

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

Jones and Wilson (1997) considered the range ability of flows in the bypass line of heat exchanger through interesting heat exchanger problems. Difficulty is immediately encountered when considering heat exchanger between two process streams; changing the flowrate of one will certainly affect the exit temperature of the other. Unfortunately, interfering with a process stream flowrate immediately upsets the plant mass balance, which is undesirable. The 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.

Luyben, Tyreus and Luyben (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 step of the proposed procedure center around the fundamental principles of plantwide control: energy management, production rate, product quality, operational, environmental and safety constraints, liquid-level and gas-pressure inventories, makeup of reactants, component balances and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, Eastman process and HDA process. The procedure produced a workable plantwide control strategy for a given process design. The control system was tested on a dynamic model built with TMODS, Dupont's in-house simulator.

Luyben (1998) presented base case of heat exchanger network (HEN) designs with 1 heat exchanger and two alternatives of control structure of Butane Isomerization plant. Disturbances are used to evaluate control structure performances: thermal disturbance and the material flow disturbance.

Kunlawaniteewat (2001) proposed the rules and procedure for design control structure of heat exchanger network using heuristic approach for to achieve outlet temperature targets and maintain maximum energy recovery (MER). The rules are categorized as following: generals, match pattern, loop placement, bypass placement, and split fraction rules.

Wongsri and Kietawarin (2002) presented a comparison among four control structures designed for withstanding disturbances that cause production rate change of HDA process. The changes had been introduced to the amount of toluene and feed temperature before entering the reactor. Compared with the reference control structure using a level control to control toluene quantity in the system, the first control scheme measured toluene flowrate in the process and adjusted the fresh toluene feed rate. This structure resulted in faster dynamic response than the reference structure. The second control scheme was modified from the first scheme by adding a cooling unit to control the outlet temperature from the reactor, instead of using internal process flow. The result was to reduce material and separation ratio fluctuations within the process. The product quality was also quite steadily. In the third control scheme, a ratio control was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process. This scheme showed that it could withstand large disturbances. Dynamic study showed that the control structure had significant effect on process behavior. A good system control should quickly response to disturbances and adjusts itself to steady state while minimizing the deviation of the product quality.

Wongsri and Thaicharoen (2004) presented the new control structures for HDA process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben's structure (CS1). The result showed that the HDA process with heat integration can reduce energy cost. Furthermore, this process can be operated well by using plantwide methodology to design the control structure. The dynamics responses of the designed control structures and the reference structure are similar. The CS2 has been limited in bypass. So, it is able to handle in small disturbances. The CS3 has been designed to improve CS2 in order to handle more disturbances by using auxiliary heater instead of bypass valve to control temperature of stabilizer column. The recycle column temperature control response of the CS4 is faster than that of the previous control structures, because reboiler duty of column can control the column temperature more effective than bottom flow. The CS5, on - demand structure has an advantage when downstream customer desires immediate responses in the availability of the product stream from this process. The energy used in CS6 control structure is less than CS1 and CS4.

Wongsri and Hermawan (2004) studied the control strategies for energy integrated HDA plant (i.e. alternative 1, 4 and 6) based on the heat pathway heuristics, i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the dynamic maximum energy recovery (DMER) can be achieved with some trade-off. In addition, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network. The new control structure with the LSS has been applied in the HDA plant.

Wongsri and Kunajitpimol (2006) presented four alternatives of heat exchanger network (HEN) designs and two alternatives of control structure of Butane Isomerization plant. The control difficulties associated with heat integration were solved by adding auxiliary utilities which was kept minimal. Heat exchanger network designs used the heat from the reactor effluent stream to provide the heat for the column reboiler. The energy saving was 24.88 % from the design without heat integration, but the capital cost raised about 0.67 % due to adding of a process to process exchanger and an auxiliary utility exchanger to the process. The plantwide control structures were designed following Luyben's heuristic method. The result showed that the control structures can reject disturbances better than base case which were designed by Luyben. The designed control structure was evaluated based on the rigorous dynamic simulation using the commercial software HYSYS.

Wongsri and Wilailak (2007) presented three new alternatives of heat exchanger networks are designed to reduce complex of heat integrated structures for Butane Isomerization plant. The resilient heat exchanger networks design follows Wongsri's resilient HEN synthesis method (1990). They used 1 feed effluent heat exchanger (FEHE) which has completely heat exchange. The plantwide control configuration of heat-integrated plant is designed following Luyben's heuristic method. Two kinds of disturbances are used to evaluate control structure performances: thermal disturbance and the material flow disturbance.

CHAPTER III

THEORY

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

3.1 Basic Knowledge for Pinch Technology

3.1.1 Pinch Technology

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

3.1.2 Basic Pinch Analysis Concept

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

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

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

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

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

where:

CP = heat capacity flow rate (kW/C)
C_p = Specific heat capacity of the stream (kJ/C.kg)
F = mass flow rate of the stream (kg/s)

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

Table 3.2 The problem table for data given in Table 3.1

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

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

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

3.2 Heat Exchanger networks (HENs)

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

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

3.2.1 Definition of HEN Resiliency

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

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

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

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

3.2.2 Heuristics for HEN Synthesis

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

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

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

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

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

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

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

Heuristic E2. Do not transfer heat across the pinch.

Heuristic E3. Do not cool above the pinch.

Heuristic E4. Do not heat below the pinch.

The laws of thermodynamics:

Heuristic T1. In a heating problem, if a supply temperature of a cold stream is less than a target temperature of a hot stream by Tmin or more and the heat capacity flow rate of a hot stream is less than or equal to the heat capacity flow rate of a cold stream, the match between these two streams is feasible.

(Immediately above the pinch temperature, the heat capacity flow rate of a cold stream must be greater than or equal to that of a hot stream.)

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

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

3.2.3 Math Classification

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

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

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

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

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

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

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

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

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

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

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

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

3.2.4 Match Patterns

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

By using the 'tick off rule' there are four match patterns for a pair of hot and cold streams according to the match position and the length (heat load) of streams. The four patterns are considered to the basic match pattern classes. The members of these classes are the patterns where other configurations and properties are specified. The four match pattern classes are simply called A, B, C and D and are shown in Figure 3.1, 3.2, 3.3 and 3.4 respectively. Any eligible match must belong to one of the four match pattern classes.

Definition 3.1 Class A Match Pattern: The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the cold end of the cold stream. The residual heat load is on the hot portion of the cold stream. (See Figure 3.1)

A match of this class is a first type match at cold end position and the heat load of the cold stream is greater than that of the hot stream. This is a upstream match. For a heating subproblem, a Class A match is favored, because it leaves a cold process stream at the hot end (Heuristic N1) and follows the pinch heuristics. (See Table 3.3)

Definition 3.2 Class B Match Pattern: The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the hot end of the hot stream. The residual heat load is on the cold portion of the hot stream. (See Figure 3.2)

A match of this class is a second type match; a hot end match and the heat load of the hot stream is greater than that of the cold stream. This is an upstream match. For a cooling subproblem, a Class B match is favored, because it leaves a hot process stream at the cold end (Heuristic N2) and also follows the pinch heuristics. (See Table 3.3)

Definition 3.3 Class C Match Pattern: The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the cold end of the hot stream. The residual heat load is on the hot portion of the hot stream. (See Figure 3.3)

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

Definition 3.4 Class D Match Pattern: The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the hot end of the cold stream. The residual heat load is on the cold portion of the cold stream. (See Figure 3.4)

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

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

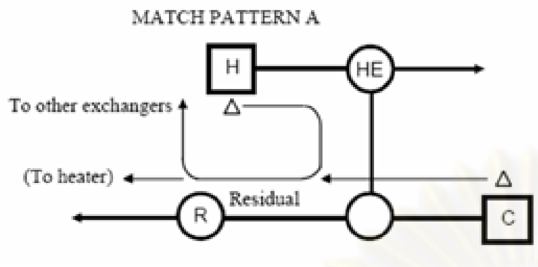


Figure 3.1 Class A Match Pattern.

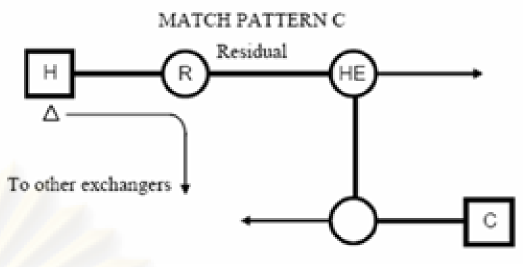


Figure 3.3 Class C Match Pattern

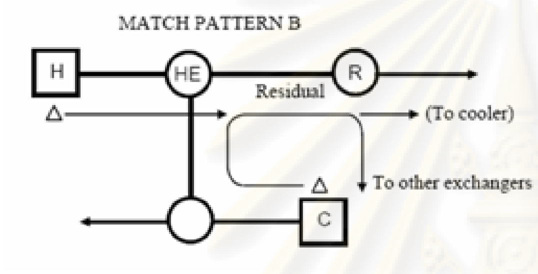


Figure 3.2 Class B Match Pattern.

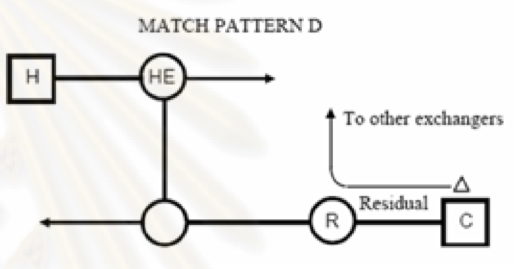
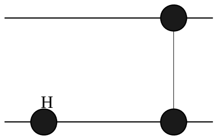
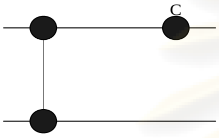
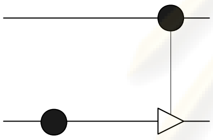
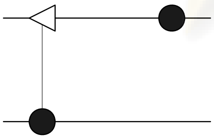
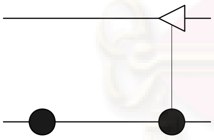
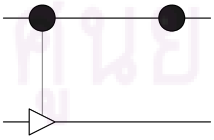


Figure 3.4 Class D Match Pattern

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

Table 3.3 Match Pattern Operators of Class A and B

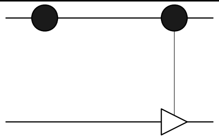
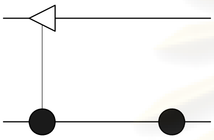
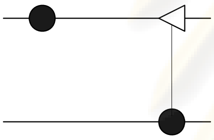
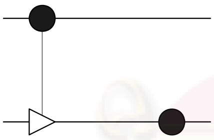
Match Operators	Conditions	Actions
 Pattern AH	$T_H^s{}^{*} \geq T_C^t{}^{**}$ $L_H \leq L_C$ $T_H^s \geq T_C^s + L_H\, W_C^{-1}$ $L_C - L_H \leq Q_{\min}^{heating}$	Match H and C Status of H $\Leftarrow$ Matched*** $T_C^s \Leftarrow T_C^s + L_H\, W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern BK	$T_H^s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

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

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

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

Table 3.4 Match Pattern Operators of Class C and D

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

3.2.5 Disturbance Propagation Design Method

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

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

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

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

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

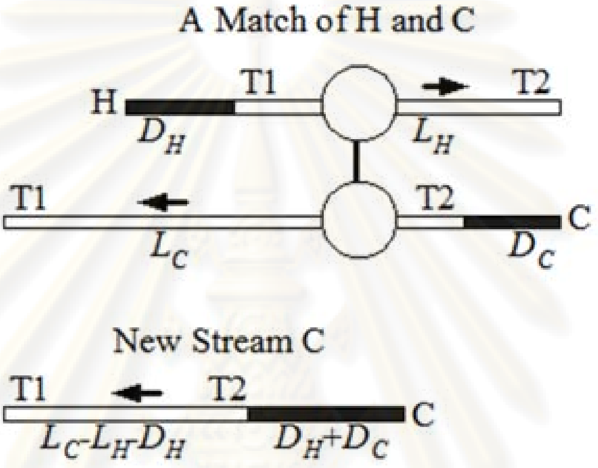


Figure 3.5 A Concept of Propagated Disturbance

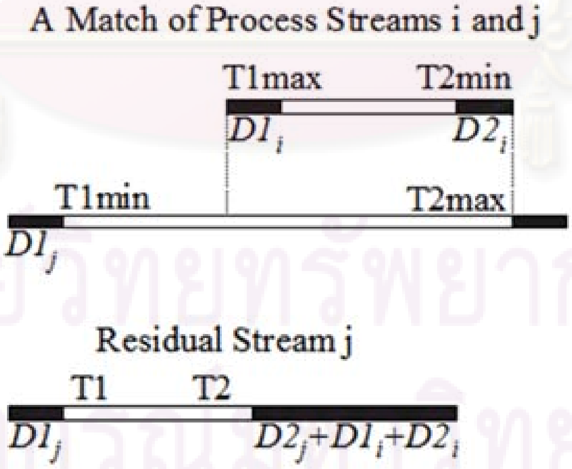


Figure 3.6 A General Concept of Propagated Disturbance

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

3.2.6 Synthesis Procedures

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

1. Push the match operators to a stack in proper order. This is a beginning of a new state.
2. While there is an operator on a stack.

   (a) Pop a match operator form a stack to operate on process streams.

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

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

3.3 Plantwide Control

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

3.3.1 Integrated Process

Figure 3.7 shows integrated process flowsheet. Three basic features of integrated chemical process lie at the root of our need to consider the entire plant's control system: the effect of material recycle, the effect of energy integration, and the need to account for chemical component inventories.

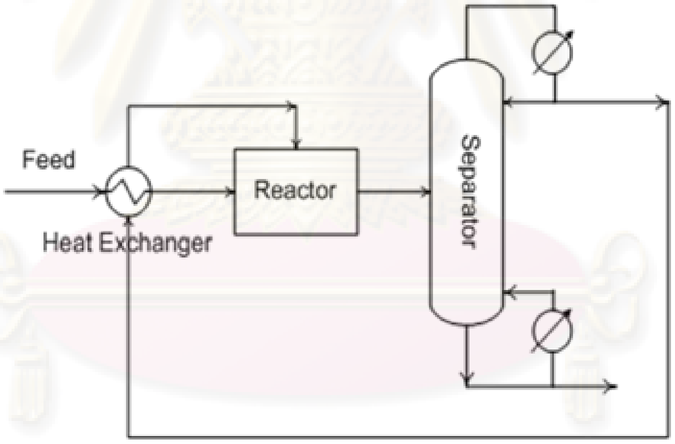


Figure 3.7 Integrated Process flowsheet

3.3.1.1 Material Recycles

Material is recycled for six basic and important reasons.

1. Increase conversion. For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent by necessity contains both reactants

and products. Separation and recycle of reactants are essential if the process is to be economically viable.

2. Improve economics. In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than it is to reach the necessary conversion level in one reactor or several in series. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

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

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

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

6. Control properties. In many polymerization reactors, conversion of monomer is limited to achieve the desired polymer properties. These include average molecular weight, molecular weight distribution, degree of branching, particle size, etc. Another reason for limiting conversion to polymer is to control the

increase in viscosity that is typical of polymer solutions. This facilitates reactor agitation and heat removal and allows the material to be further processed.

3.3.1.2 Energy Integration

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

3.3.1.3 Chemical Component Inventories

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

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

3.3.2 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex. Two basic effect of recycle is: Recycle has an impact on the dynamics of the process. The overall time constant can be much different than the sum of the time constants of the time constants of the individual units. Recycle leads to the "snowball" effect. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates.

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

The large swings in recycle flowrates are undesirable in plant because they can overload the capacity of separation section or move the separation section into a flow region below its minimum turndown. Therefore it is important to select a plantwide control structure that avoids this effect.

3.3.3 Plantwide Control Design Procedures

Step1: Establish control objectives

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

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

Step 2: Determine control degrees of freedom

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

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

Step 3: Establish energy management system

Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system.

We use the term energy management to describe two functions.

1. We must provide a control system that removes exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used elsewhere in the process by other unit operations. This heat, however, must ultimately be dissipated to utilities.

2. If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensure the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

Heat removal in exothermic reactors is crucial because of the potential for thermal runaways. In endothermic reactions, failure to add enough heat simply results in the reaction slowing up. If the exothermic reactor is running adiabatically, the control system must prevent excessive temperature rise through the reactor.

Heat integration of a distillation column with other columns or with reactors is widely used in chemical plants to reduce energy consumption. While these designs look great in terms of steady-state economics, they can lead to complex dynamic behavior and poor performance due to recycling of disturbances. If not already included in the design, trim heater/cooler or heat exchanger bypass line must be added to prevent this. Energy disturbances should be transferred to the plant utility system whenever possible to remove this source of variability from the process units.

Step 4: Set production rate

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

We often want to select a variable that has the least effect on the separation section but also has a rapid and direct effect on reaction rate in the reactor without hitting an operational constraint.

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

We should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times and large steady-state gains.

It should be note that, since product quality considerations have become more important, so it should be establish the product-quality loops first, before the material balance control structure.

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

In most process a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flows in the recycle loop are controlled by level. We have to determine what valve should be used to control each inventory variable. Inventories include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should be controlled with the manipulate variable that has the largest effect on it within that unit (Richardson rule).

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

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

Step 7: Check component balances

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

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

Step 8: Control individual unit operations

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

Step 9: Optimize economics or improve dynamic controllability

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

CHAPTER IV

PROCESS AND DESIGN

4.1 Process Description

The isomerization process is quite important in the petroleum industry because isobutane is usually more valuable as a chemical feedstock than normal butane. The typical amount of iC_4 contained in crude oil and produced in refinery operations such as catalytic cracking is sometime not enough to satisfy the demand. On the other hand the supply of nC_4 sometimes exceeds the demand, particularly in the summer when less nC_4 can be blended into gasoline because of vapor pressure limitations.

Some of the many uses of isobutane include the production of high-octane gasoline blending components by reacting it with various olefins in alkylation processes and the production of propylene oxide and tertiary butane alcohol.

The process consists of a reactor, two distillation columns, and liquid recycle stream. There are four components to consider.

Figure 4.1 shows the flowsheet of the isomerization process to convert normal butane (nC_4) into isobutane (iC_4).

$$\mathrm{nC_4} \rightleftharpoons \mathrm{iC_4}$$

The reaction of nC_4 to iC_4 occurs in the vapor phase and is run at elevated temperatures (400 ^oF) and pressures (600 psia). The reaction of is exothermic (heat of reaction -3600 Btu/lb.mol), so there is a temperature rise as the process stream flows through the adiabatic tubular reactor. Following heat exchanger with the reactor inlet stream and condensation with cooling water, the reactor effluent is introduced a large distillation column that separates the C_4's. The iso/normal separation is difficult because of the similar relative volatilities, so many tray (50) and high reflux ratio (7) are required. For the design case considered, this column ends up being 16 feet in diameter. This column is called a deisobutanizer (DIB).

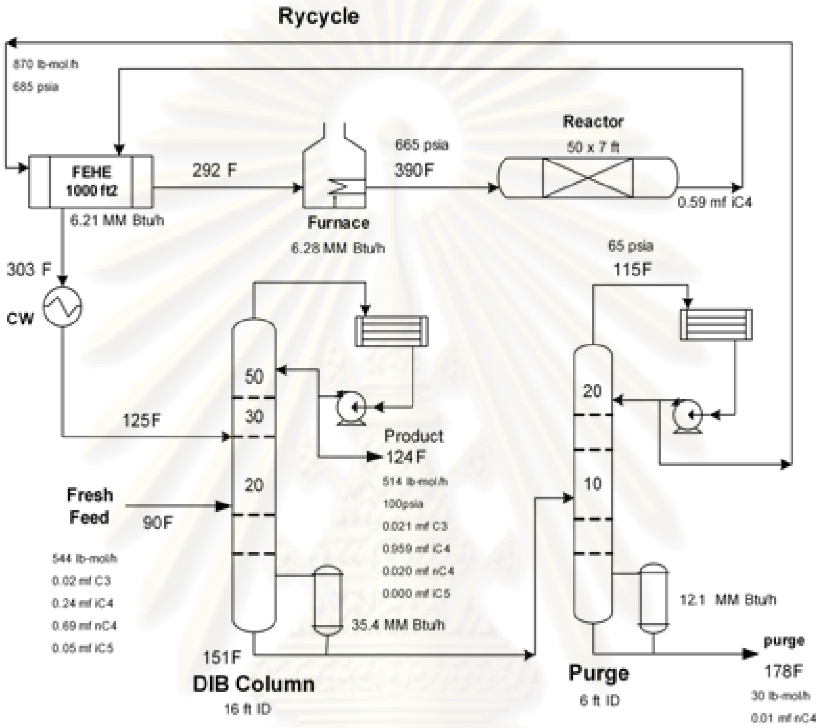


Figure 4.1 The Butane Isomerization Process for reversible reaction case (Plantwide Process Control, 1998)

The fresh feed stream is a mixture of nC_4 and iC_4 (with some propane and isopentane impurities). It is also introduced into the column, not directly into the reactor. It is fed at a lower tray in the column than the reactor effluent stream because the concentration of iC_4 in the fresh feed is lower. This enables the removal of some of the iC_4 and all of the C_3 in the fresh feed before sending the nC_4 to the reactor from the recycle stream. The ratio of the recycle flow to the fresh feed flow is about 1:2. The DIB column operates at 100 psia so that cooling water can be used in the condenser (reflux drum temperature is 124 ^oF). The base temperature is 150 ^oF, so low-pressure stream can be used.

The distillate product from the DIB is the isobutane product. It has a specification of 2 mol% nC_4. Since the fresh feed contains some propane, there is also some propane in the distillate product. All of the propane in the feed leaves the process in the distillate stream.

The bottoms from the DIB contain most of the nC_4, along with some iC_4 impurity and all of the heavy isopentane impurity. Since this heavy component will build up in the process unless it is removed, a second distillation column is used to purge out a small stream that contains the isopentane. Some nC_4 is lost in this purge stream. The purge column has 20 trays and is 6 ft in diameter. The distillate product from the second column is the recycle stream to the reactor, which is pumped up to the required pressure and sent through a feed-effluent heat exchanger and a furnace before entering the reactor in the vapor phase.

The numerical case studied is derived from a flowsheet given in Stanford Research Institute Report 91, "Isomerization of Paraffins for Gasoline". Since no kinetic information is given in this in this report, only reactor inlet and exit conditions. We assume that the reaction is reversible. The equilibrium constant decreases with increasing temperature because the reaction is exothermic. We also increase the size of the reactor so that the effluent leaves essentially at chemical equiblibrium. Table A1, Table A2 give stream data and equipment data for the butane isomerization process. In Appendix B lists the process parameter values.

4.2 Design of heat exchanger networks for reversible reaction case

At this point, the heat exchanger network design method provide by Wongsri (1990) is used to design the heat exchanger networks for Butane Isomerization process. The design procedures and definitions from previous chapters will be methods to design and compare with the preliminary stage of a process design without energy integration. The Problem Table Method is applied to find pinch temperature and reach maximum energy recovery (MER). The cost estimated will be consequence to compare and choose the best network that more optimal for the Butane Isomerization process. The information for design is shown in the following Table 4.1.

Table 4.1 The information of Butane Isomerization Process for reversible reaction case.

Stream Name	Tin (^oF)	Tout (^oF)	W (BTU/hr ^oF)	duty (BTU/hr)
H1: Reactor Product Stream	422.57	125.00	4.51E+04	1.34E+07
H2: DIB Column Condenser	122.40	121.20	2.92E+07	3.51E+07
H3: Purge Column Condenser	112.36	111.20	1.23E+07	1.43E+07
C1: Reactor Feed Stream	119.14	390.00	4.63E+04	1.25E+07
C2: DIB Column Reboiler	144.76	146.31	2.35E+07	3.64E+07
C3: Purge Column Reboiler	174.62	175.42	1.64E+07	1.31E+07

4.2.1 HEN Base Case

According to table 4.1, it can be simply translated to a heat exchanger network for Butane Isomerization Process (Base Case) in Figure 4.2.

There are two streams in the network. We do not find Pinch temperature using Problem table method.

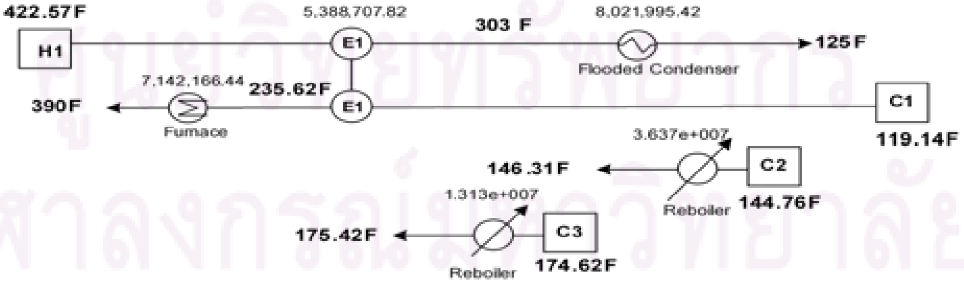


Figure 4.2 The heat exchanger network, Base Case for reversible reaction case

4.2.2 RHEN Alternative 1

There are two streams in the network. We can find Pinch temperature using Problem table method as shown in Table 4.3. At the minimum heat load condition, the pinch temperature occurs at 163.76/143.76 ^oF and 164.76/144.76 ^oF. The minimum utility requirements have been predicted 24.753x10^6 Btu/hr of hot utilities and 1.792x10^6 Btu/hr of cold utilities.

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.2. Figure 4.3 shows a design of resilient heat exchanger network for Butane Isomerization process alternative 1. In our case as shown in Figure 4.3, the minimum temperature difference in the process-to-process-heat-exchangers, ΔT_{min} is set to be 20 ^oF.

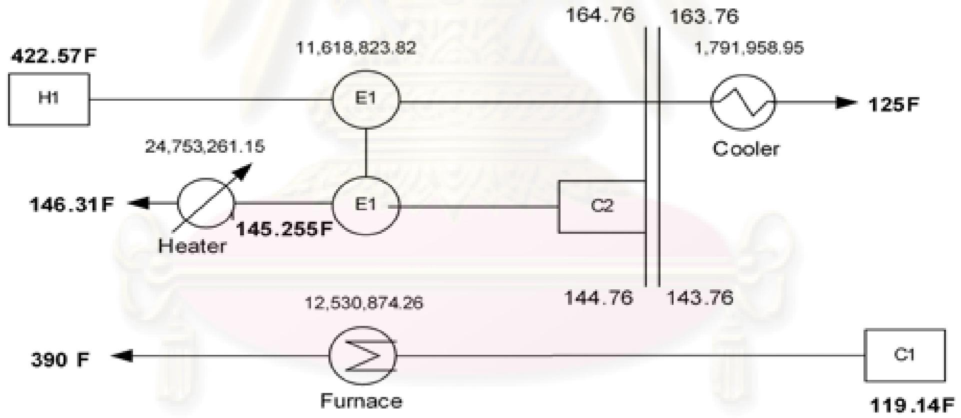


Figure 4.3 The resilient heat exchanger network alternative 1, RHEN-1

Table 4.2 Process stream data for RHEN-1

Stream	W(Btu/hr- ^oF)	Tsupply(^oF)			Ttarget(^oF)
		Nominal	Max	Min	
H1	45,067.39	422.57	442.57	412.57	125.00
C2	23,465,862.27	144.76	144.76	143.76	146.31

Synthesis Table for Cold End of RHEN-1							
Stream	Load	W	T1	T2	D1	D2	Match Action
a)	State 1 B[H]						
H1	1,746,812.04	45,067.39	163.76	125.00	45,067.39	-	to cooler
C2		23,465,862.27					
Synthesis Table for Hot End of RHEN-1							
Stream	Load	W	T1	T2	D1	D2	Match Action
a)	State 1 D[H]						
H1	11,168,149.92	45,067.39	412.57	164.76	1,352,021.70	45,067.39	Select
C2	36,372,086.52	23,465,862.27	146.31	144.76	-	23,465,862.27	Select
b)	State 2						
C2	23,851,914.90	23,465,862.27	146.31	145.29	-	24,772,816.58	to heater

Table 4.3 Problem table for RHEN-1

W		Thot	Tcold	dT	Sum W	Require	Interval	Cascade	Sum int
H1	C2								
0	0	422.57	402.57	0	0.00	**Qh**	0.00		
45,067.39	0	166.31	146.31	256.26	45067.39	24753261.15	11548969.36	36302230.51	11548969.36
45,068.39	23,465,862.27	164.76	144.76	1.55	-23420793.88	36302230.51	-36302230.51	0.00	-24753261.15
45,069.39	0	125.00	105.00	39.76	45069.39	0.00	1791958.95	1791958.95	-22961302.21
								Qc	

4.2.3 RHEN Alternative 2

There are two streams in the network. We don't need to find Pinch temperature using Problem table method. From resilient heat exchanger network design, the auxiliary heater is used in this case.

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.4. Figure 4.4 shows a design of resilient heat exchanger network for Butane Isomerization process alternative 2.

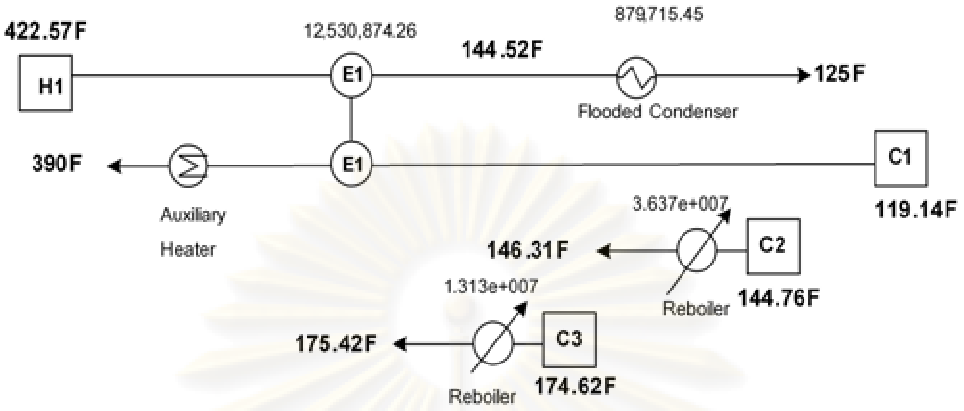


Figure 4.4 The resilient heat exchanger network alternative 2, RHEN-2

Table 4.4 Process stream data for RHEN-2

Stream	W(Btu/hr- ^oF)	Tsupply(^oF)			Ttarget(^oF)
		Nominal	Max	Min	
H1	45,067.39	422.57	442.57	412.57	125.00
C1	46,263.29	119.14	139.14	99.14	390.00

Synthesis Table of RHEN-2							
Stream	Load	W	T1	T2	D1	D2	Match Action
a)	State 1 B[H]						
H1	13,410,703.24	45,067.39	422.57	125.00	1,352,021.70	-	Select
C1	12,530,874.73	46,263.29	390.00	119.14	-	1,850,531.60	to aux heater
b)	State 2						
H1	879,828.51	45,067.39	144.523	125.00	1,352,021.70	-	to cooler

4.2.4 RHEN Alternative 3

There are two streams in the network. We can find Pinch temperature using Problem table method as shown in Table 4.6. At the minimum heat load condition, the pinch temperature occurs at 194.62/174.62^oF and 194.12/174.12^oF. The minimum utility requirements have been predicted 2.86x10^6 Btu/hr of hot utilities and 3.138x10^6 Btu/hr of cold utilities.

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.5. Figure 4.5 shows a design of resilient heat exchanger network for Butane Isomerization process alternative 3. In our case as shown in Figure 4.4, the minimum temperature difference in the process-to-process-heat-exchangers, ΔT_{min} is set to be 20 ^oF.

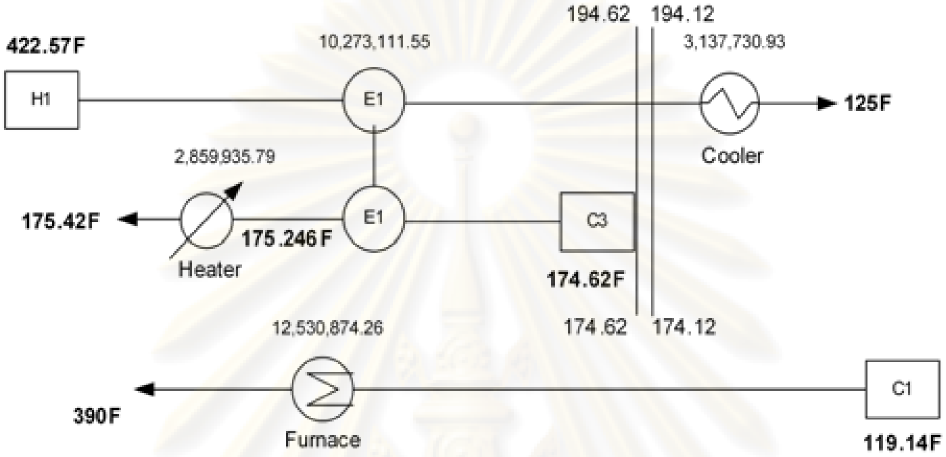


Figure 4.5 The resilient heat exchanger network alternative 3, RHEN-3

Table 4.5 Process stream data for RHEN-3

Stream	W(Btu/hr- ^oF)	Tsupply(^oF)			Ttarget(^oF)
		Nominal	Max	Min	
H1	45,067.39	422.57	442.57	412.57	125.00
C3	16,416,310.18	174.62	174.62	174.12	175.42

Synthesis Table for Cold End of RHEN-3							
Stream	Load	W	T1	T2	D1	D2	Match Action
a)	State 1 B[H]						
H1	3,115,058.00	45,067.39	194.12	125.00	22,533.70	0	to cooler
C3		16,416,310.18					
Synthesis Table for Hot End of RHEN-3							
Stream	Load	W	T1	T2	D1	D2	Match Action
a)	State 1 D[H]						
H1	9,822,437.65	45,067.39	412.57	194.62	1,352,021.70	22,533.70	Select
C3	13,133,048.14	16,416,310.18	175.42	174.62	-	8,208,155.09	Select
b)	State 2						
C3	1,958,588.79	16,416,310.18	175.42	175.30	-	9,537,643.10	to heater

Table 4.6 Problem table for RHEN-3

W		Thot	Tcold	dT	Sum W	Require	Interval	Cascade	Sum int
H1	C3								
0	0	422.57	402.57	0	0.00	**Qh**	0.00		
45,067.39	0	195.42	175.42	227.15	45067.39	2859935.79	10237057.64	13096993.43	10237057.64
45,068.39	16,416,310.18	194.62	174.62	0.8	-16371241.79	13096993.43	-13096993.43	0.00	-2859935.79
45,069.39	0	125.00	105.00	69.62	45069.39	0.00	3137730.93	3137730.93	277795.14
								Qc	

The various alternatives of heat exchanger network are designed for the Butane Isomerization process, the energy saved from the Base case as in Table 4.7

Table 4.7 Energy integration of Butane Isomerization process for reversible reaction case

	Base case	RHEN-1	RHEN-2	RHEN-3
Utilities usage (Btu/hr)				
Furnace	7,142,166.44	12,530,874.26	-	12,530,874.26
DIB reboiler	36,372,086.51	24,753,261.15	36,372,086.51	36,372,086.51
Purge reboiler	13,133,048.14	13,133,048.14	13,133,048.14	2,859,935.79
Hot utilities usage	56,647,301.09	50,417,183.55	49,505,134.65	51,762,896.56
Cold utilities usage	8,021,995.42	1,791,958.95	879,715.45	3,137,730.93
Total utilities usage	64,669,296.51	52,209,142.50	50,384,850.10	54,900,627.49
Energy saving ,%	-	19.27	22.09	15.11

4.3 The Butane Isomerization Alternatives for reversible reaction case

Three alternatives of heat exchanger networks (HEN) designs of the Butane Isomerization plant are proposed to save energy from the Base Case and use to evaluate performance of control structures are designed both simply energy-integrated plant and complex energy-integrated plant.

In Figure 4.6 show the Base Case of Butane Isomerization process with simply energy integration, we used a feed-effluent heat exchanger (FEHE) to reduce the amount of fuel burned in the furnace. The heat of reaction and the heat added in the furnace are therefore removed in the flooded condenser.

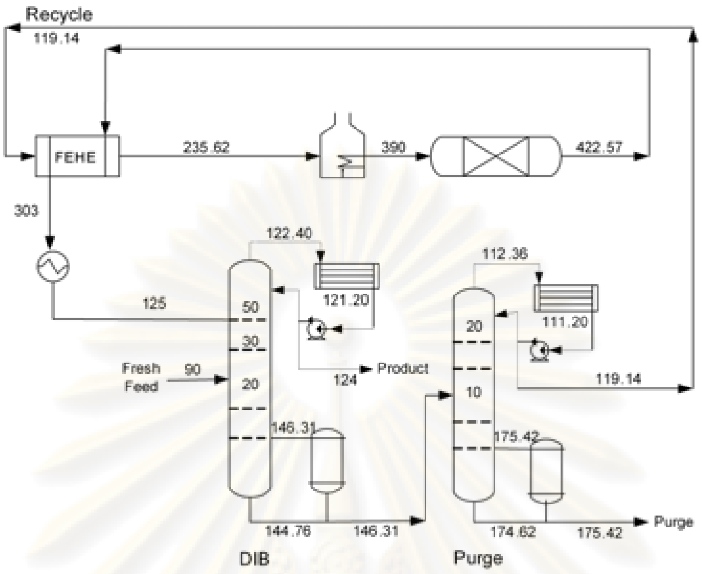


Figure 4.6 Butane Isomerization process, Base Case

In alternative 1, there is a heat exchanger for preheat the reboiler in the DIB column is driven by the reactor effluent stream. The heat of reaction and the heat added in the furnace are removed in the flooded condenser as in Figure 4.7.

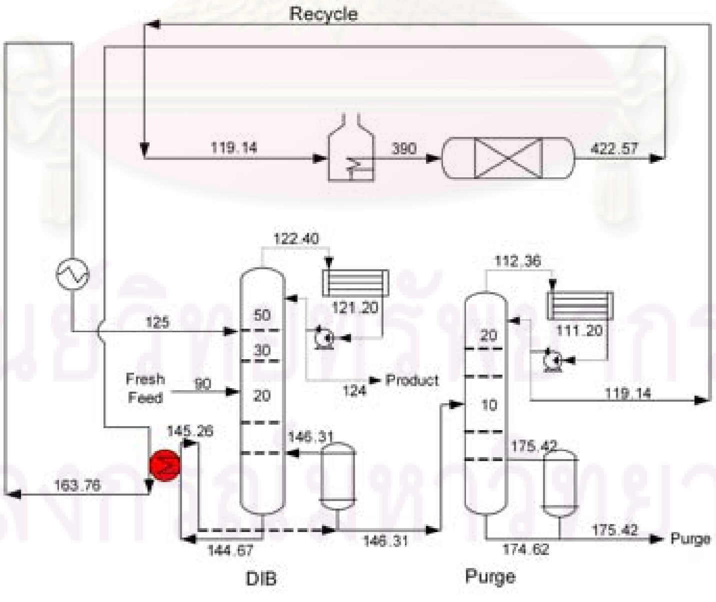


Figure 4.7 Butane Isomerization process alternative 1

In alternative 2, there is a heat exchanger for preheat the reactor feed stream. The heat of reaction and the heat added in the auxiliary heater are removed in the flooded condenser as in Figure 4.8.

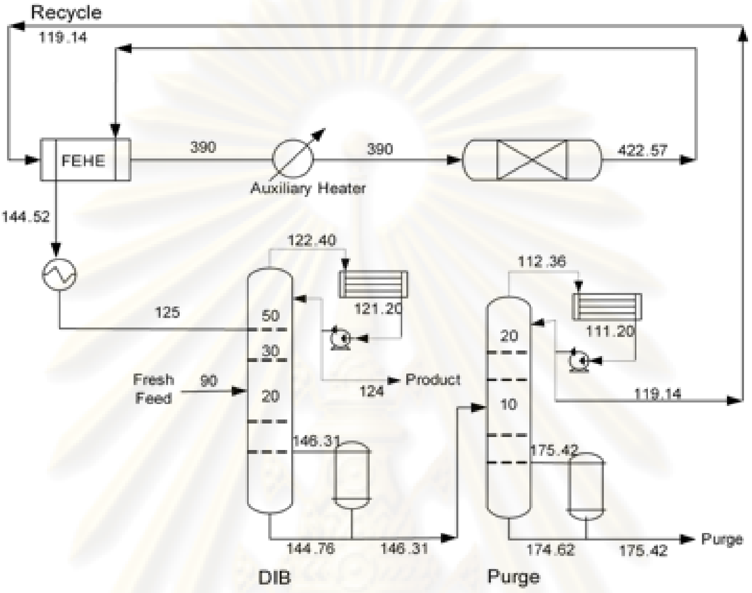


Figure 4.8 Butane Isomerization process alternative 2

In alternative 3, there is a heat exchanger for preheat reboiler in the Purge column. The reactor feed stream used the heat from the furnace and the heat from the reaction are removed in the flooded condenser as in Figure 4.9.

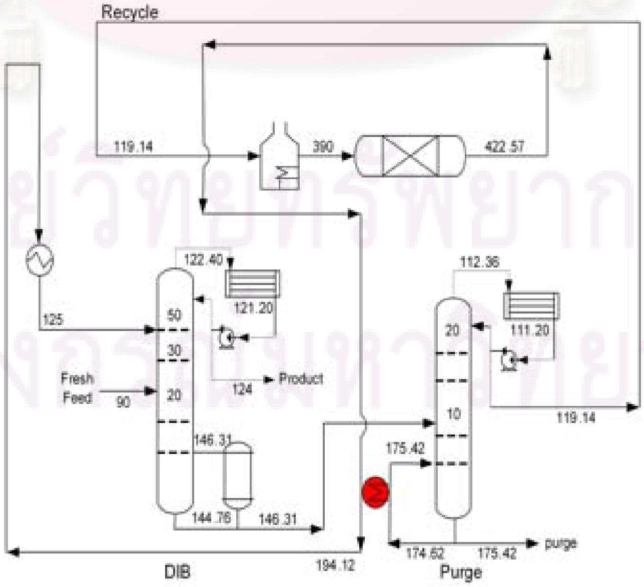


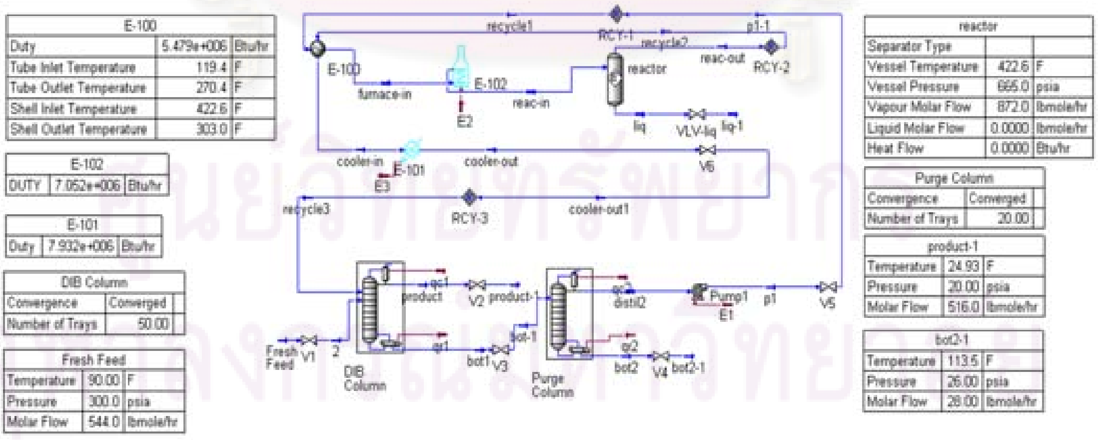
Figure 4.9 Butane Isomerization process alternative 3

4.4 Steady-State Modeling for reversible reaction case

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Luyben et al. (1998). Appendix A presents the data and specifications for the different equipment. For the simulation, the Peng-Robinson model is selected for physical property calculations because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions. The reaction kinetics of both reactions are modeled with standard Arrhenius kinetic expressions available in HYSYS.PLANT, and the kinetic data are taken from Luyben et al. (1998).

4.4.1 Steady State Simulation of Butane Isomerization Process (Base case)

Figure 4.10 shows the HYSYS flowsheet of Butane Isomerization process (Base Case). The steady state simulation results are summarized in Table A.1 and Figure 4.11.



E-100		
Duty	5.479e+006	Btu/hr
Tube Inlet Temperature	119.4	F
Tube Outlet Temperature	270.4	F
Shell Inlet Temperature	422.6	F
Shell Outlet Temperature	303.0	F

E-102		
DUTY	7.052e+006	Btu/hr

E-101		
Duty	7.932e+006	Btu/hr

DIB Column		
Convergence	Converged	
Number of Trays	50.00	

Fresh Feed		
Temperature	90.00	F
Pressure	300.0	psia
Molar Flow	544.0	lbmole/hr

reactor		
Separator Type		
Vessel Temperature	422.6	F
Vessel Pressure	665.0	psia
Vapour Molar Flow	872.0	lbmole/hr
Liquid Molar Flow	0.0000	lbmole/hr
Heat Flow	0.0000	Btu/hr

Purge Column		
Convergence	Converged	
Number of Trays	20.00	

product-1		
Temperature	24.93	F
Pressure	20.00	psia
Molar Flow	516.0	lbmole/hr

bot2-1		
Temperature	113.5	F
Pressure	26.00	psia
Molar Flow	28.00	lbmole/hr

Figure 4.10 The simulated Butane Isomerization process (Base Case for reversible reaction case) at steady-state by HYSYS

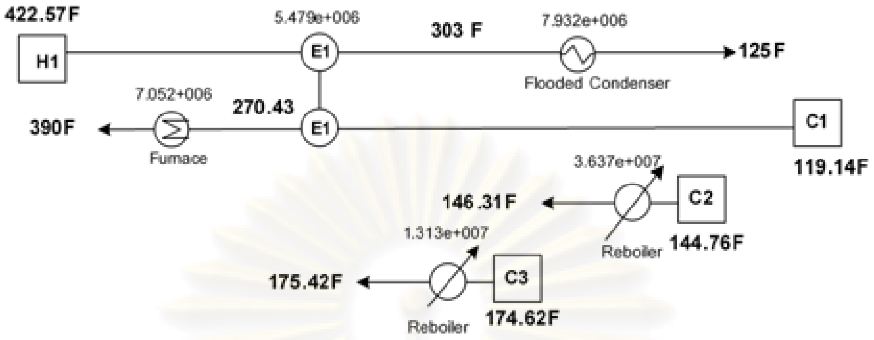


Figure 4.11 The steady state simulation results of heat exchanger network, Base Case for reversible reaction case

4.4.2 Steady State Simulation of Butane Isomerization Process Alternative 1

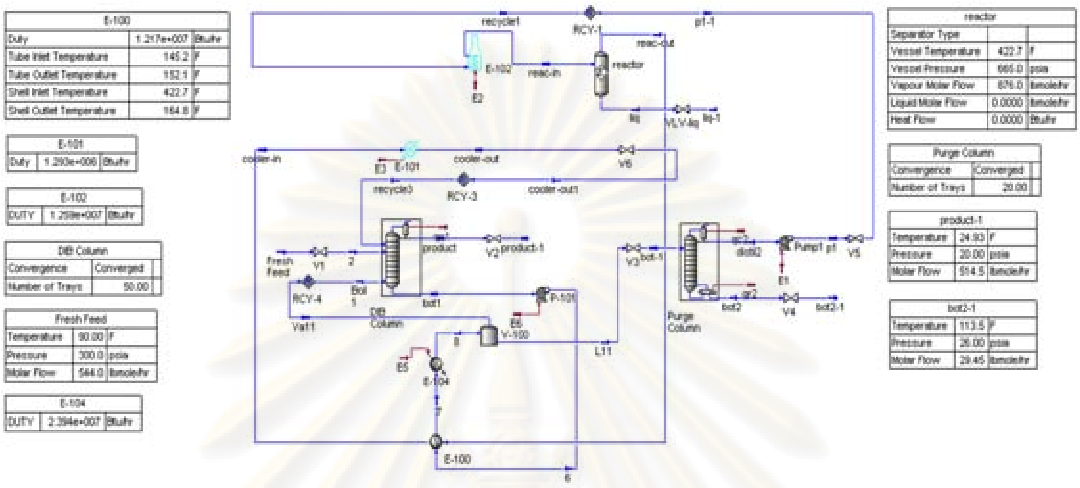
In alternative 1 there is a heat exchanger and additionally the reboiler in the DIB column is driven by the reactor effluent stream. The heat exchanger is used to reboil the DIB column. The process-to-process heat exchanger is simulated using a heat exchanger with a hot stream on the shell side and a cold stream on the tube side. Note that, a minimum ΔT of about 20 ^oF is assumed for all process-to-process heat exchangers.

The DIB column is simulated using a “refluxed absorber” that it does not include a reboiler. The Purge column is simulated using the “distillation column” module. Since a “reflux absorber” module is used, only one variable need to be specified for the columns with condenser. The overhead mole fraction is chosen to be specified for a “refluxed absorber” module.

In alternatives 1, a tank is needed to accommodate liquid from the bottom of DIB column.

Figure 4.12 shows the HYSYS flowsheets of the Butane Isomerization process with energy integration schemes for alternative 1. The selected process streams data for this alternative is not included in this chapter but listed in

Appendix A. The steady state simulation result is shown in Figure 4.13.



E-100		
Duty	1.217e+007	Btu/hr
Tube Inlet Temperature	145.2	F
Tube Outlet Temperature	152.1	F
Shell Inlet Temperature	422.7	F
Shell Outlet Temperature	164.8	F

E-101		
Duty	1.293e+006	Btu/hr

E-102		
DUTY	1.259e+007	Btu/hr

DIB Column		
Convergence	Converged	
Number of Trays	50.00	

Fresh Feed		
Temperature	90.00	F
Pressure	300.0	psia
Molar Flow	544.0	lbmole/hr

E-104		
DUTY	2.394e+007	Btu/hr

reactor		
Separator Type		
Vessel Temperature	422.7	F
Vessel Pressure	685.0	psia
Vapour Molar Flow	876.0	lbmole/hr
Liquid Molar Flow	0.0000	lbmole/hr
Heat Flow	0.0000	Btu/hr

Purge Column		
Convergence	Converged	
Number of Trays	20.00	

product-1		
Temperature	24.93	F
Pressure	20.00	psia
Molar Flow	514.5	lbmole/hr

bot2-1		
Temperature	113.5	F
Pressure	26.00	psia
Molar Flow	29.45	lbmole/hr

Figure 4.12 The simulated Butane Isomerization process (alt.1) at steady-state by HYSYS

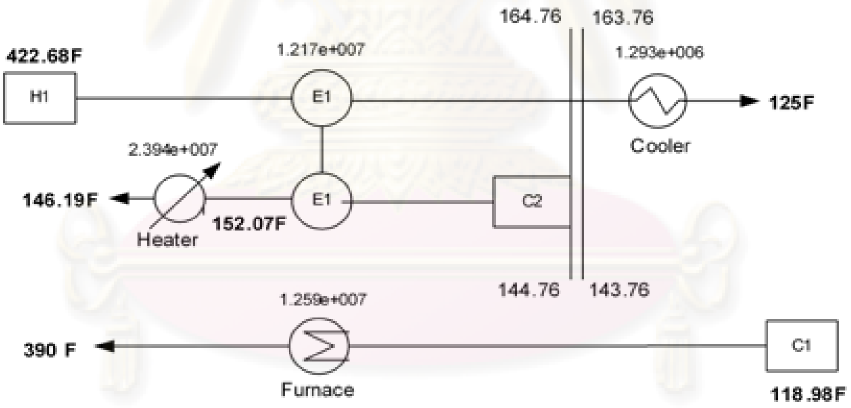
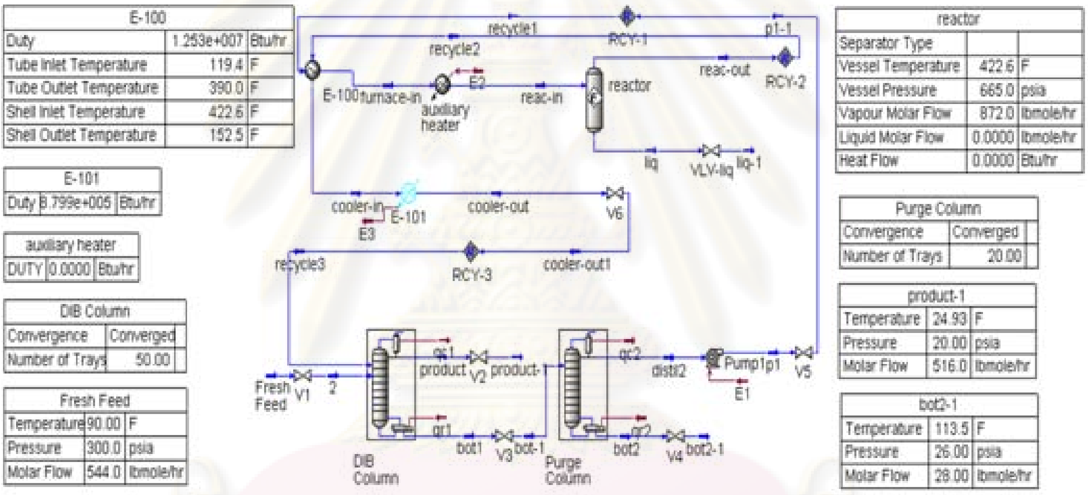


Figure 4.13 The steady state simulation results of resilient heat exchanger network, alternative 1

4.4.3 Steady State Simulation of Butane Isomerization Process Alternative 2

In alternative 2, there is a heat exchanger and is driven by the reactor effluent stream. The heat exchanger for alternative 2 is used to preheat the reactor feed stream. We add an auxiliary heater to supply the heat because the total heat from heat exchanger is not enough to heat inlet stream of reactor. The process-to-process heat exchanger is simulated using a heat exchanger with a hot stream on the shell side and a cold stream on the tube side.

Figure 4.14 shows the HYSYS flowsheets of the Butane Isomerization process with energy integration schemes for alternative 2. The selected process streams data for this alternative is not included in this chapter but listed in Appendix A. The steady state simulation result is shown in Figure 4.15.



E-100		
Duty	1.253e+007	Btu/hr
Tube Inlet Temperature	119.4	F
Tube Outlet Temperature	390.0	F
Shell Inlet Temperature	422.6	F
Shell Outlet Temperature	152.5	F

E-101		
Duty	8.799e+005	Btu/hr

auxiliary heater		
DUTY	0.0000	Btu/hr

DIB Column		
Convergence	Converged	
Number of Trays	50.00	

Fresh Feed		
Temperature	90.00	F
Pressure	300.0	psia
Molar Flow	544.0	lbmole/hr

reactor		
Separator Type		
Vessel Temperature	422.6	F
Vessel Pressure	665.0	psia
Vapour Molar Flow	872.0	lbmole/hr
Liquid Molar Flow	0.0000	lbmole/hr
Heat Flow	0.0000	Btu/hr

Purge Column		
Convergence	Converged	
Number of Trays	20.00	

product-1		
Temperature	24.93	F
Pressure	20.00	psia
Molar Flow	516.0	lbmole/hr

bot2-1		
Temperature	113.5	F
Pressure	26.00	psia
Molar Flow	28.00	lbmole/hr

Figure 4.14 The simulated Butane Isomerization process (alt.2) at steady-state by HYSYS

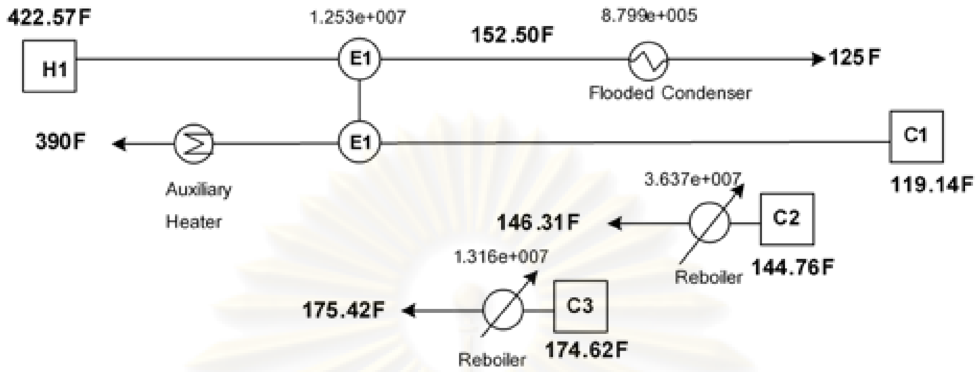


Figure 4.15 The steady state simulation results of resilient heat exchanger network, alternative 2

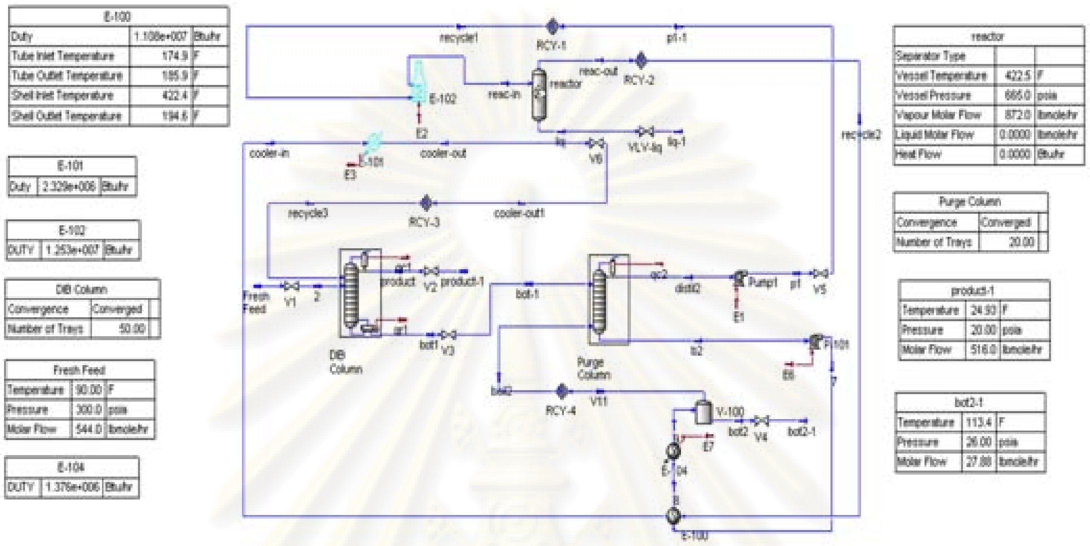
4.4.4 Steady State Simulation of Butane Isomerization Process Alternative 3

In alternative 3, there is a heat exchanger and additionally the reboiler in the Purge column is driven by the reactor effluent stream. The heat exchanger for alternative 3 is used to reboil the Purge column. The process-to-process heat exchanger is simulated using a heat exchanger with a hot stream on the shell side and a cold stream on the tube side. Note that, a minimum ΔT of about 20 ^oF is assumed for all process-to-process heat exchangers.

The DIB column is simulated using the “distillation column” module. The Purge column is simulated using “refluxed absorber” that it does not include a reboiler. Since a “reflux absorber” module is used, only one variable need to be specified for the columns with condenser. The overhead mole fraction is chosen to be specified for a “refluxed absorber” module.

In alternative 3, a tank is needed to accommodate liquid from the bottom of Purge column.

Figure shows 4.16 the HYSYS flowsheets of the Butane Isomerization process with energy integration schemes for alternative 3. The selected process streams data for this alternative is not included in this chapter but listed in Appendix A. The steady state simulation result is shown in Figure 4.17.



E-100		
Duty	1.108e+007	Btu/hr
Tube Inlet Temperature	174.9	F
Tube Outlet Temperature	185.9	F
Shell Inlet Temperature	422.4	F
Shell Outlet Temperature	194.6	F

E-101		
Duty	2.329e+006	Btu/hr

E-102		
DUTY	1.253e+007	Btu/hr

DIB Column		
Convergence	Converged	
Number of Trays	50.00	

Fresh Feed		
Temperature	90.00	F
Pressure	300.0	psia
Molar Flow	544.0	lbmole/hr

E-104		
DUTY	1.376e+006	Btu/hr

reactor		
Separator Type		
Vessel Temperature	422.5	F
Vessel Pressure	665.0	psia
Vapour Molar Flow	872.0	lbmole/hr
Liquid Molar Flow	0.0000	lbmole/hr
Heat Flow	0.0000	Btu/hr

Purge Column		
Convergence	Converged	
Number of Trays	20.00	

product-1		
Temperature	24.93	F
Pressure	20.00	psia
Molar Flow	516.0	lbmole/hr

bot2-1		
Temperature	113.4	F
Pressure	26.00	psia
Molar Flow	27.88	lbmole/hr

Figure 4.16 The simulated Butane Isomerization process (alt.3) at steady-state by HYSYS

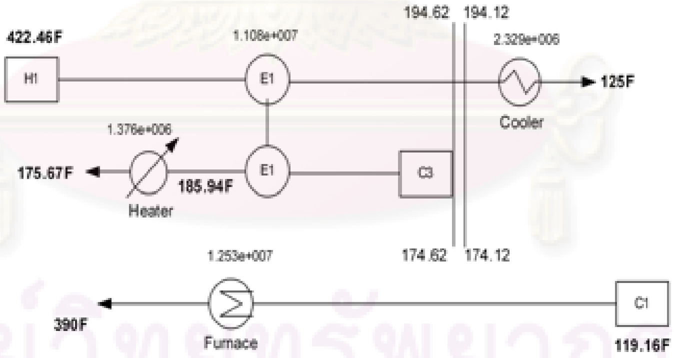


Figure 4.17 The steady state simulation results of resilient heat exchanger network, alternative 3

4.4.5 Energy Integration from Steady State Simulation of Butane Isomerization Process for reversible reaction case

From steady state simulation results by HYSYS, the energy saved from the base case heat consumption as shown in Table 4.8.

Table 4.8 Energy integration of Butane Isomerization process for reversible reaction case (steady state simulation)

	Base case	RHEN-1	RHEN-2	RHEN-3
Utilities usage (Btu/hr)				
Furnace	7,052,243.29	12,587,636.95	-	12,531,675.15
DIB reboiler	36,372,179.93	23,938,394.93	36,372,300.46	36,290,520.50
Purge reboiler	13,164,814.31	18,940,967.25	13,164,814.30	1,376,188.60
Hot utilities usage	56,589,237.53	55,466,999.13	49,537,114.76	50,198,384.25
Cold utilities usage	7,932,186.94	1,293,091.15	879,943.60	2,328,709.68
Total utilities usage	64,521,424.47	56,760,090.28	50,417,058.36	52,527,093.93
Energy saving ,%	-	12.03	21.86	18.59

4.5 The Butane Isomerization Process for irreversible reaction case

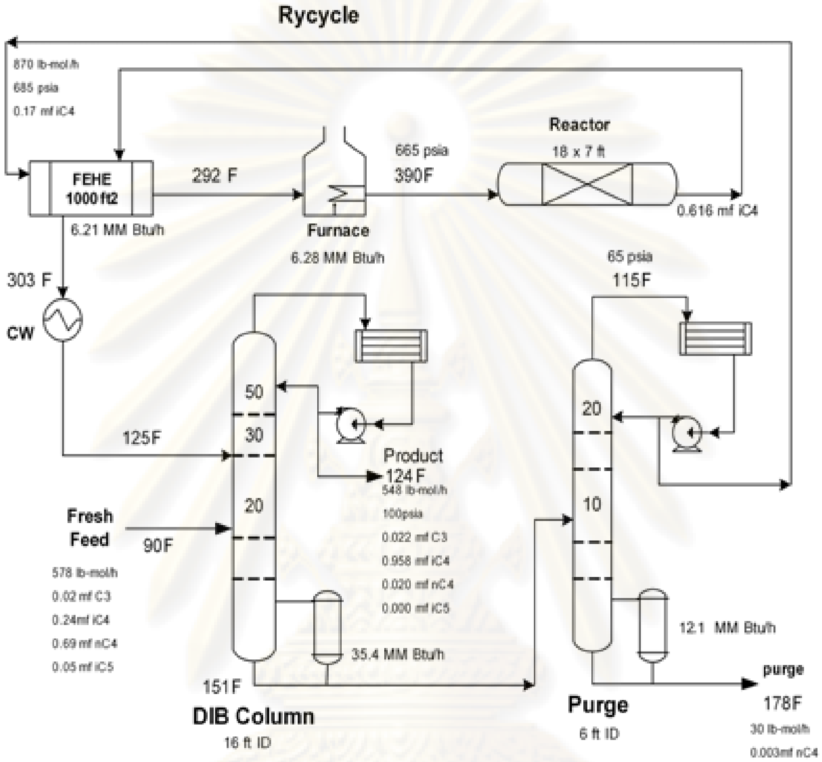


Figure 4.18 The Butane Isomerization Process for irreversible reaction case (Plantwide Process Control, 1998)

The information for design is shown in the following Table 4.9.

Table 4.9 The information of Butane Isomerization Process for irreversible reaction case

Stream Name	Tin (^oF)	Tout (^oF)	W (BTU/hr ^oF)	duty (BTU/hr)
H1: Reactor Product Stream	424.10	125.00	4.46E+04	1.34E+07
H2: DIB Column Condenser	122.40	121.20	2.47E+07	2.97E+07
H3: Purge Column Condenser	110.38	108.92	9.09E+06	1.33E+07
C1: Reactor Feed Stream	117.67	390.10	4.57E+04	1.25E+07
C2: DIB Column Reboiler	142.08	143.87	1.73E+07	3.10E+07
C3: Purge Column Reboiler	171.50	173.76	5.39E+06	1.22E+07

4.5.1 HEN Base Case for irreversible reaction case

According to table 4.9 it can be simply translated to a heat exchanger network for Butane Isomerization Process (Base Case) in Figure 4.18.

There are two streams in the network. We do not find Pinch temperature using Problem table method.

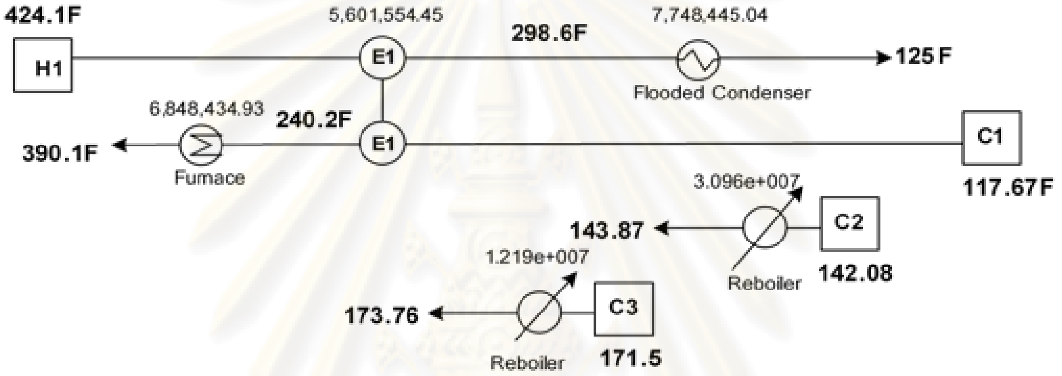
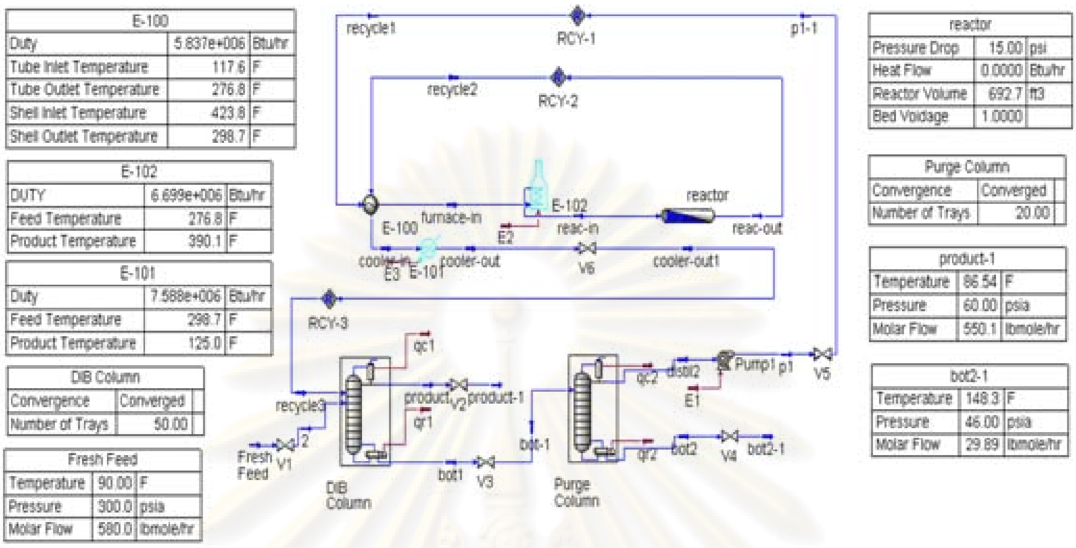


Figure 4.19 The heat exchanger network, Base Case for irreversible reaction case

4.5.2 Steady State Simulation of Butane Isomerization Process (Base Case for irreversible reaction case)

Figure 4.20 shows the HYSYS flowsheet of Butane Isomerization process (Base Case for irreversible reaction case). The steady state simulation results are summarized in Table A.1 and Figure 4.21.



E-100		
Duty	5.837e+006	Btu/hr
Tube Inlet Temperature	117.6	F
Tube Outlet Temperature	276.8	F
Shell Inlet Temperature	423.8	F
Shell Outlet Temperature	298.7	F

E-102		
DUTY	6.699e+006	Btu/hr
Feed Temperature	276.8	F
Product Temperature	390.1	F

E-101		
Duty	7.588e+006	Btu/hr
Feed Temperature	298.7	F
Product Temperature	125.0	F

DIB Column		
Convergence	Converged	
Number of Trays	50.00	

Fresh Feed		
Temperature	90.00	F
Pressure	300.0	psia
Molar Flow	580.0	lbmole/hr

reactor		
Pressure Drop	15.00	psi
Heat Flow	0.0000	Btu/hr
Reactor Volume	692.7	ft3
Bed Voidage	1.0000	

Purge Column		
Convergence	Converged	
Number of Trays	20.00	

product-1		
Temperature	86.54	F
Pressure	60.00	psia
Molar Flow	550.1	lbmole/hr

bot2-1		
Temperature	148.3	F
Pressure	46.00	psia
Molar Flow	29.89	lbmole/hr

Figure 4.20 The simulated Butane Isomerization process (Base Case for irreversible case) at steady-state by HYSYS

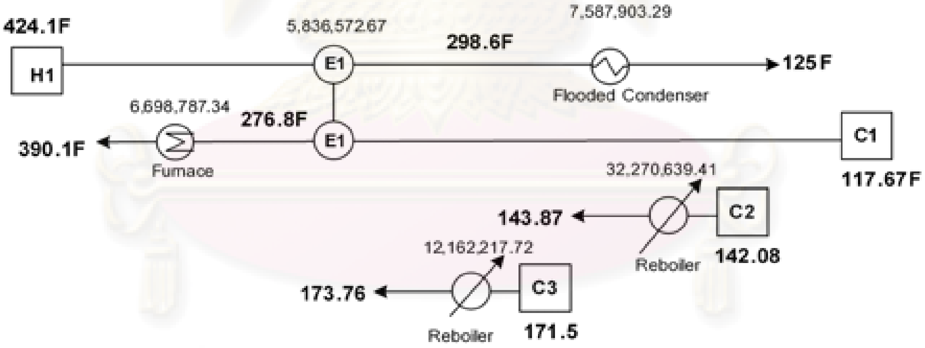


Figure 4.21 The steady state simulation results of heat exchanger network, Base Case for irreversible reaction case

CHAPTER V

CONTROL STRUCTURE DESIGN AND DYNAMIC SIMULATION

5.1 Plantwide control design procedure

5.1.1 Nine-step approach of Luyben

This approach is used to design the first, second and third control structure (CS1-3) of the Butane Isomerization process.

Step 1: Establish control objectives

In this process we want to achieve the desired production rate and control the impurity of normal butane in the isobutene product at 2 mol %. Reactor pressure cannot exceed the design operating pressure of 700 psia. We assume that we are free to choose the production rate handle. Neither the fresh feed nor product flowrates are fixed other plant considerations. In the pentane purge column, we do not want to lose too much nC_4.

Step 2: Determine control degrees of freedom

The Butane Isomerization process for Base case has 14 control degrees of freedom. They include fresh feed valve; DIB column stream, cooling water, reflux, distillate, and bottoms valve; Purge column stream, cooling water, reflux, distillate, and bottom valve; furnace fuel valve; flooded condenser cooling water valve; and DIB column feed valve. For the resilient heat exchanger networks, each has a bypass valve of heat exchanger. So there are 15 degrees of freedom for a heat exchangers (RHEN-1, RHEN-2 and RHEN-3)

Step 3: Establish energy management system

The exothermic heat of reaction must be removed, and the reactor feed must be heated to a high enough temperature to initiate the reaction. Since the heat of reaction is not large and complete one pass conversion is not achieved, the reactor exit temperature is only 32 ^oF higher than the reactor inlet temperature. Since heat transfer coefficients in gas-to-gas systems are typically quite low, this small temperature differential would require a very large heat exchanger if only the reactor effluent is used to heat the reactor feed and no furnace is used. Therefore, a furnace is required to bring the reactor inlet up to the desired level.

The use of a feed-effluent heat exchanger (FEHE) reduces the amount of fuel burned in the furnace. So form a steady-state viewpoint, the economic trade-off between utility and capital costs would produces a fairly large heat exchanger and a small furnace. However, the exothermic heat of reaction and the heat of vaporization supplied in the furnace must be dissipated to utilities at the flooded condenser. If the FEHE is too large, reactor heat will be recycled. Also the large heat exchanger, the smaller heat input in the furnace. This could potentially be solved using a bypass around the FEHE on the cold side. This should enable us to prevent reactor runaway to high temperature and would guarantee that the furnace is in operation at all times. However, unless the furnace is large enough, there is no guarantee that the system will never quench to low temperature when a large disturbance occurs to drop the reactor inlet temperature.

A second difficulty that can occur with a large FEHE is a hydraulic problem. The recycle stream entering the heat exchanger is subcooled liquid (115 ^oF) at the pressure in the reactor section (685 psia). As this stream is heated to the required reactor inlet temperature of 390 ^oF, it begins to vaporize. It is superheated vapor when fed into the reactor (390 ^oF at 665 psia). When a small FEHE is used, the exit is 292 ^oF for the recycle stream, which means the stream is still all liquid. All the vaporization occurs in the furnace. If a large heat exchanger were used, vaporization would begin to occur in the heat exchanger. This would make the hydraulic design of this FEHE much more difficult. The dynamic response could also be adversely affected as changes in flowrates and temperature make the stream go in and out of the two-phase region.

The same problem occurs on the hot side of FEHE. As the hot reactor effluent is cooled, it starts to condense at some temperature. And this dewpoint temperature could occur in the heat exchanger and not in the flooded condenser if a large area is used.

Because of both the heat dissipation and hydraulic concerns, we use a relatively small FEHE: 1000 ft^2 compared to the Stanford Research Report's listed area of 3100 ft^2. So the energy management system consists of controlling reactor inlet temperature by furnace firing and controlling the rate of removal in the flooded condenser by cooling water flowrate. The heat of reaction and the heat added in the furnace are therefore removed in the flooded condenser. Because of this design we do not need a bypass around the FEHE.

In this work, we designed the new heat exchanger network to be chosen for each proper control structure. For RHEN-1, RHEN-2 and RHEN-3 are simply heat-integrated process, they use a large FEHE to save energy from Base Case.

Step4: Set production rate

We are not constrained either by reactant supply or product demand to set production rate at a certain point in the process. We need to examine which variables affect reactor productivity.

The kinetic expression for the isomerization reaction is relatively simple. For the irreversible case, reaction rate depends upon the forward rate constant, reactor volume, and normal butane concentration.

$$\mathrm{R} = \mathrm{k}_F \mathrm{V}_R \mathrm{C}_{nC4}$$

Form this expression we see that only three variables could possibly be dominant: temperature, pressure, and mole fraction of nC_4 in the reactor feed.

Pressure affects productivity through its influence on the reactant concentration. Since the normal operating reactor pressure is close to the design limit, we are constrained in how much we can move pressure to achieve the desired production rate change. The nC_4 mole fraction in the reactant feed is about 0.81. Therefore large absolute changes in the reactant feed mole fraction would have to be made to be achieve a significant relative change in throughput.

Finally, we are then left with temperature. The relative change in reaction rate depends upon the temperature through the activation energy. For a 10 ^oF change in temperature, the reaction rate increases by 20 percent. Clearly temperature is a dominant variable for reactor productivity.

For the reversible case, reaction rate depends upon the forward and reverse rate constants, reactor volume, and nC_4 and iC_4 concentrations:

$$\mathrm{R} = \mathrm{k}_F\mathrm{V}_R\mathrm{C}_{nC4} - \mathrm{k}_R\mathrm{V}_R\mathrm{C}_{iC4}$$

The activation energy of the reverse reaction is always greater than the activation energy of the forward reaction since the reaction is exothermic. Therefore the reverse reaction will increase more quickly with an increase in the temperature than will the forward reaction. Temperature may still dominate for reactor productivity, but in the opposite direction compared with the irreversible case, since conversion increases with lower temperature. However, when the temperature becomes too low, both reaction rates slow down such that we cannot achieve the desired production rate with this variable alone. Instead, the concentrations of nC_4 and iC_4 dominate the rate through the relationship imposed by the equilibrium constant $\mathrm{K}_{eq} = \mathrm{C}_{iC4} / \mathrm{C}_{nC4}$.

Therefore we choose the reactor inlet temperature setpoint as the production rate handle for the irreversible case. However, for the reversible case we need to look for variables that affect the ratio of nC_4 to iC_4 in the recycle stream. For this case we will not have unit control for the reactor since these concentrations depend upon operation in other parts of the process.

Note that setting the production rate with variables at the reactor or within the process specifies the amount of fresh reactant feed flow required at steady state. The choices for the control system made in Steps 6 and 7 must recognize this relationship between production rate and fresh reactant feed flowrate.

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

The final isobutene product is the distillate from the DIB column, and we want to keep the composition of the nC_4 impurity at 2 mol %. Nothing can be done about the propane impurity. Whatever propane is in the fresh feed must leave in the product stream. Because the separation involves two isomers, the temperature profile is flat in the DIB column. Use of an overhead composition analyzer is necessary.

The choice of manipulated variables that can be used to control nC_4 composition in the DIB distillate include reflux flowrate, distillate flowrate and reboiler heat input. If the reflux ratio is high, control of reflux drum level using distillate flow may be ineffective, particularly if the distillate were going directly to a downstream process. If we use reflux flow to control reflux drum level, we must control distillate composite by manipulating the distillate flowrate. The reason is that distillate flow must math production rate, which is dependently set in the reactor. However, in this case we assume that the distillate is going to a storage tank or cavern, so large changes in distillate flowrate are not important. Distillate can then be used for reflux drum level control, allowing us to consider other variables for composition control.

Most distillate column responds more quickly to vapor rate changes than to changes in liquid rates. Therefore, we can select reboiler heat input to control nC_4 impurity in the distillate but this choice is poor because we are controlling something at the top of the column by changing a variable near the base. However, vapor changes affect all trays in the column quite quickly, so tight control of distillate composition should be possible by manipulating vapor boilup. A viable alternative is to control distillate composition with distillate flowrate and control reflux drum level with reflux flowrate.

To avoid the high-pressure safety constraint, we must control reactor pressure. We can use the distillate valve from the purge column, the flooded condenser cooling water valve, or the DIB column feed valve. The most logical variable to use for control of the flooded condenser (reactor) pressure is the DIB column feed valve. Base upon the discussion in step 3, we would then use the flooded condenser cooling water valve to keep the liquid leveling a good control range.

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

We have only two choices, DIB column base valve or purge column distillate valve, for fixing a flow in the recycle loop. Either of these would work. The rationale for picking one is based upon avoiding disturbances to the unit downstream of the fixed flow location. Since the purge column is not critical from the viewpoint of product quality, we elect to fix the flow upstream of reactor (purge column distillate flow) so that we minimize disturbance in reactor temperature and pressure.

We must control the two column pressure. This is best done by manipulating the condenser cooling water flowrates.

There are four liquid levels to be controlled i.e. DIB column base level, DIB column reflux drum, Purge column base level and Purge column reflux drum. The choices of manipulated variables that can be used to control DIB column reflux drum level include distillate product flowrate and reflux flowrate. We must also control the level in the DIB column base and in the purge column reflux drum and base.

Having made the choice to fix the purge column distillate flow, we are faced with the problem of how to control purge column reflux drum level. We have two primary choices: reflux flow or heat input. We choose the latter because the flowrate of the purge column reflux is small relative to the vapor coming overhead from the top of the column. Remember the Richardson rule, which says we select the largest stream. So we choose the heat input manipulating to control the Purge column reflux drum.

The flowrate of the purge stream from the base of the purge column is quite small, so it would not do a good job in controlling base level. This is especially true when the large stream flow has been selected to control the reflux drum level. Base level in the purge column can be controlled by manipulating the bottoms flowrate from the DIB column.

We are then left with controlling base level in the DIB column. The only remaining valve is the fresh nC_4 feed flowrate into the column. The feed is liquid and there only 20 trays between the lower feed point and the column base, so base level control using feed should be possible. This base level is also an indication of the nC_4 inventory within the process.

The material balance control structure works opposite to the direction of flow. Purge column distillate is fixed; purge column reflux drum level is controlled by vapor boilup; purge column base level is controlled by feed to the purge column; and DIB column base level is controlled by the fresh feed to the DIB column.

Had we started to assign the DIB column base level control first, we would have ended up with the same inventory control structure. The reason is as follow. Assume we had chosen the DIB column base valve to control base level. After resolving the purge column inventory loops, we would have found that we need to control the purge column base or reflux drum level with the fresh feed flow to the DIB column. The dynamic lags associated with these loops would have forced us back to the control strategy as described above.

Step 7: Check component balances

Four components need to be accounted for; they are C_3, iC_4, nC_4 and iC_5. The light inert propane leaves in the product stream. The heavy inert component isopentane (iC_5) leaves in the purge stream. Any the iC_4 coming into the process in the fresh feed and the iC_4 produced by the reaction can leave in the product stream.

The amount of reactant the nC_4 fed into the system must somehow be exactly balance by the amount of the nC_4 converted to product the iC_4. The process acts almost like a purge integration in term of the moles of the nC_4. The way this balancing of the nC_4 is accomplished in the control structure shown in Figure 5.1 is by using the level in the base of the DIB column to indicate if the nC_4 is building up in the system or is being depleted. The material in the DIB base is mostly the nC_4. There is a little the iC_4 (16 percent) and a little the iC_5 (5 percent), and the remained is the nC_4. So DIB base level changes reflect changes in the nC_4 inventory in the process. If the level is decreasing, fresh feed should be increased because we are consuming more reactant than we are feeding.

Step 8: Control individual unit operations

The previous steps have left us at this point with two unassigned control valves, which are the reflux flows to each column (case of the DIB reflux flow is not used). We may need dual composition control in the DIB column for the reversible case.

Step 9: Optimize economics or improve dynamic controllability

This step is not considered in this work.

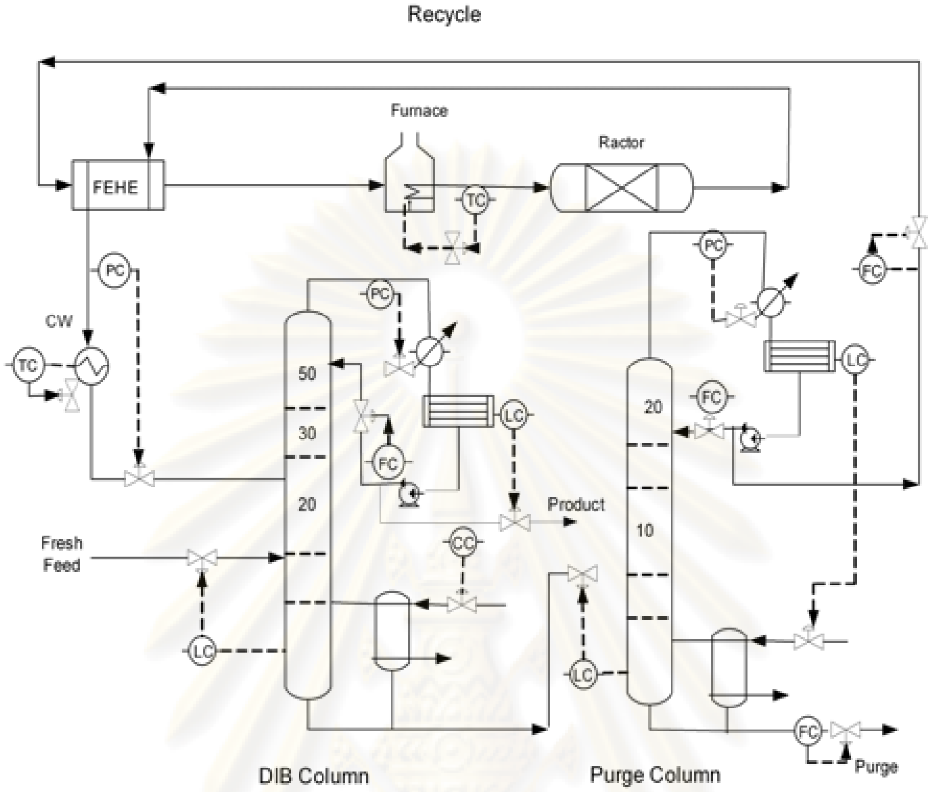


Figure 5.1 Control structure for Isomerization process (Plantwide Process Control, 1998)

5.1.2 Fixture Point Theorem

For the forth control structure, we use the Fixture point theorem (Wongsri, 2008).

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

Fixture point theorem analysis

1. Consideration in dynamic mode of simulation until process set up to steady state.
2. Control variable (CV) can be arranged to follow the most sensibility of the process variable by step change the MV (change only one MV, the other

should be fixed then alternate to other until complete). Study the magnitude of integral absolute error (IAE) of all process variables that deviates form steady state.

3. Consider CV that give the most deviation from steady state (high IAE score) to match with MV. CV and MV should be directing interactive together, after that will consider the next CV to match with other MV.

5.2 Design of plantwide control structures

In this current work, we apply the first control structure of Luyben (1998) namely control structure 1 (CS1), the second control structure of Wilailak (2007) namely control structure 2 (CS2) to the Butane Isomerization process with energy integration schemes for RHEN-1, RHEN-2, RHEN-3 and Base Case. The new plantwide control structures CS3 and CS4 are designed for all processes. In all of these control structures, the same loops are used as follows:

- The DIB column reboiler level is controlled by manipulating the fresh feed valve.
- The Purge column reboiler level is controlled by manipulating the Purge column feed valve.
- The flowrate of recycle stream is controlled by manipulating the Purge column distillate valve.
- The flooded condenser pressure is controlled by manipulating the DIB column feed recycle valve.
- The flooded condenser outlet temperature is controlled by manipulating the cooler duty.
- The reactor inlet temperature is controlled by manipulating the furnace duty.

- The DIB column pressure is controlled by manipulating the DIB column condenser duty.
- The Purge column pressure is controlled by manipulating the Purge column condenser duty.
- The Purge column condenser level is controlled by manipulating the Purge column reboiler duty.

5.2.1 Reference control structure I (CS1)

For DIB column of this control structure, the impurity of nC_4 in the product stream is controlled by manipulating the DIB column reboiler duty. The DIB column reflux drum level is controlled by manipulating the DIB column distillate valve. The reflux flow is fixed with reflux valve. This control structure is designed to reduce the effects of disturbance in order to achieved impurity of normal butane in product and desired production rate. For the Purge column, the condenser level is controlled by manipulating the Purge column reboiler duty.

5.2.2 Reference control structure II (CS2)

This control structure uses the DIB column distillate valve to control impurity liquid of nC_4 in the top of DIB column (tray 50), DIB column reflux flow is manipulated to control reflux drum level, and DIB column reboiler duty is manipulated to control the temperature on tray 1 of DIB column. We choose the level of purge column condenser is controlled by manipulating the Purge column reboiler duty.

5.2.3 Design of control structure III (CS3)

This control structure uses the DIB column distillate valve to control impurity liquid of nC_4 in the top of DIB column (tray 50), DIB column reflux flow is manipulated to control reflux drum level, and DIB column reboiler duty is manipulated to control the temperature on tray 1 of DIB column. We choose the level of purge column condenser is controlled by manipulating the Purge column reboiler duty. Since there is a fairly large temperature change in the purge column, controlling the temperature on some suitable trays (tray 1 to 7) are controlled at the average temperature by purge bottom stream valve.

5.2.4 Design of control structure IV (CS4)

For DIB column of this control structure, the impurity of nC_4 in the product stream is controlled by manipulating the DIB column reboiler duty. The DIB column reflux drum level is controlled by manipulating the DIB column distillate valve. The reflux flow is fixed with reflux valve. This control structure is designed to reduce the effects of disturbance in order to achieved impurity of normal butane in product and desired production rate. For the Purge column, the condenser level is controlled by manipulating the Purge column reboiler duty. The control structure 4 (CS4) is the same structure as control structure (CS1).

For all of the control structures, we apply them to the 5 alternatives of the heat exchanger networks (Base case for reversible and irreversible reaction case and RHEN-1 to 3 for reversible reaction case). So, there are 15 alternatives of the heat exchanger networks with control structures for Butane Isomerization plant include Base case for reversible and irreversible reaction case with 3 control structures.The RHEN-1 to 3 for reversible reaction case with 3 control structures as show in Figures 5.8 to 5.22.

5.3 Energy management of heat integrated Butane Isomerization Plant

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

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

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

5.3.1 Heat Pathways and HEN control configuration designs for RHEN-1

The design of the heat pathways for RHEN-1 shown in Figures 5.2 shifts the positive and negative disturbance loads of C2 to reboiler of DIB column. Thus, the negative disturbance load of a cold stream will result in decrease of the reboiler duty which is good. The positive disturbance load will result in increase of the reboiler duty which is ruled by constraint. The negative or positive disturbance load of H1 is directed to the reboiler; the reboiler duty of corresponding column is increased or decreased accordingly.

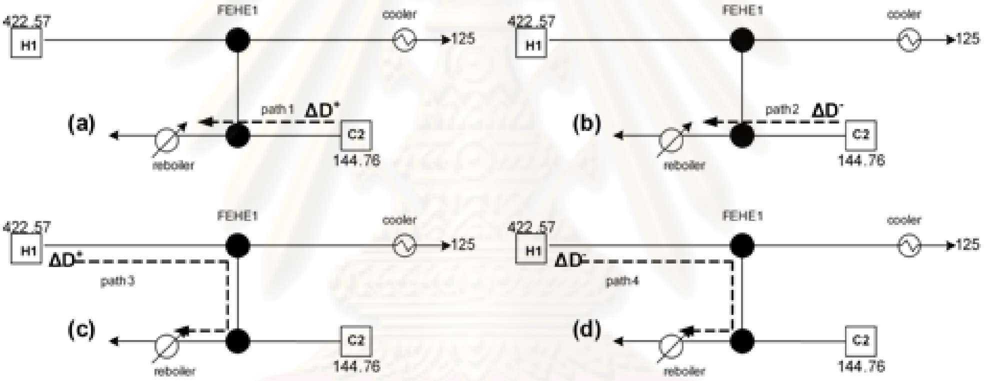


Figure 5.2 Heat pathways through RHEN-1, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C2 to the reboiler, (b) path 2 is used to shift the negative disturbance load of the cold stream C2 to the reboiler, (c) path 3 is used to shift the positive disturbance load of the hot stream H1 to the reboiler and (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to the reboiler

The control systems for RHEN-1 work as follows: Figure 5.3 shows the hot outlet temperature of FEHE1 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP). At the same time, the hot outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the reboiler duty at a good level. Whenever the hot outlet temperature of FEHE1 drops below the allowable limit due to, for example, a negative disturbance load entering the hot stream H1, the control action to the hot temperature control (TC-h) open the valve VBP. As a result, the hot outlet temperature of FEHE1 will rise to its normal temperature and the cold outlet temperature of FEHE1 will be further decreased, so the reboiler duty will also be increased. If the hot outlet temperature of FEHE1 increases above a lower limit, i.e., a desired-condition during operation, due to the positive disturbance load entering the hot stream H1, the control action to TC-h close the valve VBP. Consequently, the hot outlet temperature of FEHE1 will drop to its normal temperature and the cold outlet temperature of FEHE1 will be increased, so the reboiler duty will also be decreased. At the same time, the hot outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the cooler duty at a good level.

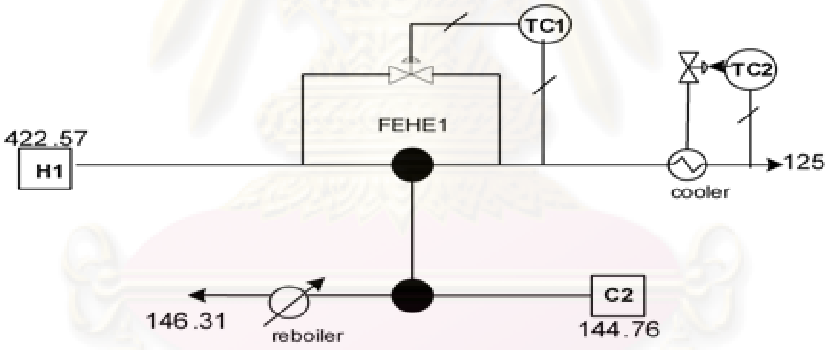


Figure 5.3 Control configuration of RHEN-1

5.3.2 Heat Pathways and HEN control configuration designs for RHEN-2

The design of the heat pathways for RHEN-2 shown in Figures 5.4 shifts the positive and negative disturbance loads of C1 to cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty which good. The negative disturbance load will result in increase of the cooler duty. The negative or positive disturbance loads of H1 are shifted to the cooler.

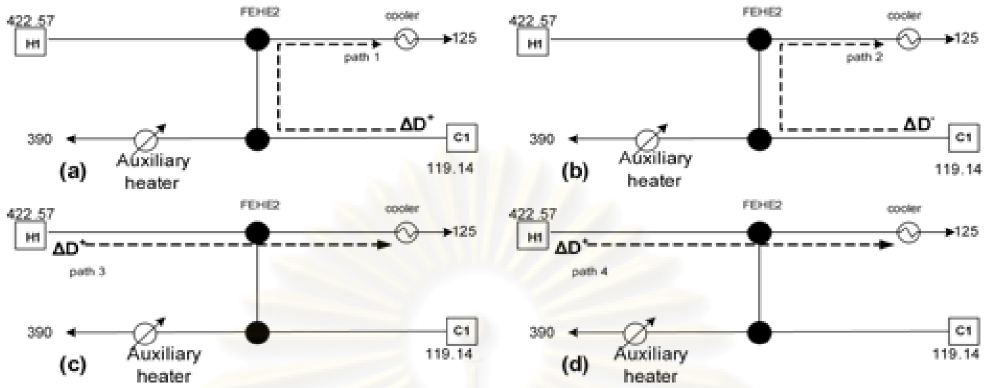


Figure 5.4 Heat pathways through RHEN-2, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C1 to the cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream C1 to the cooler, (c) path 3 is used to shift the positive disturbance load of the hot stream H1 to the cooler and (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to the cooler

The control systems for RHEN-2 work as follows: Figure 5.5 shows the cold outlet temperature of FEHE1 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP). Whenever the cold outlet temperature of FEHE1 drops below the allowable limit due to, for example, a negative disturbance load entering the hot stream H1, the control action to the cold temperature control (TC-h) close the valve VBP. 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. If the cold outlet temperature of FEHE1 increases above a lower limit, i.e., a desired-condition during operation, due to the positive disturbance load entering the hot stream H1, the control action to TC-h open the valve VBP. Consequently, the cold outlet temperature of FEHE1 will drop to its normal temperature and the hot outlet temperature of FEHE1 will be increased, so the cooler duty will also be increased. At the same time, the cold outlet temperature of FEHE1 should not be allowed to rise above an upper limit value, which is necessary to keep the cooler duty at a good level.

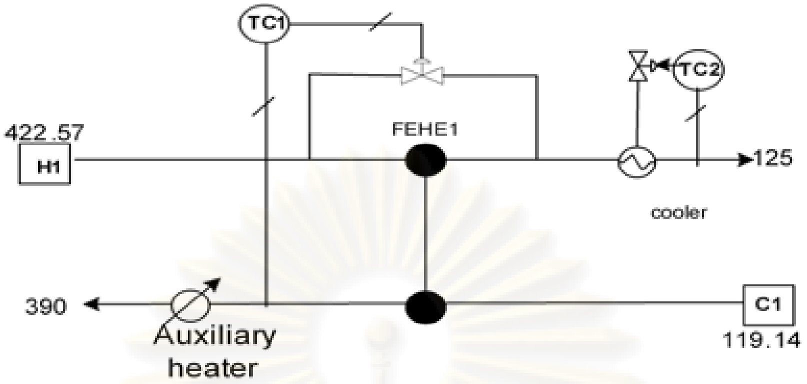


Figure 5.5 Control configuration of RHEN-2

5.3.3 Heat Pathways and HEN control configuration designs for RHEN-3

The design of the heat pathways for RHEN-3 shown in Figures 5.6 shifts the positive and negative disturbance loads of C3 to reboiler of Purge column. Thus, the negative disturbance load of a cold stream will result in decrease of the reboiler duty which is good. The positive disturbance load will result in increase of the reboiler duty which is ruled by constraint. The negative or positive disturbance load of H1 is directed to the reboiler; the reboiler duty of corresponding column is increased or decreased accordingly.

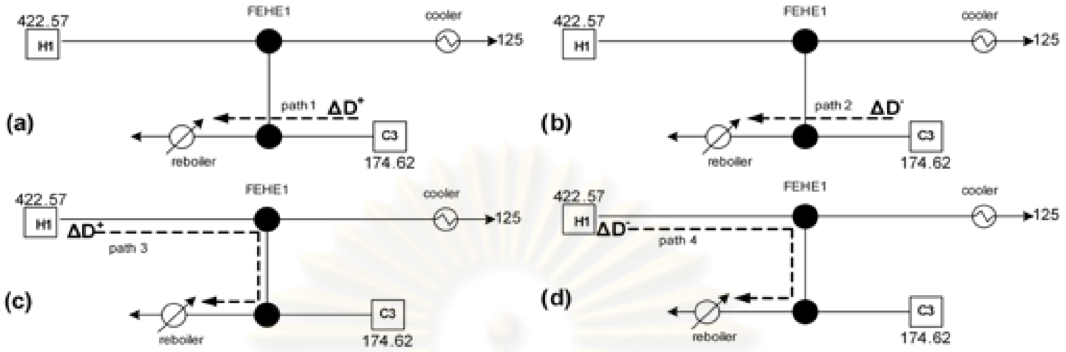


Figure 5.6 Heat pathways through RHEN-3, where: (a) path 1 is used to shift the positive disturbance load of the cold stream C2 to the reboiler, (b) path 2 is used to shift the negative disturbance load of the cold stream C2 to the reboiler,(c) path 3 is usedto shift the positive disturbance load of the hot stream H1 to the reboiler and (d) path 4 is used to shift the negative disturbance load of the hot stream H1 to the reboiler.

The control systems for RHEN-3 work as follows: Figure 5.7 shows the hot outlet temperature of FEHE1 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP). At the same time, the hot outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the reboiler duty at a good level. Whenever the hot outlet temperature of FEHE1 drops below the allowable limit due to, for example, a negative disturbance load entering the hot stream H1, the control action to the hot temperature control (TC-h) open the valve VBP. As a result, the hot outlet temperature of FEHE1 will rise to its normal temperature and the cold outlet temperature of FEHE1 will be further decreased, so the reboiler duty will also be increased. If the hot outlet temperature of FEHE1 increases above a lower limit, i.e., a desired-condition during operation, due to the positive disturbance load entering the hot stream H1, the control action to TC-h close the valve VBP. Consequently, the hot outlet temperature of FEHE1 will drop to its normal temperature and the cold outlet temperature of FEHE1 will be increased, so the reboiler duty will also be decreased. At the same time, the hot outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the cooler duty at a good level

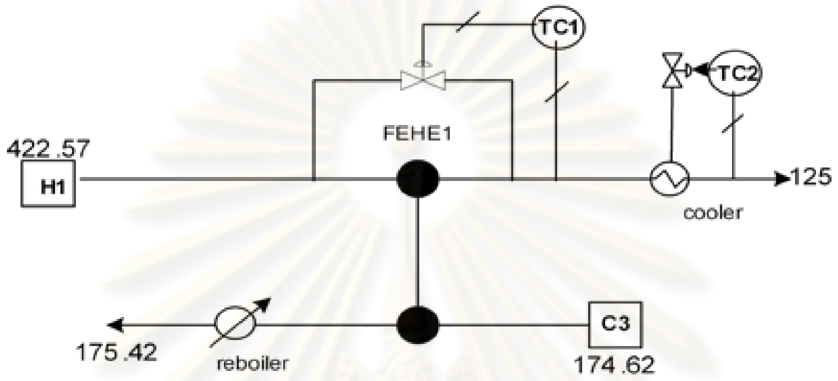


Figure 5.7 Control configuration of RHEN-3

For all the heat integration units, the bypass streams are designed to control the outlet temperatures of FEHE. 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 rate of about 5 % 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.

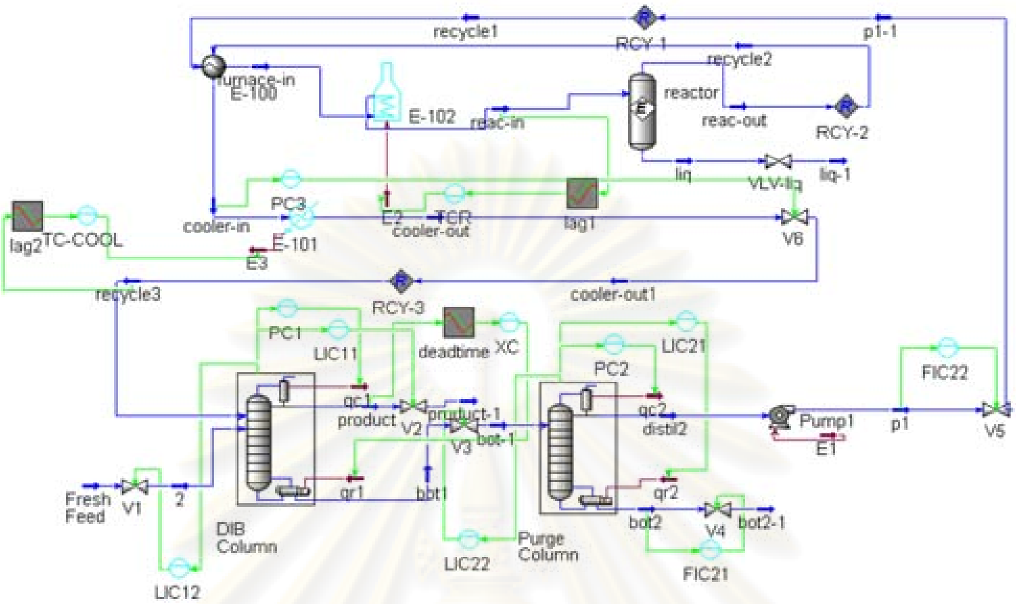


Figure 5.8 Application of reference control structure 1 (CS1) to the Butane Isomerization plant (Base Case for reversible reaction)

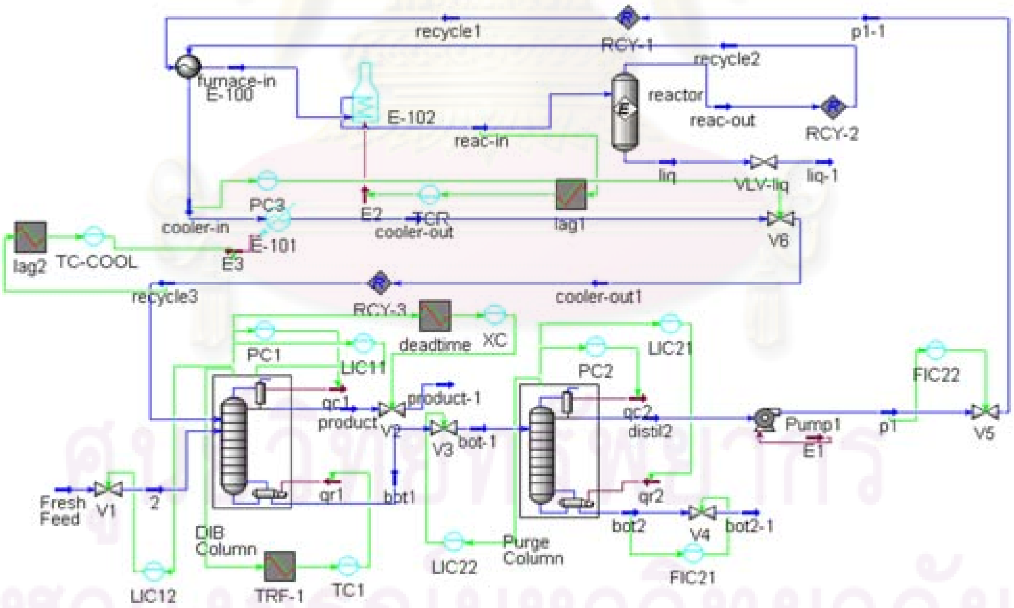


Figure 5.9 Application of reference control structure 2 (CS2) to the Butane Isomerization plant (Base Case for reversible reaction)

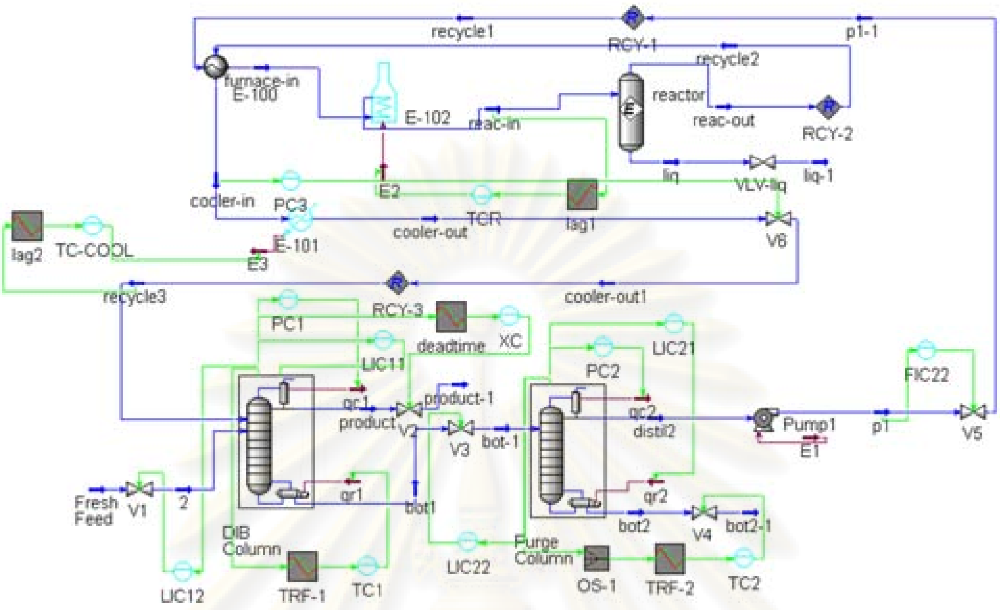


Figure 5.10 Application of design control structure 3 (CS3) to the Butane Isomerization plant (Base Case for reversible reaction)

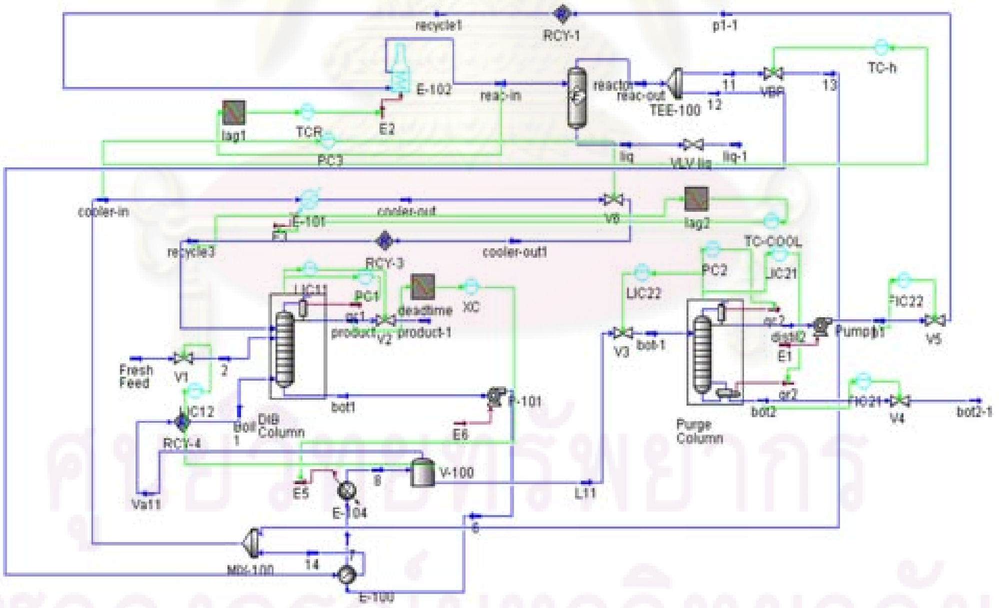


Figure 5.11 Application of reference control structure 1 (CS1) to the Butane Isomerization plant alternative 1 for reversible reaction (RHEN-1)

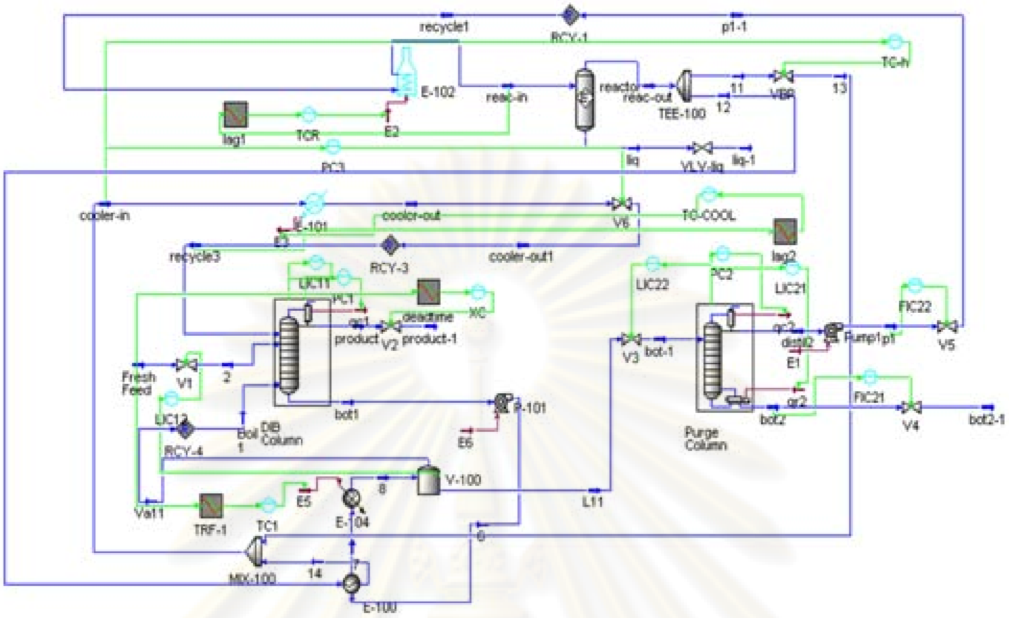


Figure 5.12 Application of reference control structure 2 (CS2) to the Butane Isomerization plant alternative 1 for reversible reaction (RHEN-1)

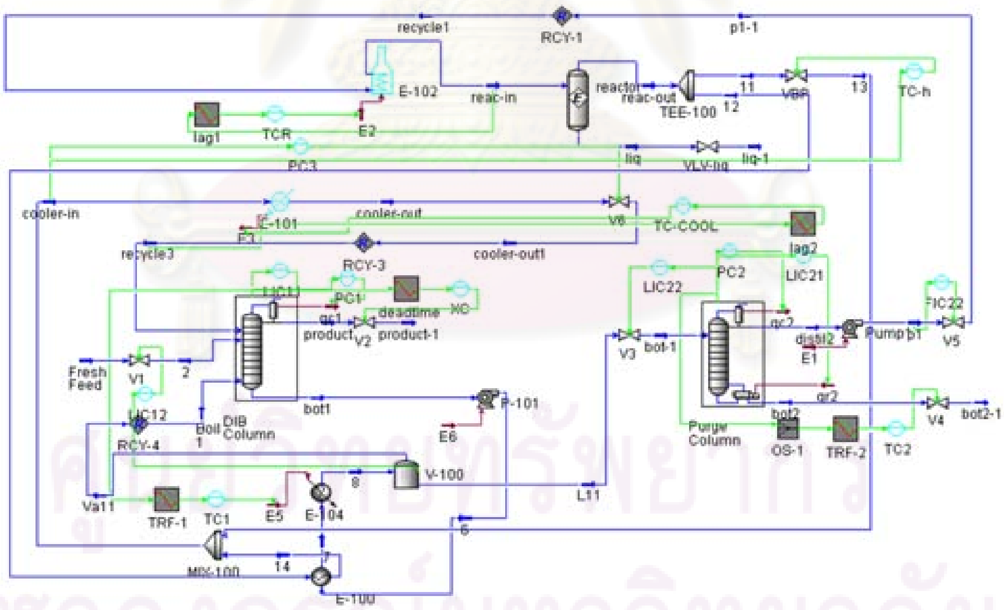


Figure 5.13 Application of design control structure 3 (CS3) to the Butane Isomerization plant alternative 1 for reversible reaction (RHEN-1)

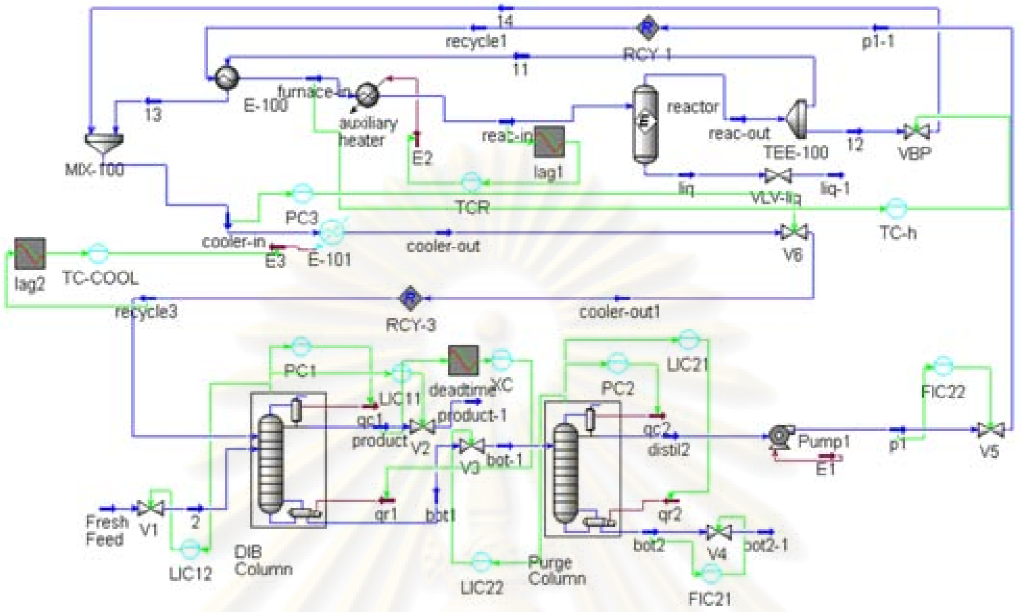


Figure 5.14 Application of reference control structure 1 (CS1) to the Butane Isomerization plant alternative 2 for reversible reaction (RHEN-2)

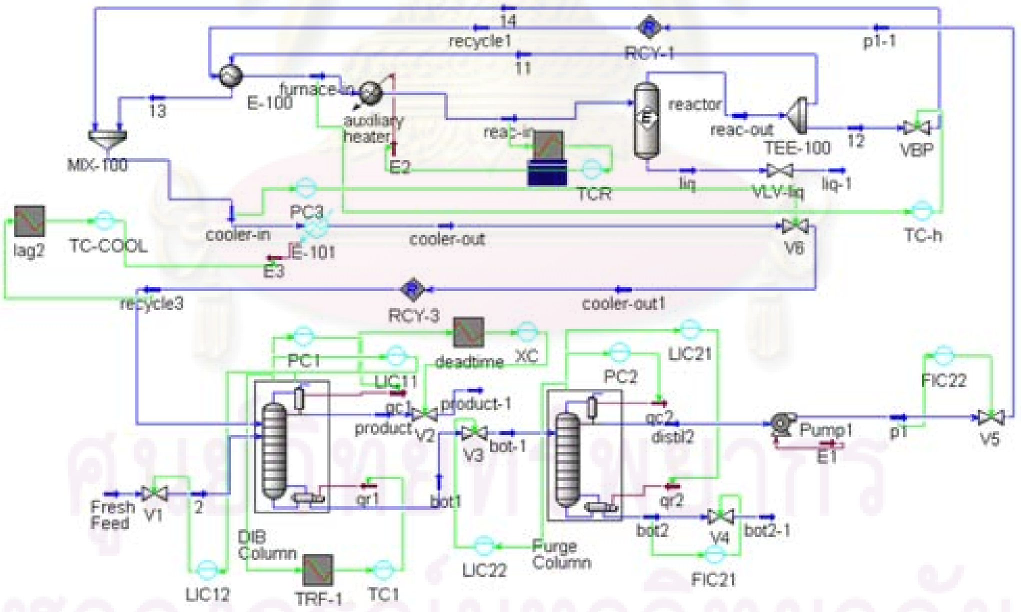


Figure 5.15 Application of reference control structure 2 (CS2) to the Butane Isomerization plant alternative 2 for reversible reaction (RHEN-2)

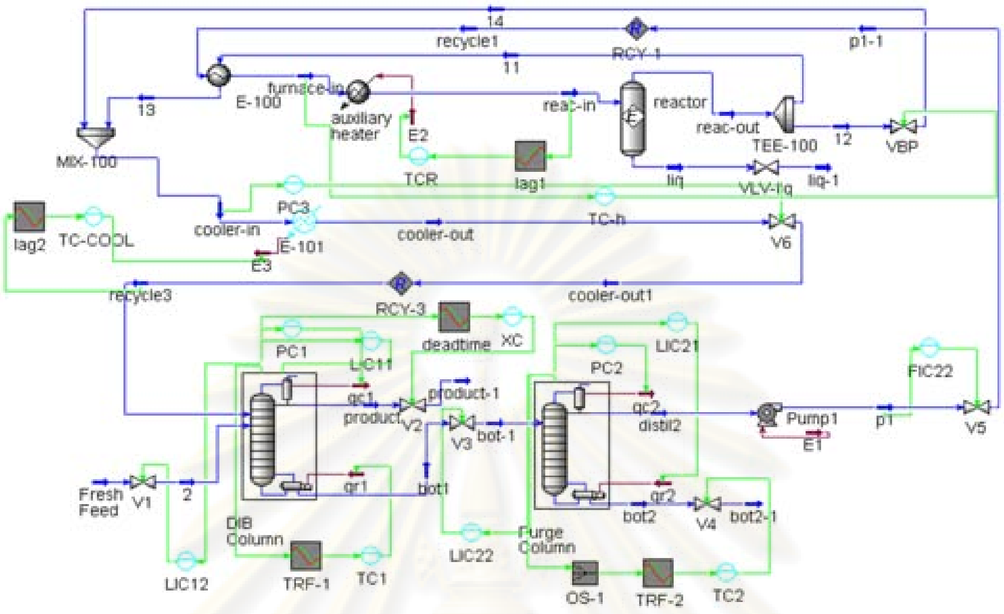


Figure 5.16 Application of design control structure 3 (CS3) to the Butane Isomerization plant alternative 2 for reversible reaction (RHEN-2)

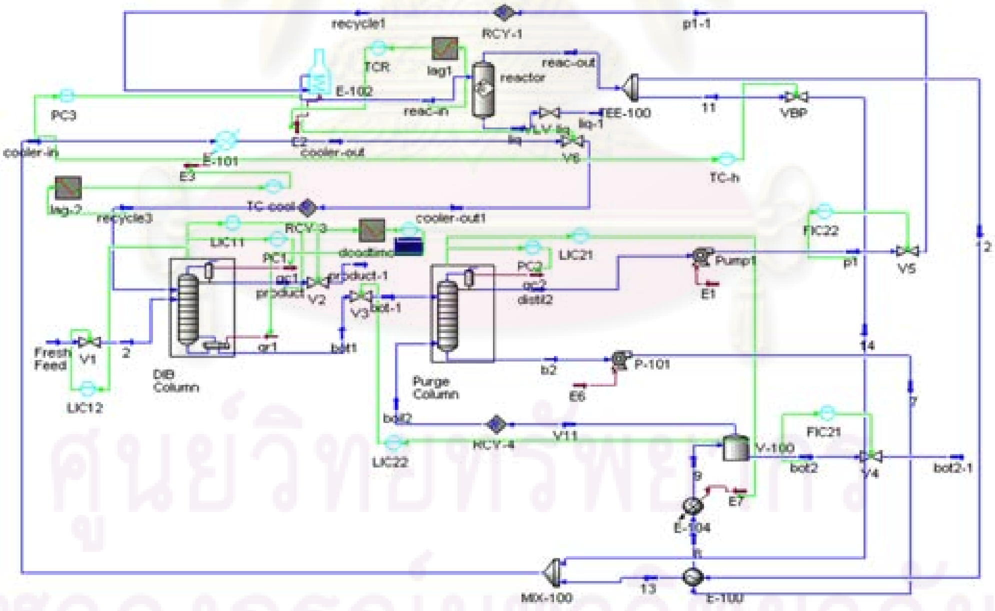


Figure 5.17 Application of reference control structure 1 (CS1) to the Butane Isomerization plant alternative 3 for reversible reaction (RHEN-3)

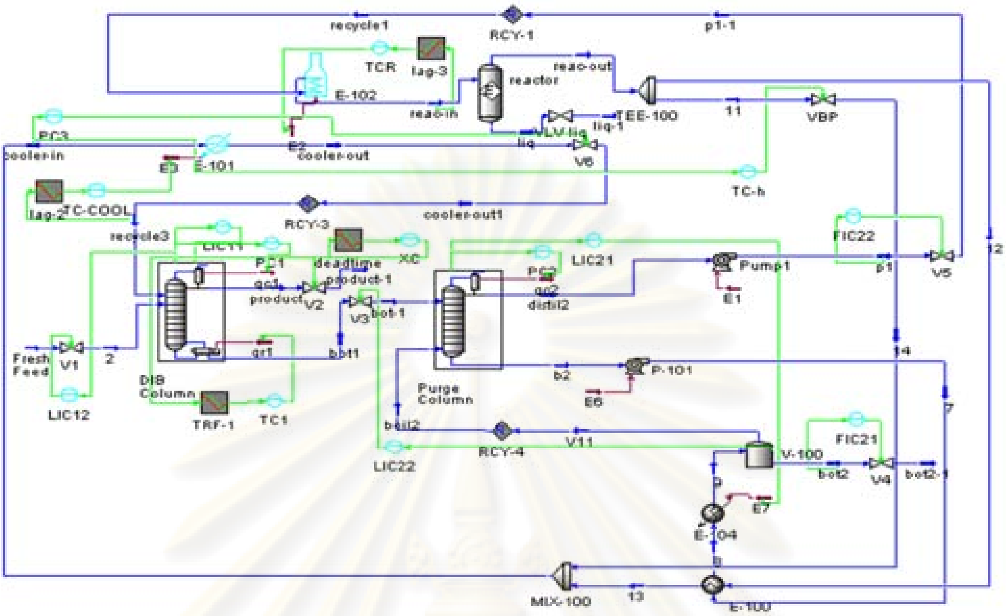


Figure 5.18 Application of reference control structure 2 (CS2) to the Butane Isomerization plant alternative 3 for reversible reaction (RHEN-3)

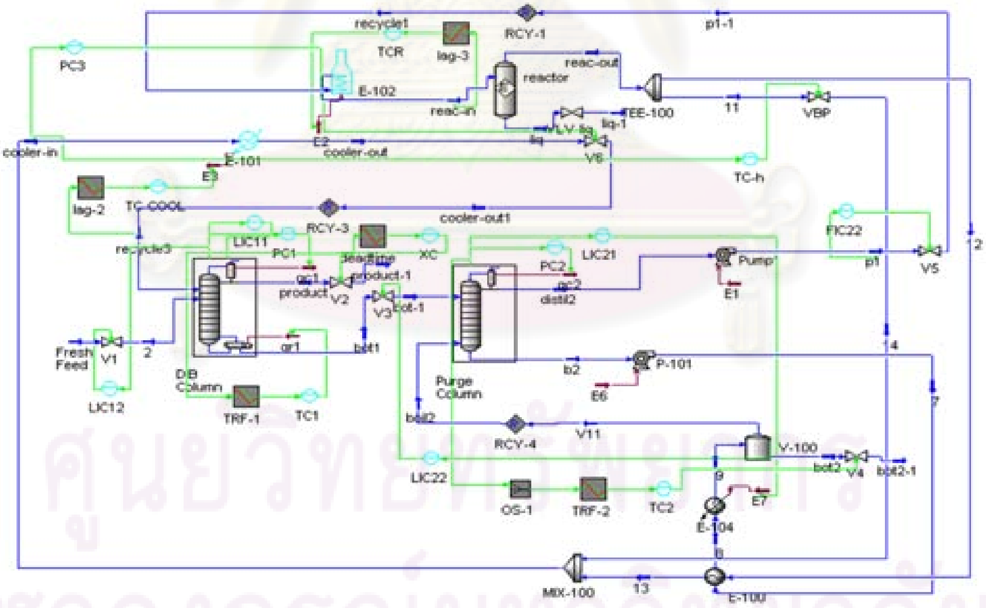


Figure 5.19 Application of design control structure 3 (CS3) to the Butane Isomerization plant alternative 3 for reversible reaction (RHEN-3)

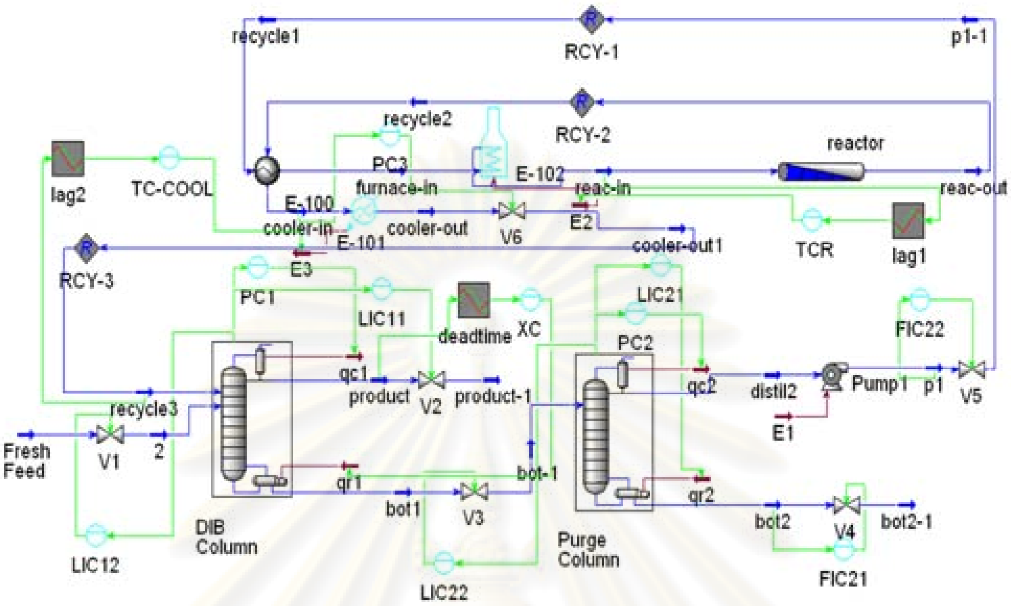


Figure 5.20 Application of reference control structure 1 (CS1) to the Butane Isomerization plant (Base case for irreversible reaction)

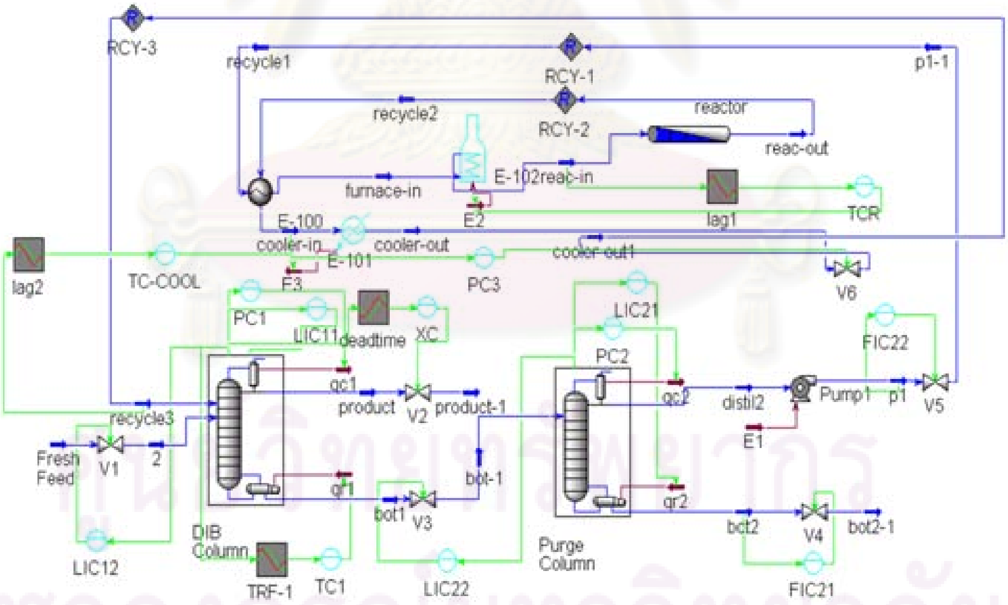


Figure 5.21 Application of reference control structure 2 (CS2) to the Butane Isomerization plant (Base case for irreversible reaction)

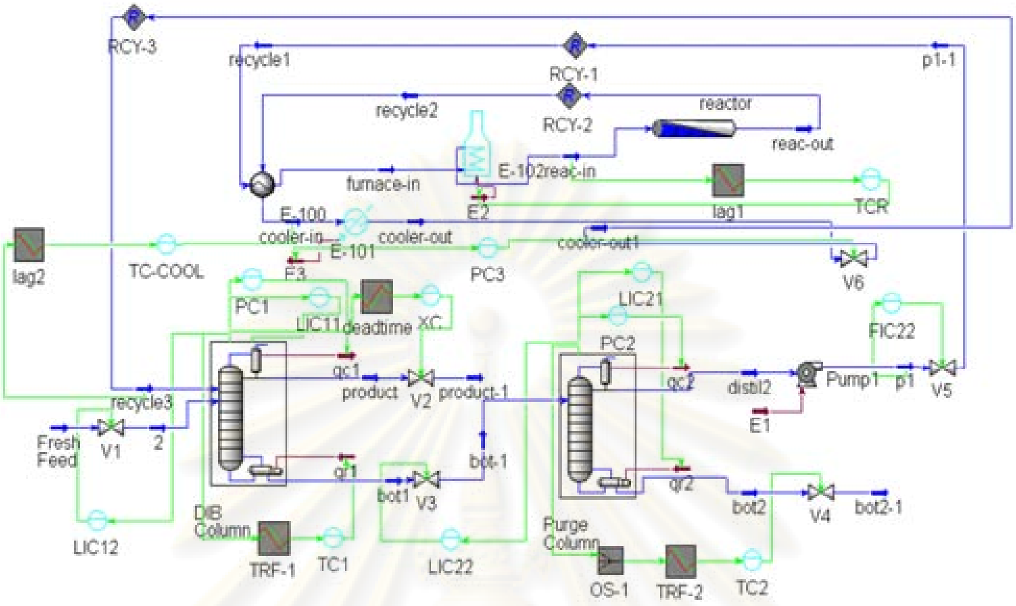


Figure 5.22 Application of design control structure 3 (CS3) to the Butane Isomerization plant (Base case for irreversible reaction)

5.4 Dynamic simulation results

In order to illustrate the dynamic behaviors of our control structures and the previous control structures (Luyben et al., 1998 and Wilailak S, 2007), two types of disturbance are used to test response of the system: inlet reactor temperature step increase 10 ^oF for reversible and irreversible reaction case, recycle flowrate increases from 872.5 lb mol/hr to 942.5 lb mol/hr for reversible reaction case and recycle flowrate increases from 870.1 lb mol/hr to 940.1 lb mol/hr for irreversible reaction case. Temperature controllers are PIDs which are tuned using relay feedback. Two temperature measurement lags of 0.1 minute are included in the two temperature loops (reactor inlet temperature and DIB feed temperature). A 3-minute deadtime is assumed in the product composition measurement (distillate from the DIB). Flow and pressure controller are PIs and their parameters are heuristics values. Proportional-only level controllers are used and their parameters are heuristics values. Butane composition is measured and controlled using PID controller. All control valves are half-open at nominal operating condition.

5.4.1 Change in the heat load disturbance of hot stream for CS1 to CS3 in Butane Isomerization plant for Base Case (reversible reaction case ;Luyben et al., 1998)

Figure 5.23 show results when the reactor inlet temperature is changed by step increases 10 ^oF (from 390 ^oF to 400 ^oF), occurring at time equals 60 minutes.

The normal butane (nC_4) for all of control structures increase at first and decrease to its set point afterwards as show in Figure 5.23a. The dynamic responses of CS2 and CS3 are faster than CS1 because there is the base temperature controller of DIB column and the reflux flow can control the reflux drum level more effective than the distillate flow.

The product flowrates decrease due to reaction rate decreases (the kinetic parameters to give a decrease in the equilibrium constant) as temperature increases, such as would occur with exothermic reversible reaction. For CS1, the purity of the DIB distillate improve (more nC_4 in the over head product), which causes the reboiler heat input to decrease. The base level is high and fresh feed flowrates are fed to the column decreasingly.

The IAEs impurity, nC_4, composition loops at the top of DIB column is shown in Table 5.1. Control structures CS3 handle the change better than CS1 and CS2.

Table 5.1 IAEs of nC_4 composition loops at the top of DIB column (Base case for reversible reaction case)

Integral Absolute Error		
CS1	CS2	CS3
3.13571	0.10331	0.10092

It is interesting to note that CS3 reject the thermal disturbance by keeping the base temperature constant, its resulted DIB reboiler duty is lower and resulted furnace duty is higher than that of CS1, CS2. The product stream is decreased; in the case of CS3, it is lower than in the case of CS1 and CS2. Figure 5.23d shows dynamic responses of the temperature on tray 1 of DIB column.

Control structure(CS3) control the impurity in the product by manipulating distillate flowrate, control temperature at DIB column by manipulating reboiler duty and control temperature at purge column by manipulating purge bottom stream.

As can be seen, the dynamic responses of CS3 are faster than the others resulting in lower in IAEs. However, large change in the product flow is not important since it is assumed that the distillate is going to a storage tank or cavern

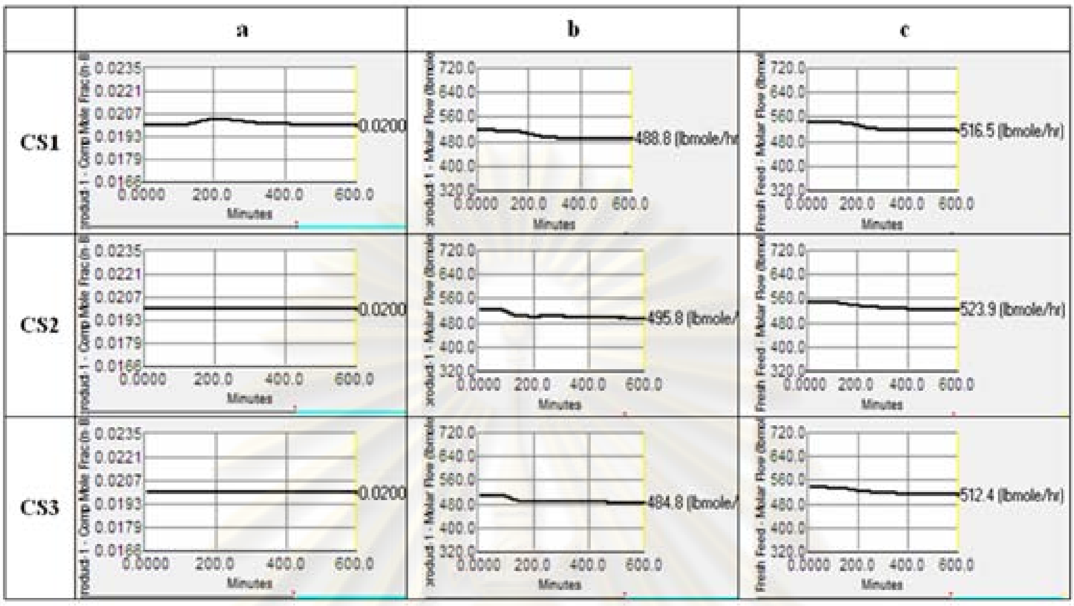


Figure 5.23 Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base case (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

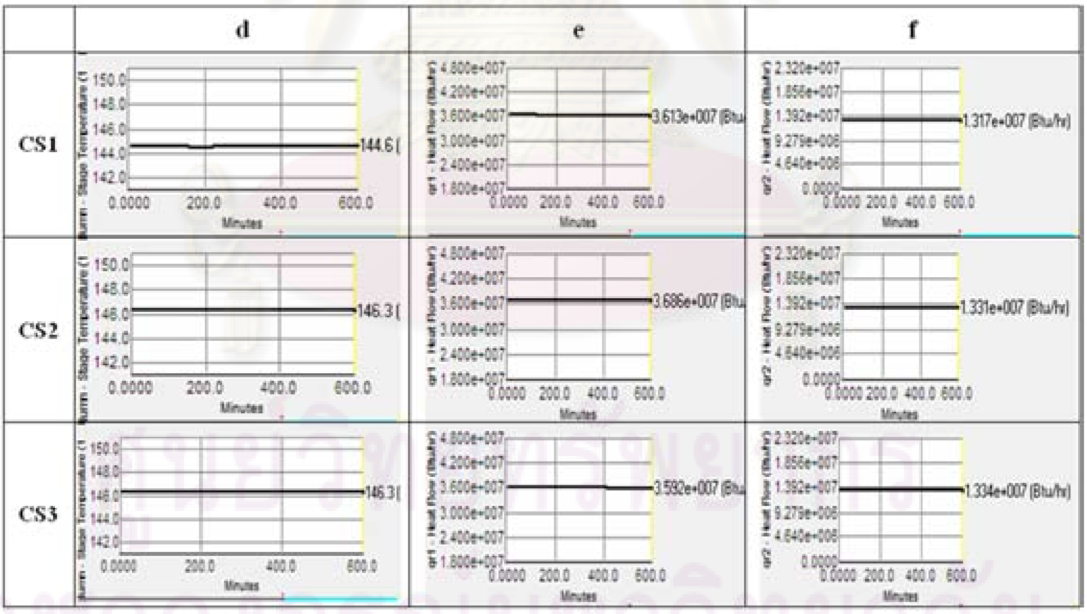


Figure 5.23 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base Case (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

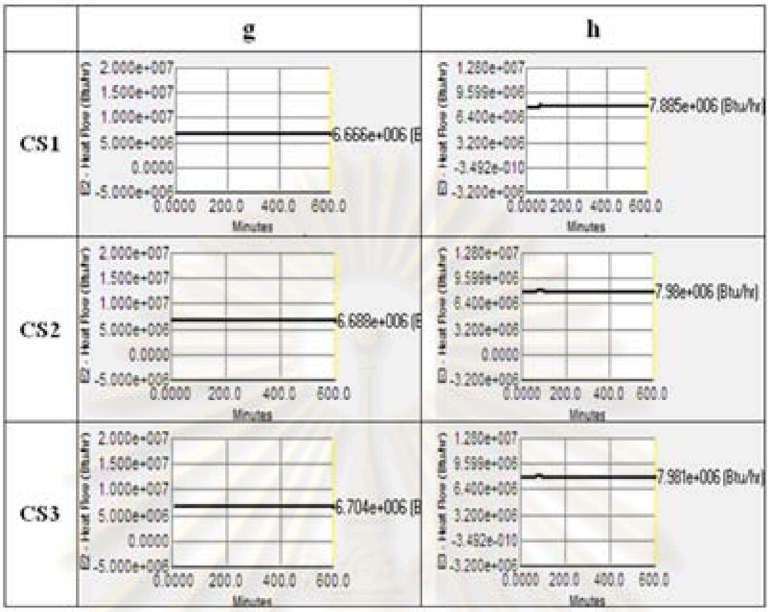


Figure 5.23 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base Case (reversible), where (g) furnace duty and (h) cooler duty

5.4.2 Change in the heat load disturbance of hot stream for CS1 to CS3 in the new designed resilient heat exchanger network: RHEN-1, RHEN-2 and RHEN-3 for reversible reaction case

Figure 5.24-5.26 show dynamic responses of the Butane Isomerization plant RHEN1-3 when the reactor inlet temperature is changed by step increases 10 ^oF (from 390 ^oF to 400 ^oF), occurring at time equals 60 minutes.

The resilient heat exchanger network structure RHEN-1, normal butane (nC_4) of all control structures increase at first and decrease to its set point over 400 minutes for CS1, while CS2 and CS3 are going to its set point over 200 minutes as show in Figure 5.24a. The product flowrates decrease due to reaction rate decreases (the kinetic parameters to give a decrease in the equilibrium constant) as temperature increases, such as would occur with exothermic reversible reaction.

For CS1, the purity of the DIB distillate improve (more nC_4 in the over head product), which causes the reboiler heat input to decrease. The base level is high and fresh feed flowrates are fed to the column decreasingly as show in Figure 5.24b-c.

Similar conclusion can be drawn for resilient heat exchanger network structure RHEN-2 and RHEN-3 with control structures CS1-CS3. (see Figure 5.25-5.26).

In this work, we design 3 new resilient heat exchanger network (RHEN-1, RHEN-2 and RHEN-3). The thermal disturbance for RHEN-1 is shifted to heater of DIB column. For RHEN-2 shift the thermal disturbance to cooler and RHEN-3 is shifted to heater of Purge Column.

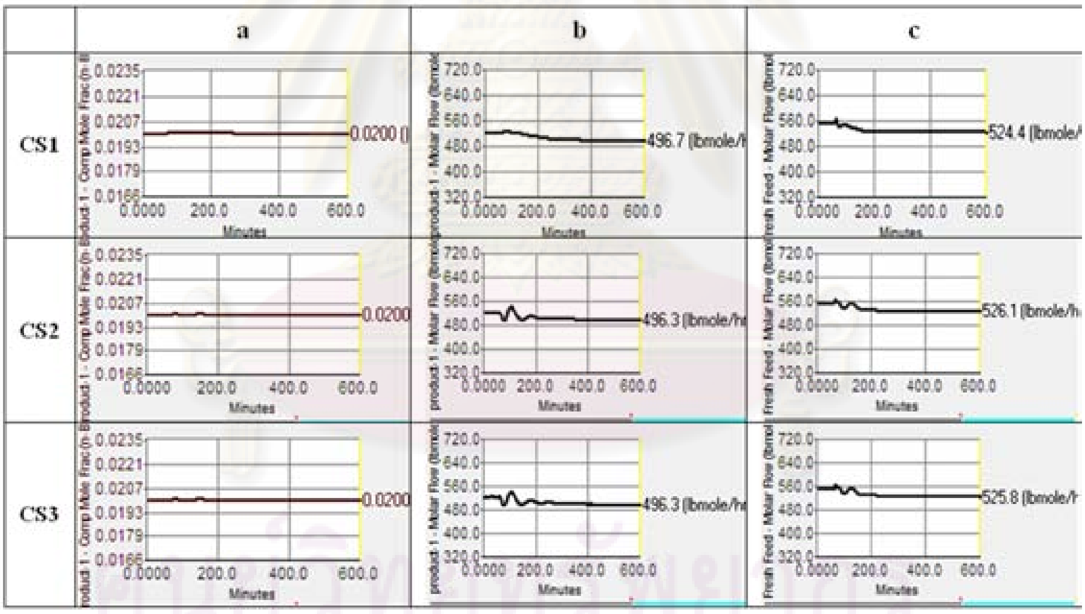


Figure 5.24 Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-1 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

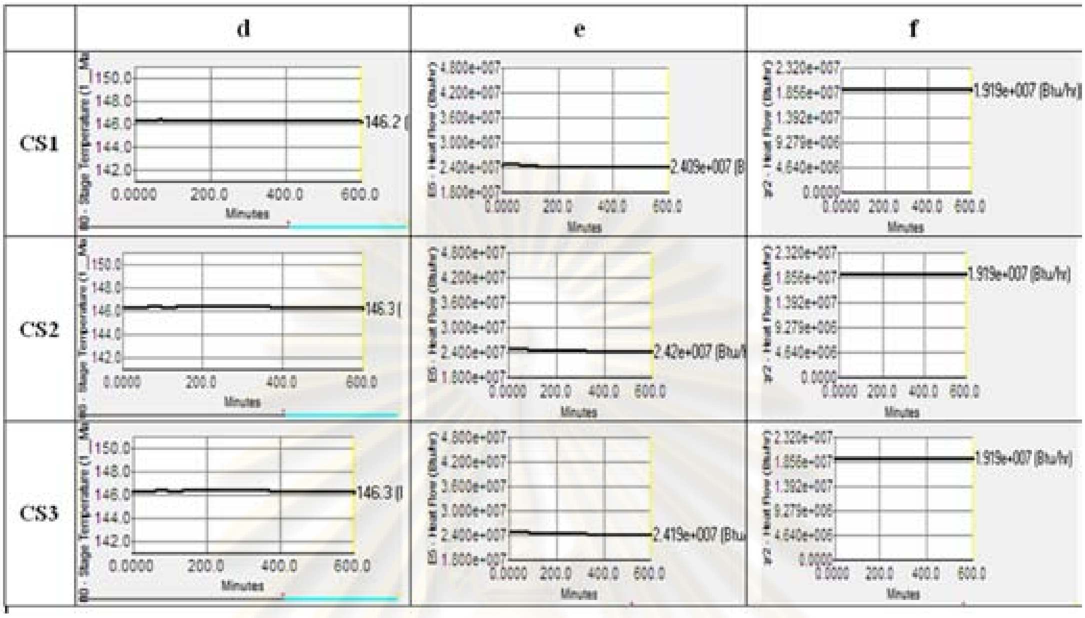


Figure 5.24 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-1 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

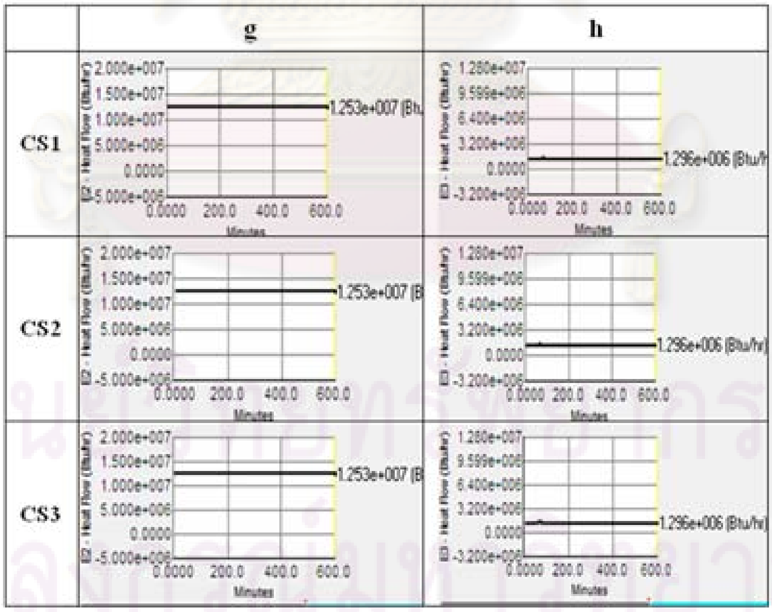


Figure 5.24 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-1 (reversible), where (g) furnace duty and (h) cooler duty

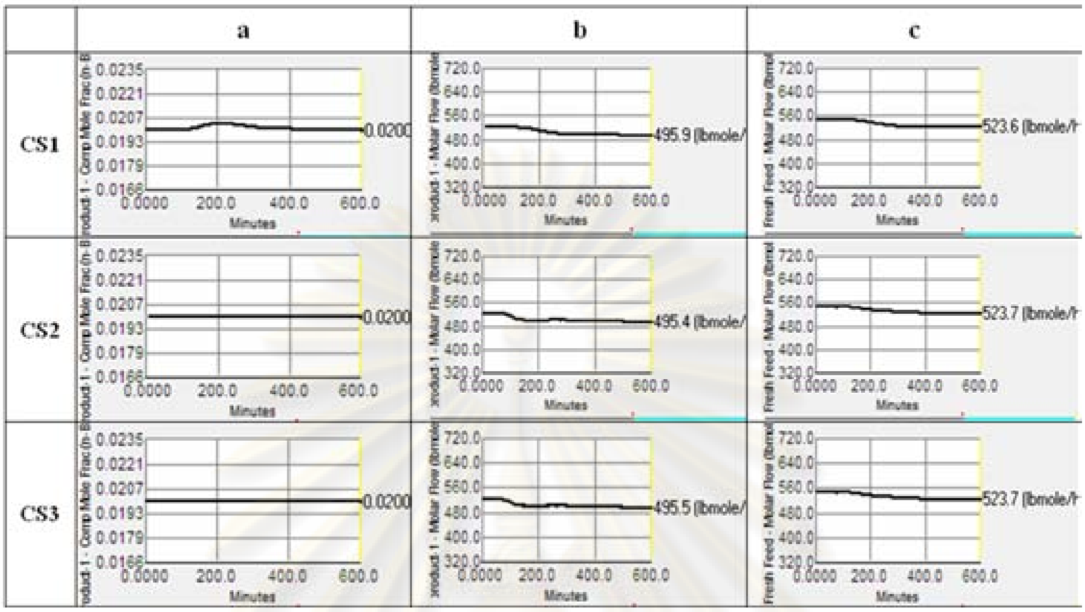


Figure 5.25 Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-2 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

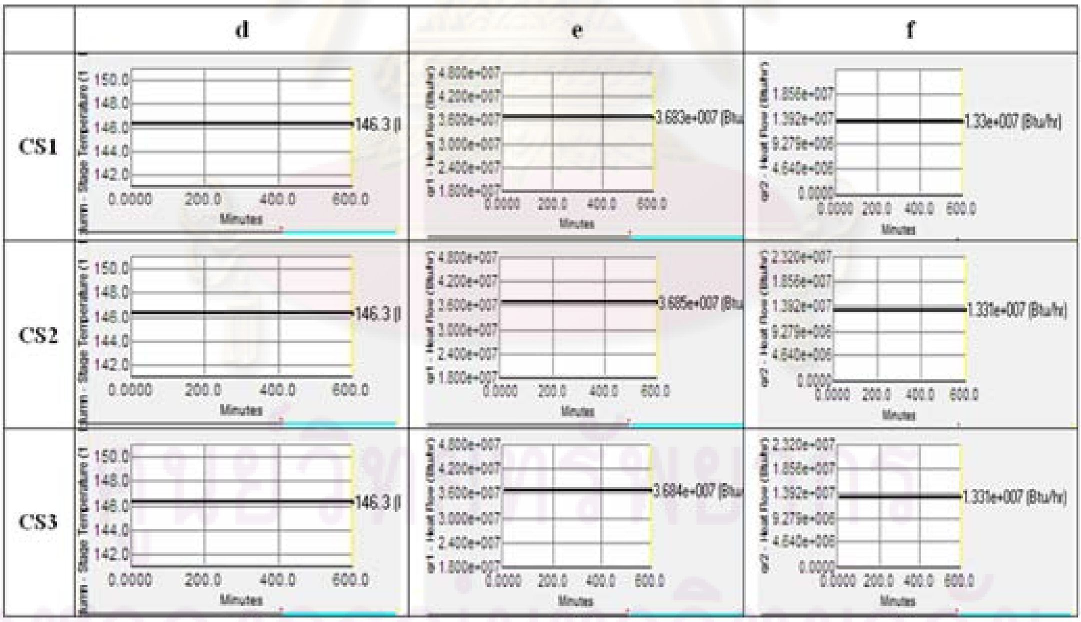


Figure 5.25 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-2 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

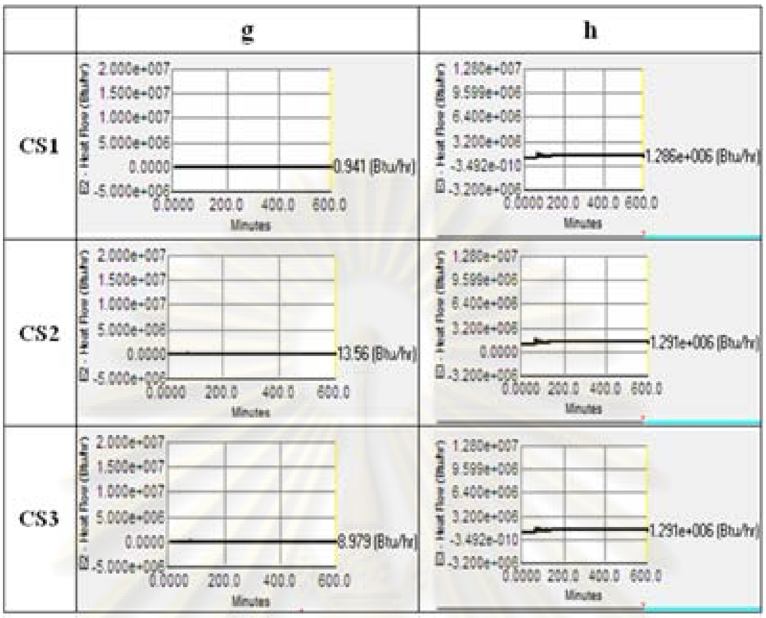


Figure 5.25 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-2 (reversible), where (g) furnace duty and (h) cooler duty

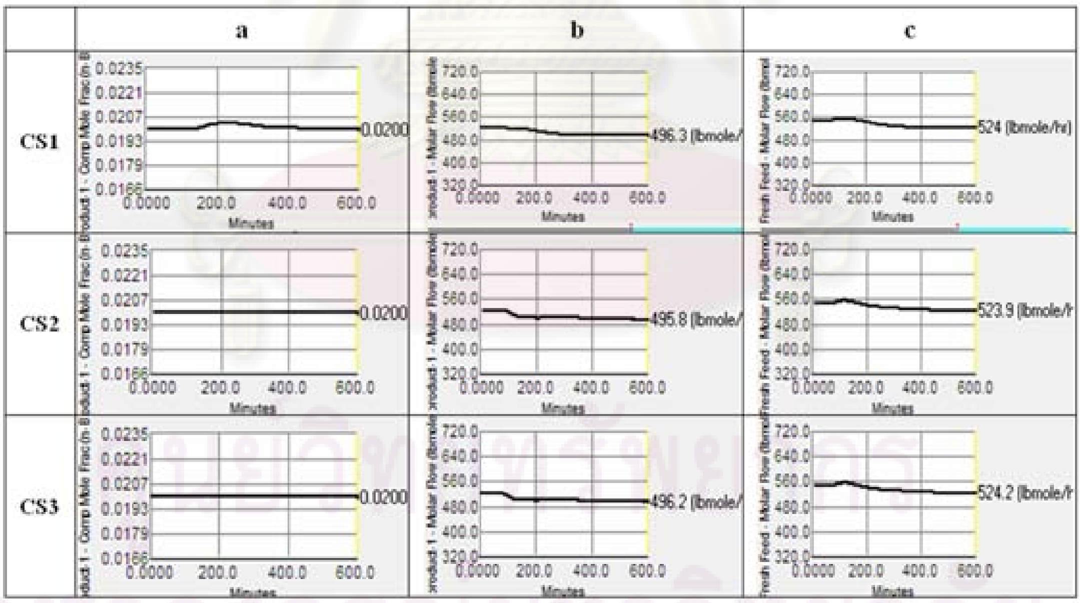


Figure 5.26 Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-3 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

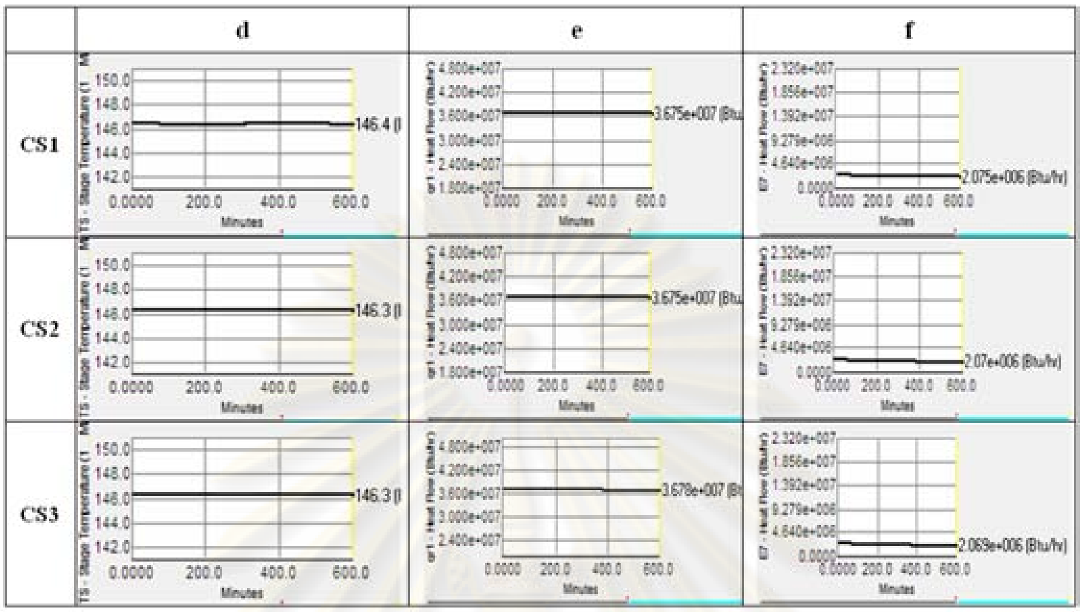


Figure 5.26 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-3 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

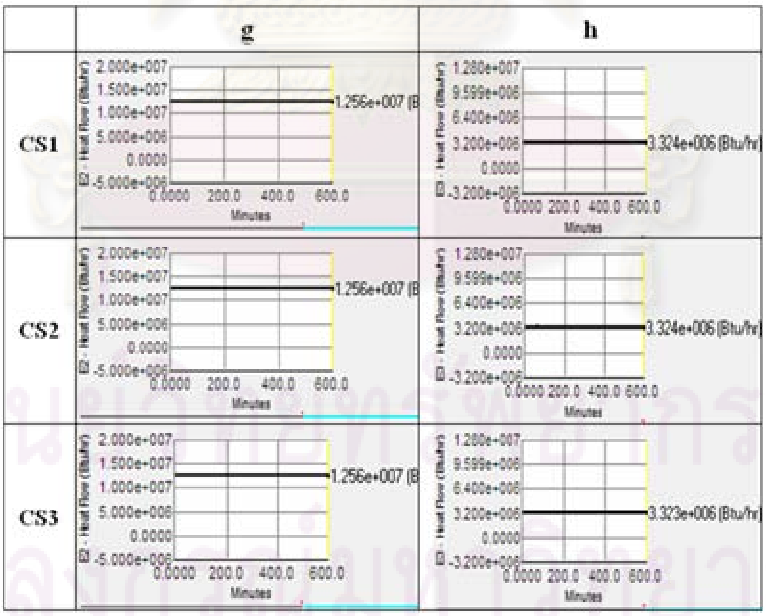


Figure 5.26 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of RHEN-3 (reversible), where (g) furnace duty and (h) cooler duty

5.4.3 Comparison of control structures for change the heat load disturbance of hot stream: CS1, CS2 and CS3 with RHEN1-3 for reversible reaction case

From the dynamic simulation results for all resilient heat exchanger network with control structures CS1-CS3 when the reactor inlet temperature is changed, we can conclude that CS3 are the proper control structures. Because the base DIB column and base Purge column temperature are controlled so they reject the thermal disturbance by keeping the base temperature constant. The product flowrate decreases due to reaction rate decreases as temperature increasingly. The nC4 impurity in product are slowly increased and return to its set point which CS3 are less variable than CS1 and CS2. Also the control structures CS3 give the better response for all resilient heat exchanger network structure as show in Table 5.2 and Figure 5.27.

Table 5.2 The IAE results of the control systems to 10 ^oF increase in the setpoint of the reactor inlet temperature

		Integral Absolute Error			
		BC	RHEN-1	RHEN-2	RHEN-3
CCDt	CS1	3.13571	0.65902	3.08288	3.03287
	CS2	0.10331	0.25196	0.10703	0.10498
	CS3	0.10092	0.24937	0.1072	0.10331
TCR	CS1	0.67392	0.0432	4.11625	0.09455
	CS2	0.6669	0.0446	4.16368	0.09437
	CS3	0.67013	0.04444	4.16873	0.09457
TCC	CS1	0.04896	0.07704	2.41691	0.07735
	CS2	0.09925	0.0777	2.44672	0.07728
	CS3	0.08644	0.07716	2.43733	0.0773
PCD	CS1	1.42806	1.75874	1.40116	1.36743
	CS2	0.60369	1.74508	0.63583	0.70959
	CS3	0.58996	1.73283	0.63878	0.66817
PCP	CS1	0.02101	0.03394	0.02806	4.87549
	CS2	0.02541	0.05488	0.02919	4.87899
	CS3	0.02732	0.05413	0.02817	4.8835
Total	CS1	2.17195	1.91292	7.96238	6.41482
	CS2	1.39525	1.92226	7.27542	5.76022
	CS3	1.37385	1.90856	7.27301	5.72353

Note CC = Composition Control, TC = Temperature Control, PC= Pressure Control, R = Reactor, D = DIB, P = Purge, C = Cooler, t = top, b = bottom

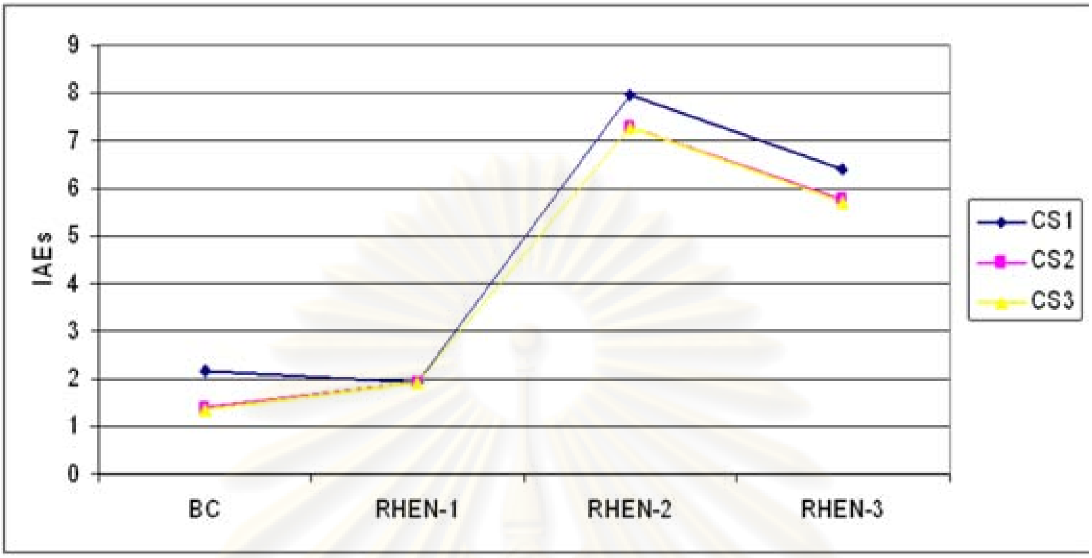


Figure 5.27 The IAE re1sults of the control systems to 10 ^oF increase in the setpoint of the reactor inlet temperature

5.4.4 Change in the heat load disturbance of hot stream for CS1 to CS3 in Butane Isomerization plant for Base Case (irreversible reaction case; Luyben et al., 1998)

Figure 5.28 show dynamic responses of the Butane Isomerization plant when the reactor inlet temperature is changed by step increases 10 ^oF (from 390 ^oF to 400 ^oF), occurring at time equals 60 minutes of base case with CS1-3, produces an increase in product flowrate. For CS1, as more iC4 is produced in the reactor with the increase in reaction rate at higher temperature, the purity of DIB column (less nC4 in the overhead product), which causes the reboiler heat input to increase. This lower the base level and pull in more fresh feed. Also the control structures CS2 and CS3 give the better response than CS1.

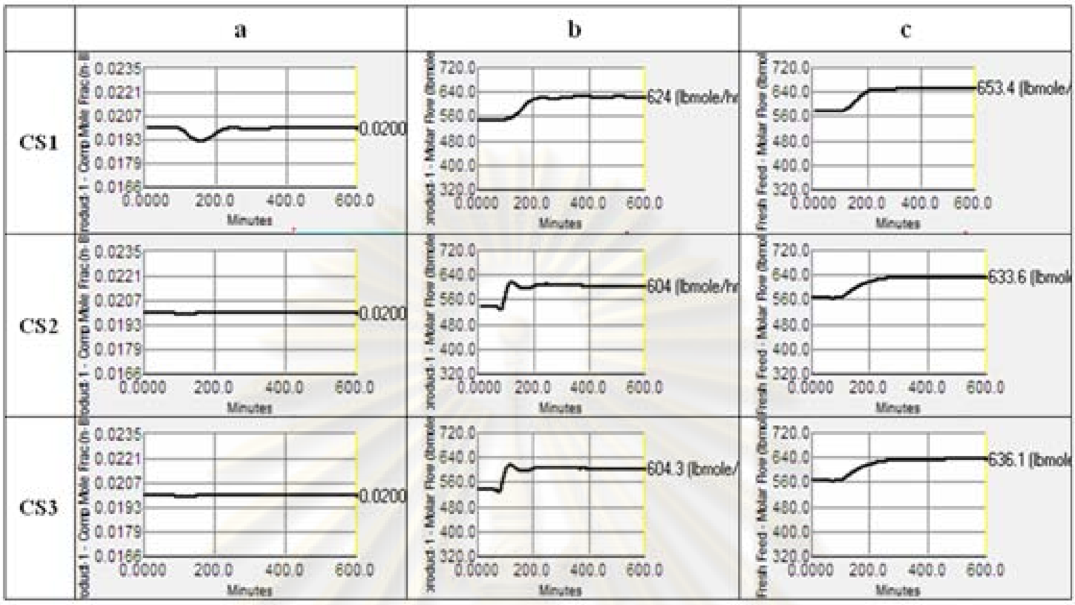


Figure 5.28 Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base case (irreversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

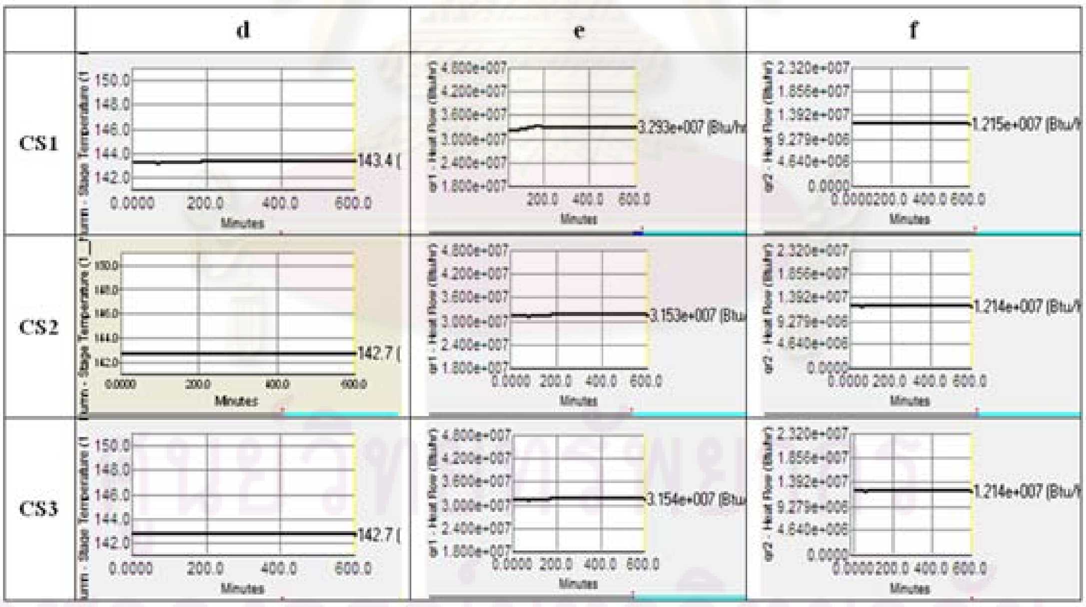


Figure 5.28 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base Case (irreversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

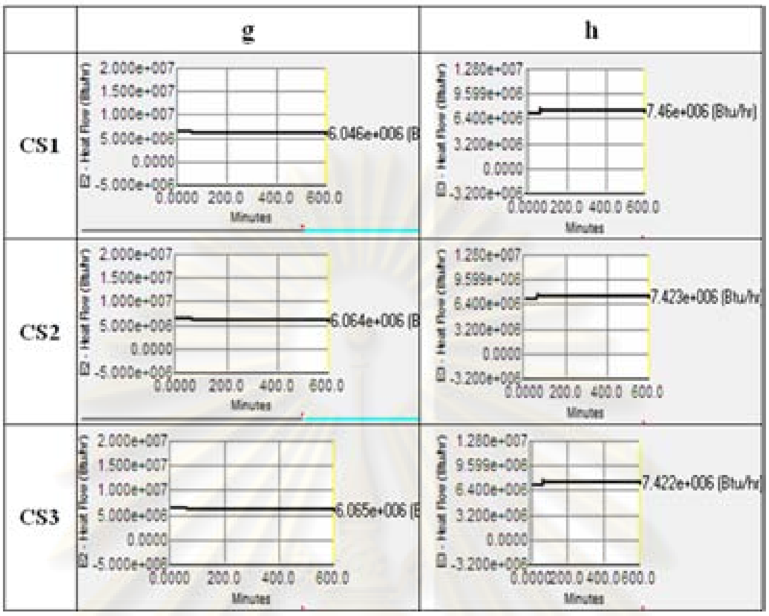


Figure 5.28 Continued Dynamic responses to 10 ^oF increase in reactor inlet temperature of Base Case (irreversible), where (g) furnace duty and (h) cooler duty

5.4.5 Comparison of Base case for change the heat load disturbance of hot stream: irreversible and reversible reaction case

Table 5.3 and Figure 5.29 show the IAE results of the control system when the reactor inlet temperature is changed by step increases 10 ^oF to compare the dynamic responses between irreversible and reversible reaction case.

As can be seen, irreversible and reversible reaction case show the IAE results the control system are different value. Also the different process gives the responsible difference.

Table 5.3 The IAE results of the control systems to 10 ^oF increase in the setpoint of the reactor inlet temperature : irreversible and reversible reaction case

		Integral Absolute Error	
		BC irreversible	BC reversible
CCDt	CS1	3.095554	3.1357105
	CS2	0.432848	0.1033109
	CS3	0.433023	0.1009248
TCR	CS1	0.041679	0.6739153
	CS2	0.041492	0.6668951
	CS3	0.041504	0.6701342
TCC	CS1	2.345505	0.0489639
	CS2	2.327576	0.0992502
	CS3	2.327479	0.0864355
PCD	CS1	0.983854	1.4280574
	CS2	0.368144	0.603688
	CS3	0.36868	0.5899604
PCP	CS1	0.020774	0.0210139
	CS2	0.019319	0.025414
	CS3	0.019801	0.0273205
Total	CS1	3.391811	2.1719505
	CS2	2.756531	1.3952472
	CS3	2.757464	1.3738506

Note CC = Composition Control, TC = Temperature Control, PC= Pressure Control, R = Reactor, D = DIB, P = Purge, C = Cooler, t = top, b = bottom

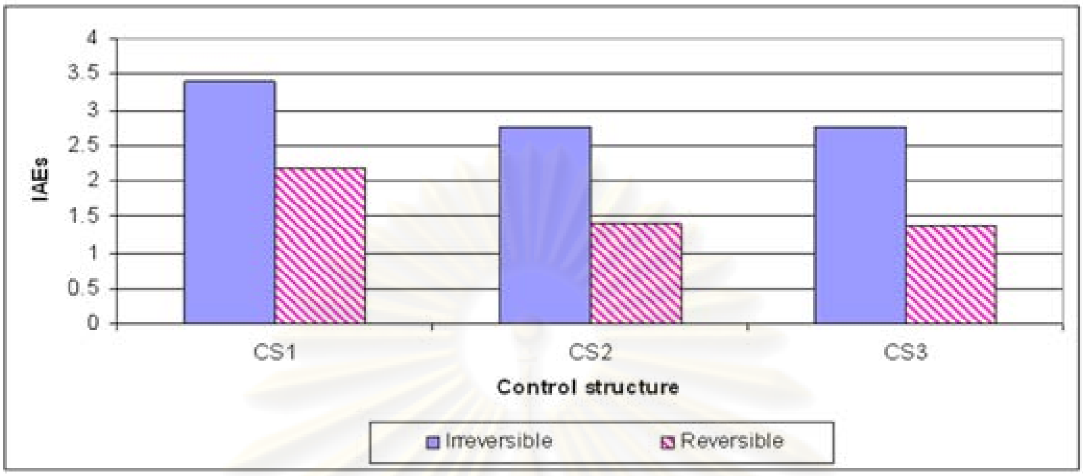


Figure 5.29 The IAE results of the control systems to 10 ^oF increase in the setpoint of the reactor inlet temperature: irreversible and reversible reaction case

5.4.6 Change in the recycle flowrates for CS1 to CS3 in Butane Isomerization plant for Base Case (reversible reaction case ;Luyben et al., 1998)

Figure 5.30 shows the dynamic responses of CS1-CS3 for the effect of increasing the recycle flowrate from 872.5 to 942.5 lb-mol/h. In CS1, production rate increase from 515.5 to 522.3 lb-mol/h. In CS2, production rate increase from 521.7 to 555.5 lb-mol/hr and CS3, production rate increase from 509.85 to 543.2 lb-mol/hr.

The product flowrates increase due to recycle flow increase. For CS1, the purity of the DIB distillate improve (less nC_4 in the over head product), which causes the reboiler heat input to increase. This lower the base level, and pulls in more fresh feed.

The IAEs impurity, nC_4, composition loops at the top of DIB column is shown in Table 5.4. Control structures CS2 and CS3 handle the change better than CS1.

Table 5.4 IAEs of nC_4 composition loops at the top of DIB column (Base case for reversible reaction case)

Integral Absolute Error		
CS1	CS2	CS3
1.860026	0.250683	0.252103

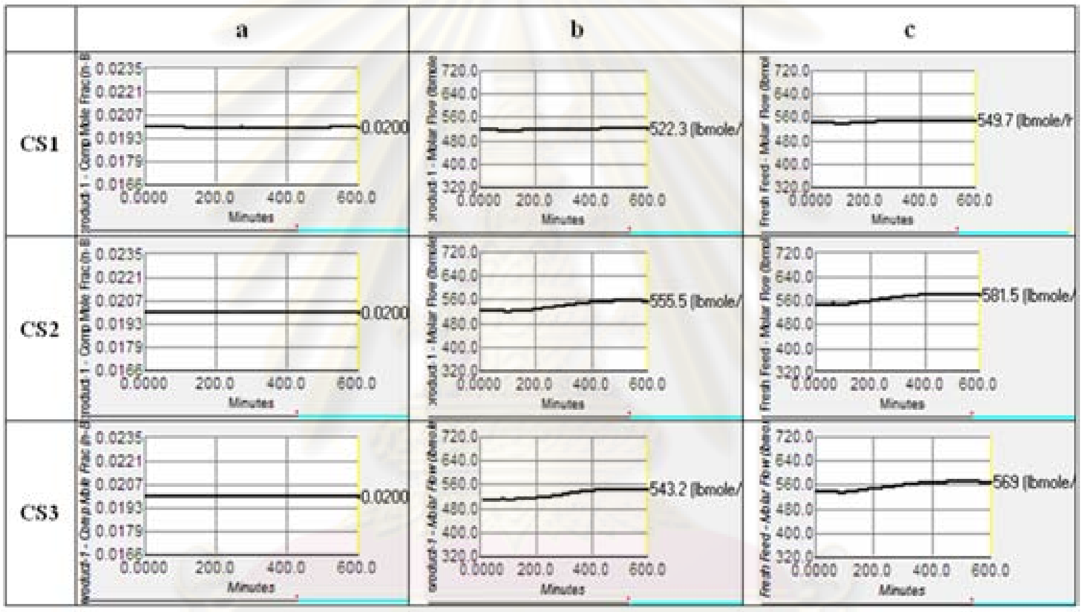


Figure 5.30 Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of Base Case (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

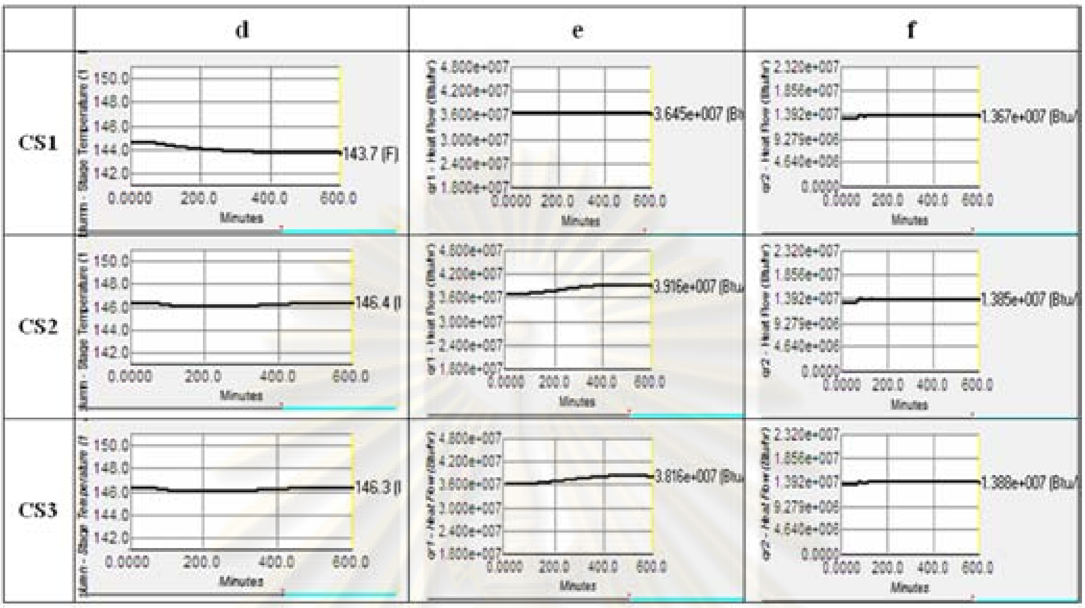


Figure 5.30 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of Base Case (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

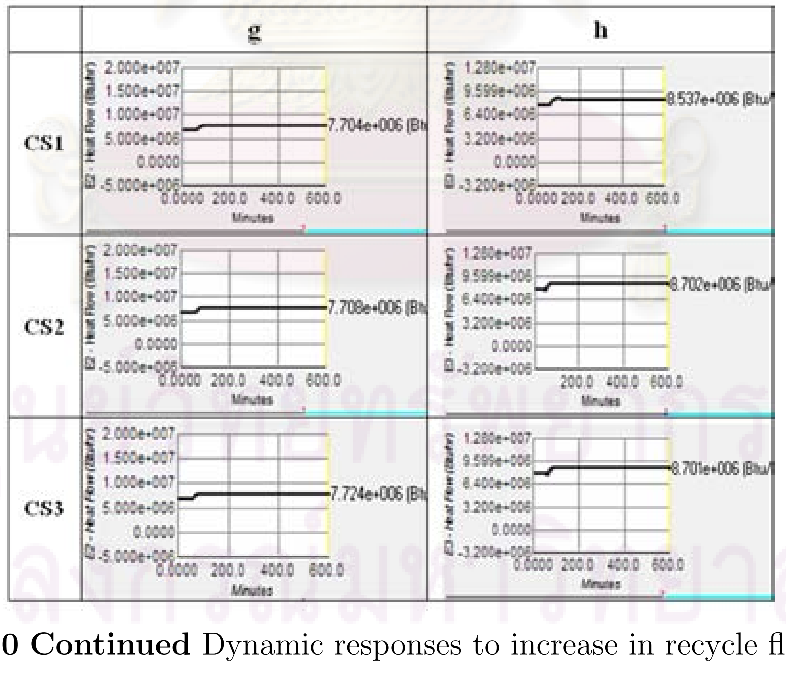


Figure 5.30 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of Base Case (reversible), where (g) furnace duty and (h) cooler duty

5.4.7 Change in the recycle flowrates for CS1 to CS3 in the new designed resilient heat exchanger network: RHEN-1, RHEN-2 and RHEN-3 for reversible reaction case

Figures 5.31-5.33 show dynamic responses of RHEN1-3 when the recycle flowrate is changed from 872.5 to 942.5 lb-mol/hr occurring at time equals 60 minutes. The results of CS1-3 with network structure RHEN-1, for CS1 show the product increases from 521 to 530 lb-mol/hr, for CS2 show the product increases from 521 to 550.4 lb-mol/hr, for CS3 show the product increases from 521 to 550.6 lb-mol/hr. The energy consumption of Purge column reboiler, funace and cooler increases as the recycle flowrate increases.

The results of CS1-3 with network structure RHEN-2, for CS1 show the product increases from 521 to 529.2 lb-mol/hr, for CS2 show the product increases from 521 to 555.5 lb-mol/hr, for CS3 show the product increases from 521 to 556 lb-mol/hr. The energy consumption of Purge column reboiler and cooler increases as the recycle flowrate increases.

The results of CS1-3 with network structure RHEN-3, for CS1 show the product increases from 521 to 529.3 lb-mol/hr, for CS2 show the product increases from 521 to 557.5 lb-mol/hr, for CS3 show the product increases from 521 to 558.2 lb-mol/hr. The energy consumption of funace and cooler increases as the recycle flowrate increases.

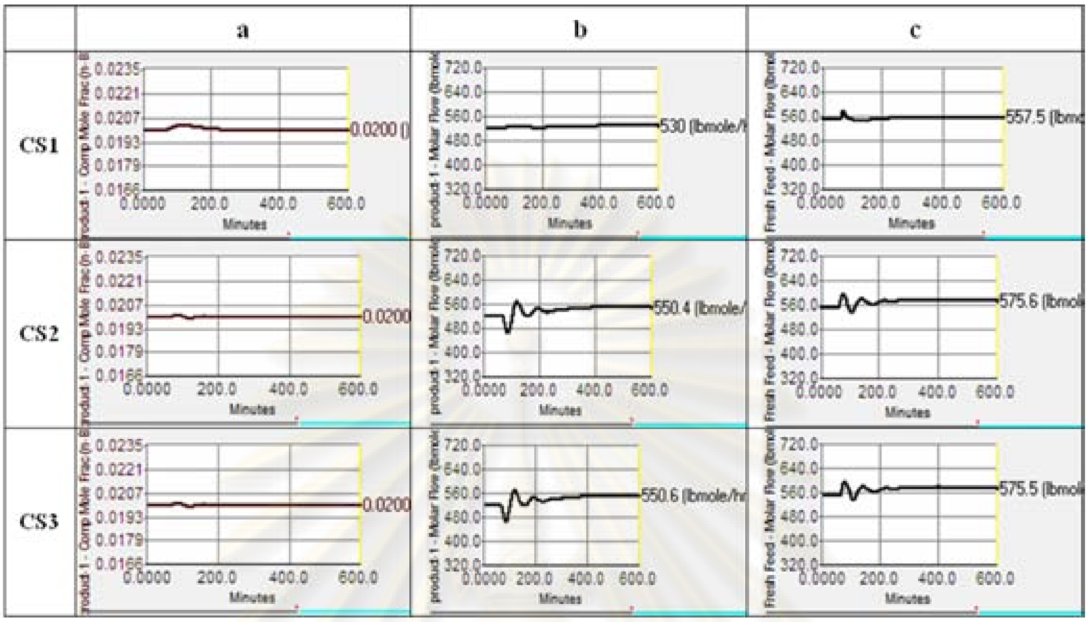


Figure 5.31 Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-1 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

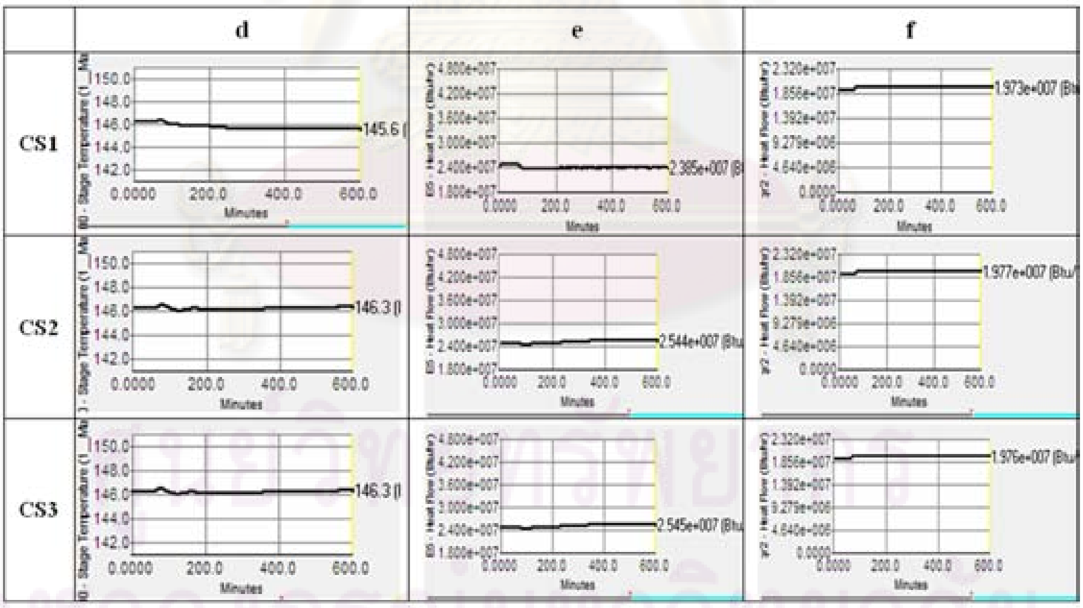


Figure 5.31 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-1 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

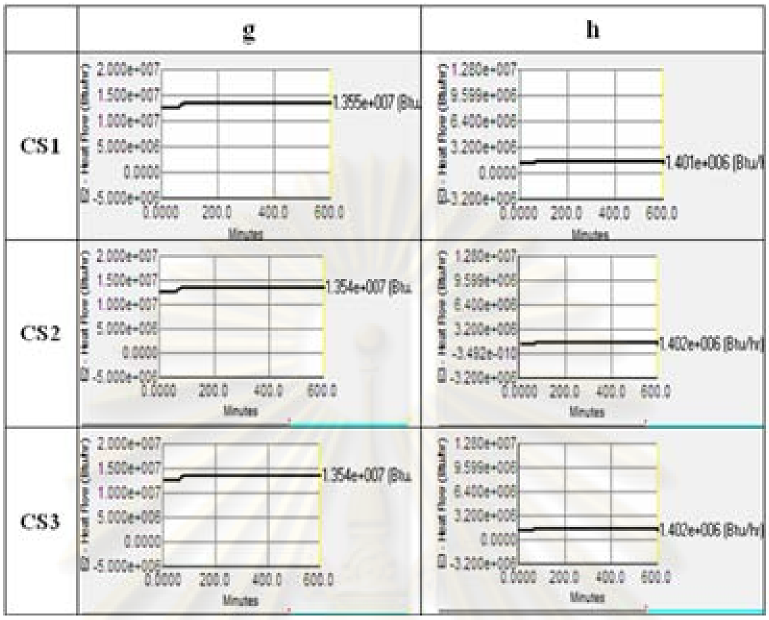


Figure 5.31 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-1 (reversible), where (g) furnace duty and (h) cooler duty

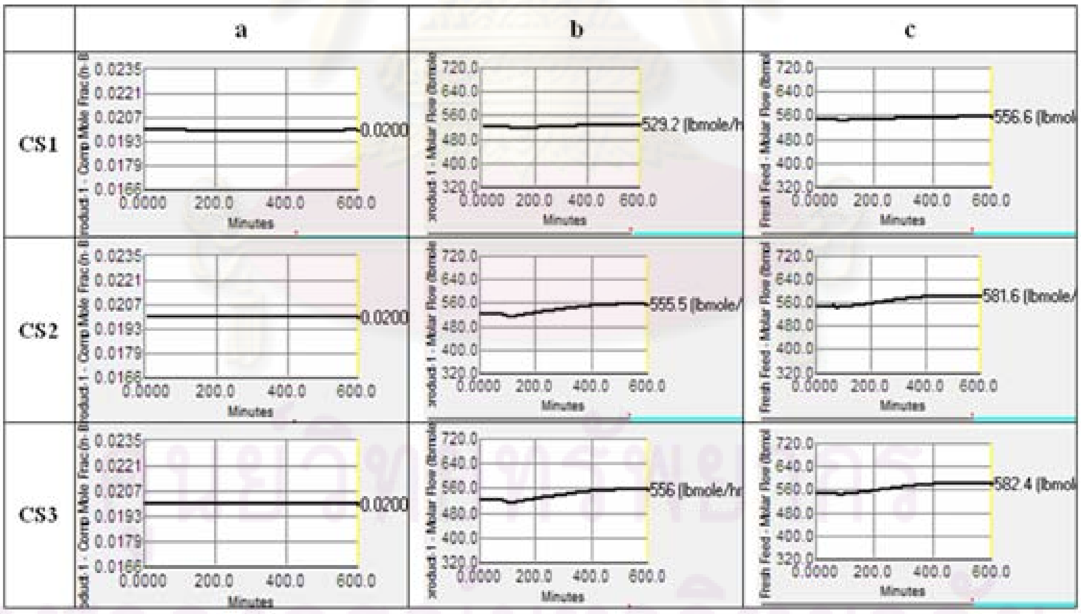


Figure 5.32 Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-2 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

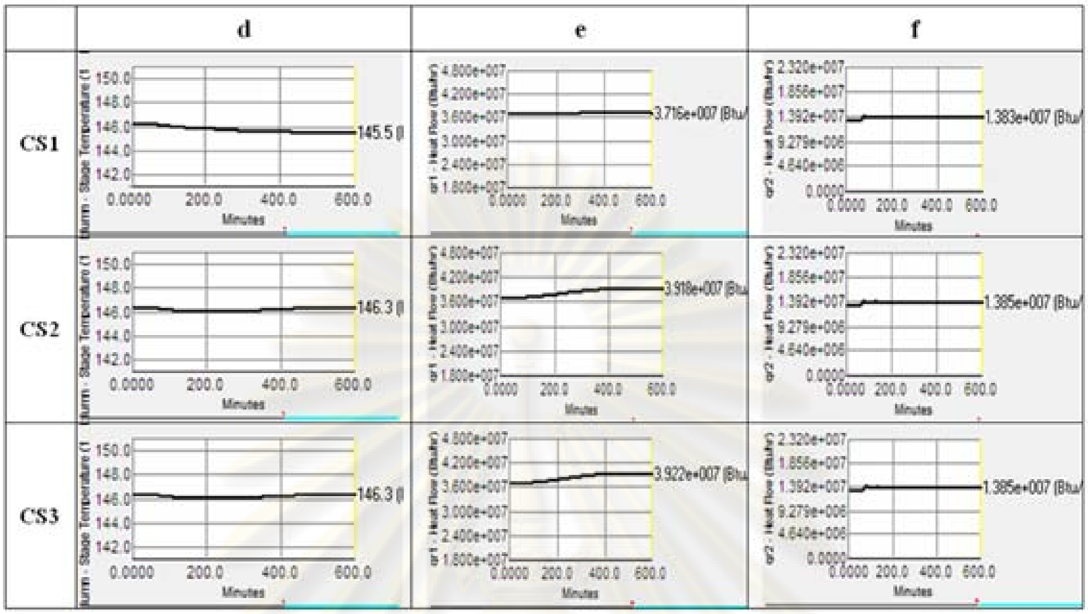


Figure 5.32 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-2 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

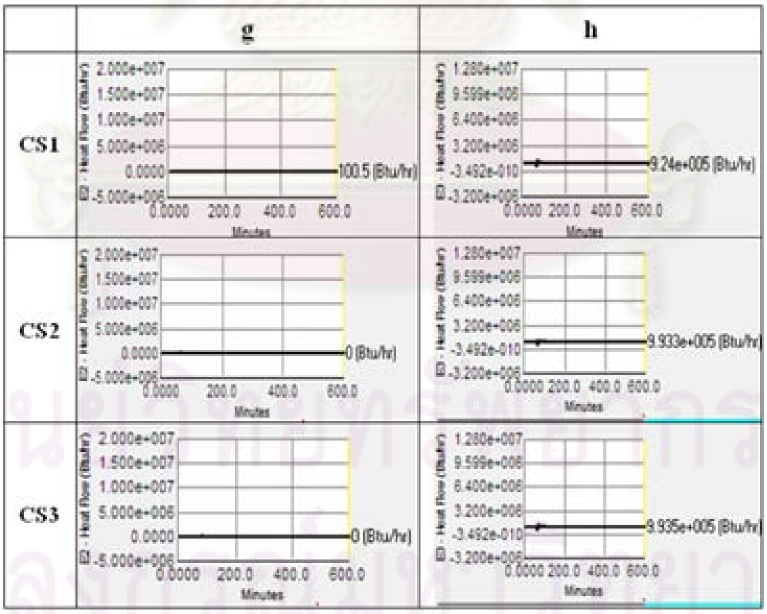


Figure 5.32 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-2 (reversible), where (g) furnace duty and (h) cooler duty

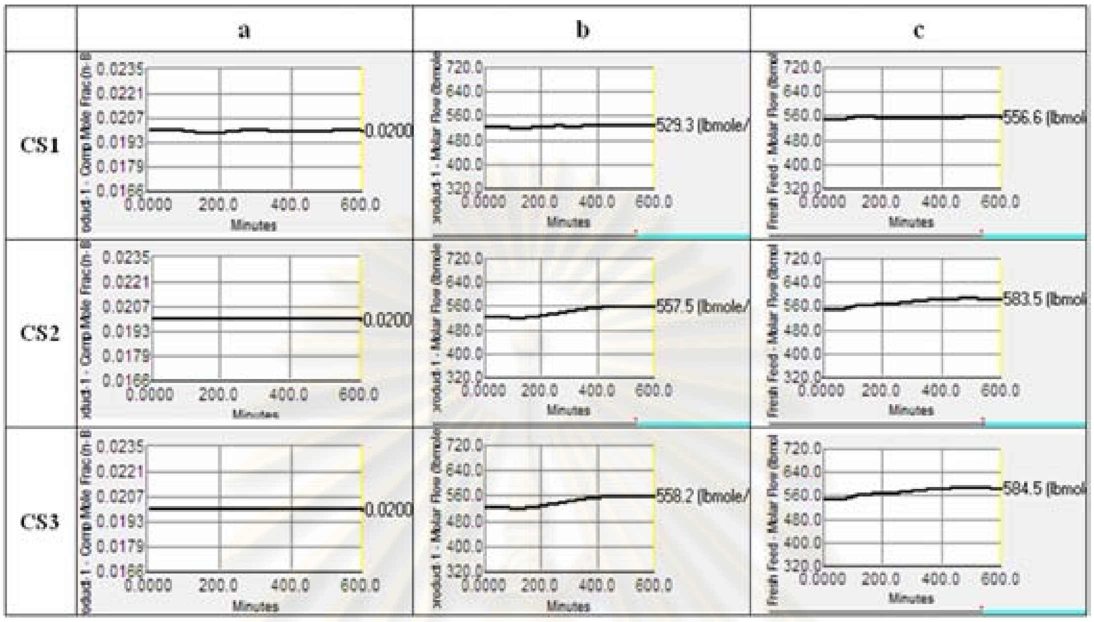


Figure 5.33 Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-3 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

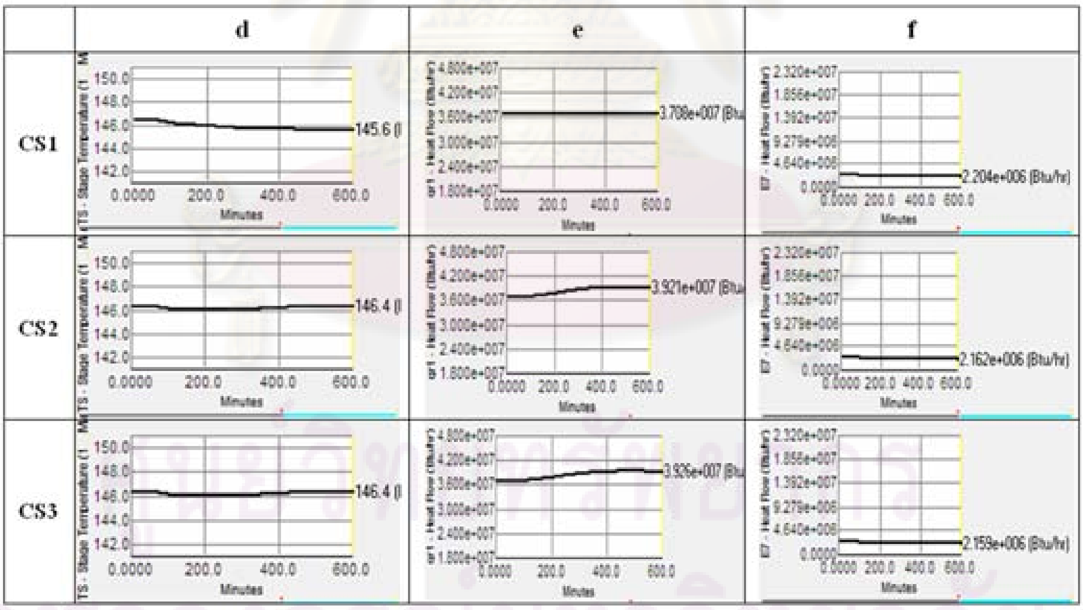


Figure 5.33 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-3 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

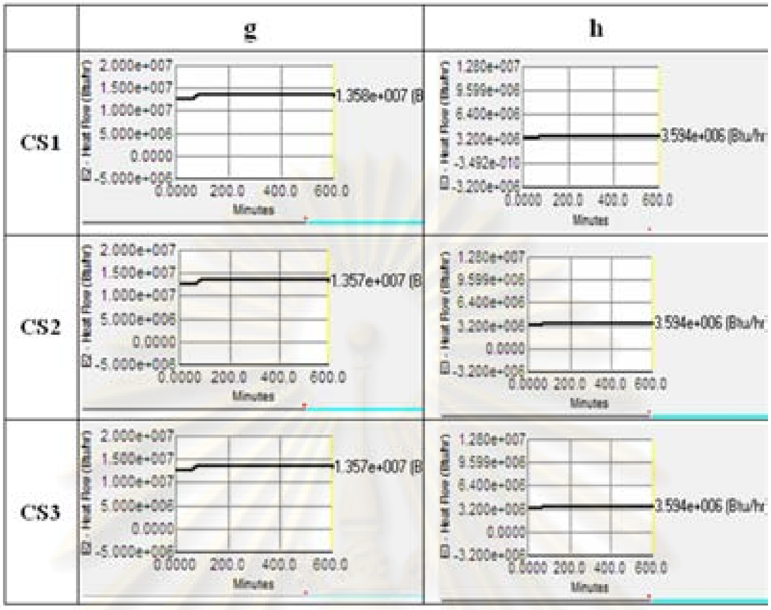


Figure 5.33 Continued Dynamic responses to increase in recycle flows from 872.5 to 942.5 lb-mol/hr of RHEN-3 (reversible), where (g) furnace duty and (h) cooler duty

5.4.8 Comparison of control structures for change in the recycle flowrates: CS1, CS2 and CS3 with RHEN-1, RHEN-2 and RHEN-3 for reversible reaction case

Figure 5.31-5.33 show the effect of increasing the recycle flowrate from 872.5 to 942.5 lb-mol/h at time equals 60 minutes of RHEN1-3 with CS1-3. As discussed before the effect is a slight increase in production rate with CS1. For CS3 with base temperature controlled give the similar increase in product rate as CS2. The base temperature control holds the impurity of the bottoms, thus there is an increase iC_4 in the distillate. Control structures of CS2 and CS3, their responses give the same results.

It is interesting that CS2 and CS3 control better than CS1. It means that the temperature column control is necessary for structure with heat integration at column to reduce complication from disturbed stream. The integral absolute errors of important control loops are shown in Table 5.5 and Figure 5.34.

Table 5.5 The IAE results of the control systems to increase in recycle flowrates from 872.5 to 942.5 lb-mol/h.

		Integral Absolute Error			
		BC	RHEN-1	RHEN-2	RHEN-3
CCDt	CS1	1.860026	1.970411	2.309931	2.337332
	CS2	0.250683	0.812172	0.31601	0.287388
	CS3	0.252103	0.815446	0.318964	0.291784
TCR	CS1	1.673473	1.045529	1.182963	1.050203
	CS2	1.647819	1.039288	1.204973	1.046194
	CS3	1.650665	1.039303	1.205783	1.046382
TCC	CS1	0.123166	0.065628	2.269661	0.074577
	CS2	0.131188	0.065493	2.254881	0.074713
	CS3	0.136838	0.065538	2.232147	0.074849
PCD	CS1	0.275358	0.493795	0.264398	0.305414
	CS2	1.582737	1.507395	1.576598	1.737883
	CS3	1.531768	1.513787	1.591401	1.762519
PCP	CS1	0.670061	0.449258	0.720289	3.001447
	CS2	0.70437	0.467214	0.728968	2.901828
	CS3	0.705665	0.467444	0.72874	2.911073
Total	CS1	4.602084	4.024621	6.747243	6.768974
	CS2	4.316797	3.891562	6.08143	6.048005
	CS3	4.27704	3.901516	6.077035	6.086607

Note CC = Composition Control, TC = Temperature Control, PC= Pressure Control, R = Reactor, D = DIB, P = Purge, C = Cooler, t = top, b = bottom

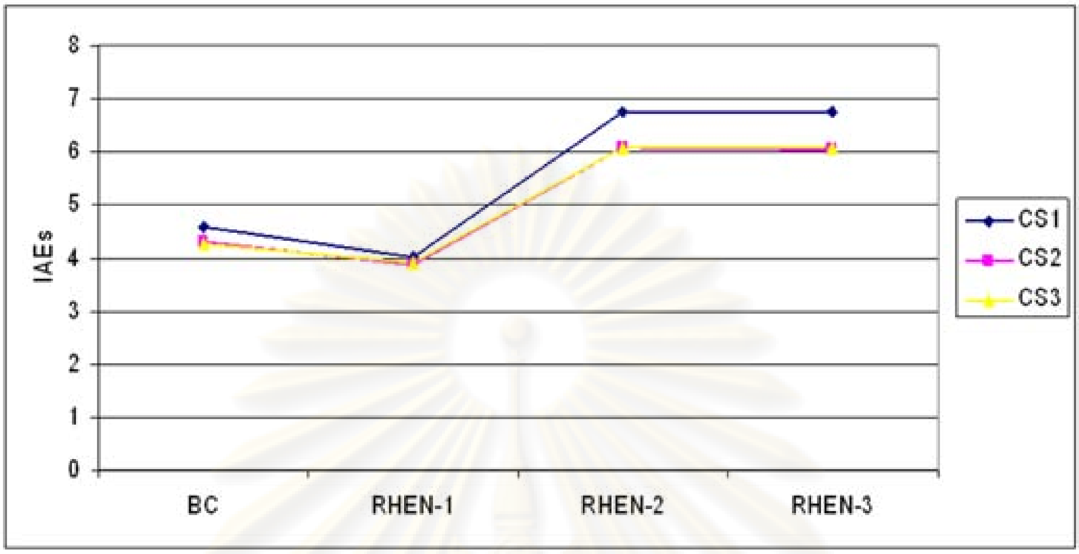


Figure 5.34 The IAE results of the control systems to increase in recycle flowrates from 872.5 to 942.5 lb-mol/h.

5.4.9 Change in the recycle flowrates for CS1 to CS3 in Butane Isomerization plant for Base Case (irreversible reaction case ; Luyben et al., 1998)

Figure 5.35 show the effect of increasing the recycle flowrate from 870.1 to 940.1 lb-mol/h at time equals 60 minutes of base case with CS1-3. In CS1, the effect (increase in recycle flowrates) is a slight decrease in production rate because of the reactor inlet composition to have a lower reactant (nC_4) concentration. The result is a slight drop in the overall reaction rate. In CS2 and CS3, the effect (increase in recycle flowrates) is increase in production flowrates.

The dynamic responses of control structure CS2 and CS3 are faster than CS1 because the reflux flow can control the reflux drum level more effective than the distillate flow.

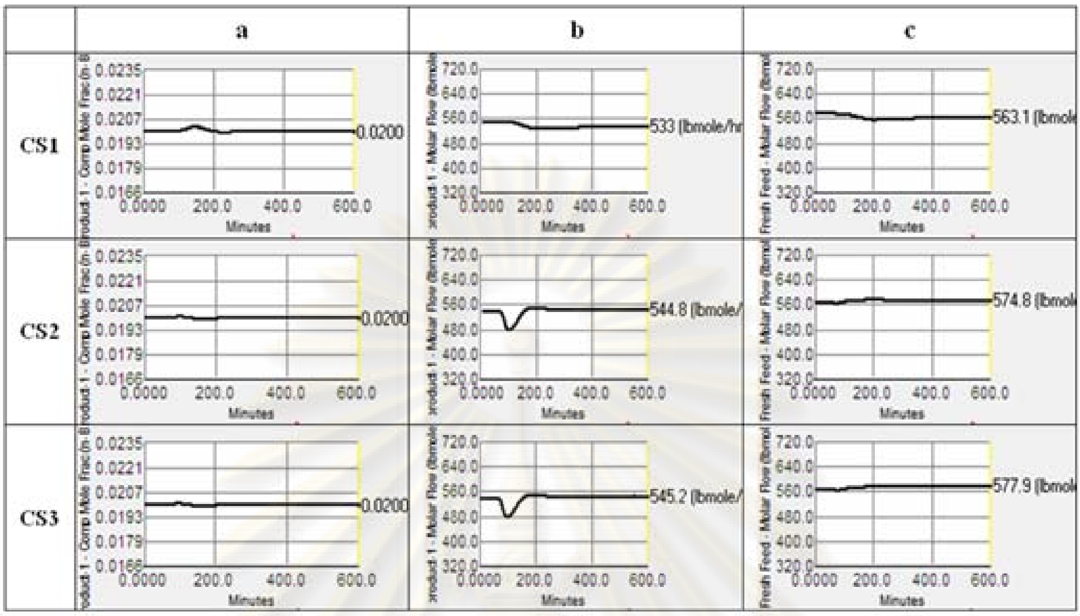


Figure 5.35 Dynamic responses to increase in recycle flows from 870.1 to 940.1 lb-mol/hr of Base case (irreversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

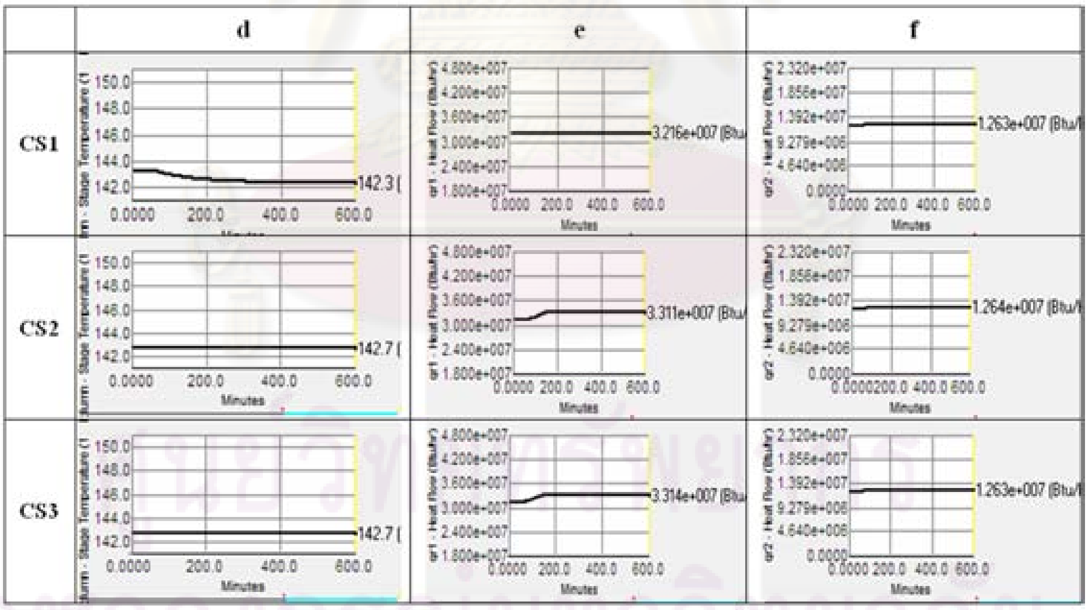


Figure 5.35 Continued Dynamic responses to increase in recycle flows from 870.1 to 940.1 lb-mol/hr of Base case (irreversible), where (d) tray 1 temperature of DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

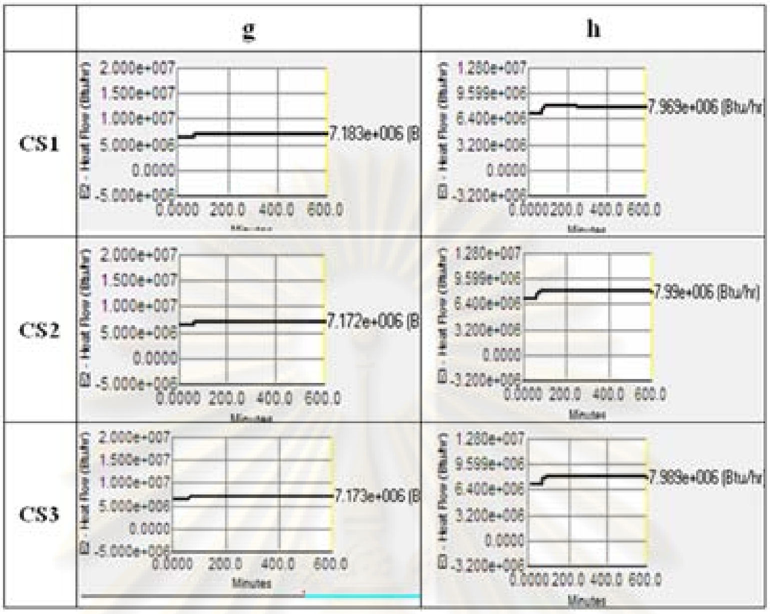


Figure 5.35 Continued Dynamic responses to increase in recycle flows from 870.1 to 940.1 lb-mol/hr of Base case (irreversible), where (g) furnace duty and (h) cooler duty

5.4.10 Comparison of Base case for change in the recycle flowrates: irreversible and reversible reaction case

Table 5.6 and Figure 5.36 show the IAE results of the control system when the recycle flowrate increase from 870.1 to 940.1 lb-mol/hr for irreversible and increase from 872.5 to 942.5 lb-mol/hr for reversible reaction case and compare the dynamic responses between irreversible and reversible reaction case.

As can be seen, for irreversible and reversible reaction case show the IAE results the control system are different value. Also the different process gives the response diferrence.

Table 5.6 The IAE results of the control systems to increase in recycle flowrates : irreversible and reversible reaction case

		Integral Absolute Error	
		BC irreversible	BC reversible
CCDt	CS1	1.683966	1.8600259
	CS2	0.746909	0.2506832
	CS3	0.746873	0.2521034
TCR	CS1	0.056467	1.6734731
	CS2	0.055475	1.6478189
	CS3	0.055483	1.6506654
TCC	CS1	2.555993	0.1231657
	CS2	2.437167	0.1311884
	CS3	2.438161	0.1368382
PCD	CS1	0.088102	0.2753576
	CS2	0.384244	1.5827366
	CS3	0.384602	1.5317682
PCP	CS1	0.183052	0.6700613
	CS2	0.180089	0.7043701
	CS3	0.180502	0.7056647
Total	CS1	4.567581	4.6020836
	CS2	3.803884	4.3167972
	CS3	3.805622	4.2770398

Note CC = Composition Control, TC = Temperature Control, PC= Pressure Control, R = Reactor, D = DIB, P = Purge, C = Cooler, t = top, b = bottom

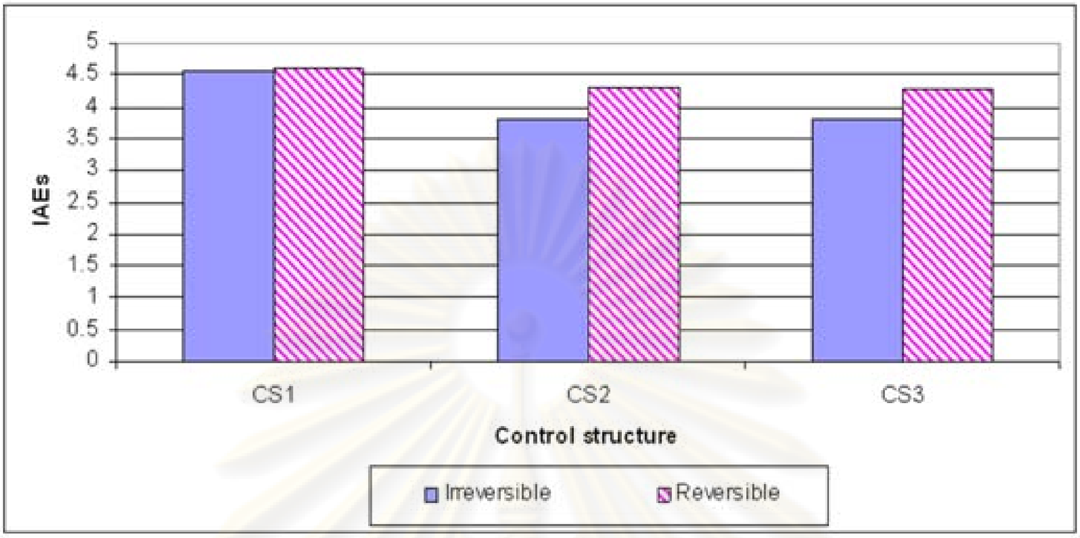


Figure 5.36 The IAE results of the control systems to increase in recycle flowrates : irreversible and reversible reaction case

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

This study considers the heat integrated process design altogether with plantwide control structure selection for reduction of energy consumption and maintaining good control performance. We look at 4 alternatives of various heat integrated processes (base case by Luyben's design and 3 new designs) and 4 plantwide control structures (1 Luyben's previous design, 1 Wilailak's design and 2 new design). Two kinds of disturbances are used: thermal disturbance and the material flow disturbance. The HEN design follows Wongsri's resilient HEN synthesis method (1990). The energy saved is 15.11-22.09% from the base case. The thermal load management of the resilient HEN, in and out, and to thermal sinks and sources uses Heat Pathway Heuristics (Wongsri and Hermawan, 2005). In general the HPH is very useful in terms of heat load or disturbance management to achieve the highest possible dynamic MER.

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

For the thermal disturbance, Control structure CS3 is the proper control structure with all alternatives because the DIB column reflux flow is manipulated to control reflux drum level, nC_4 composition is controlled by distillate valve and the base DIB column and the purge column temperature are controlled so they reject the thermal disturbance by keeping the base temperature constant.

For the material flow disturbance, we can conclude that the control structures CS2 and CS3 are better than other structures because the material disturbance entered is immediately directed out of the DIB column through distillate.

For all disturbances testing, the RHEN-1 show the IAE value less than other alternatives. Consequently, RHEN-1 is the proper heat exchanger network for all control structures.

We can conclude that we can avoid the control difficulties associated with the heat integration by choosing the suitable heat integrated structure and proper control structures.

6.2 Recommendations

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

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APPENDICES

APPENDIX A

Table A.1 Data of Butane Isomerization process (Base Case for reversible reaction case) for simulation

Name	Fresh feed	Product	Purge	Reactor inlet	Reactor outlet
Temperature [F]	90	124	178	390	422
Pressure [psia]	300	100	66	665	665
Molar Flow [lbmole/hr]	544	514	30	870	870
Mole Frac (C_3)	0.02	0.02	0	0	0
Mole Frac (iC_4)	0.24	0.96	0	0.17	0.59
Mole Frac (nC_4)	0.69	0.02	0.01	0.82	0.40
Mole Frac (iC_5)	0.05	0	0.99	0.01	0.01

Table A.2 Data of Butane Isomerization process (Base Case for irreversible reaction case) for simulation

Name	Fresh feed	Product	Purge	Reactor inlet	Reactor outlet
Temperature [F]	90	124	178	390	422
Pressure [psia]	300	100	66	665	650
Molar Flow [lbmole/hr]	580	550	30	870	870
Mole Frac (C_3)	0.02	0.02	0	0	0
Mole Frac (iC_4)	0.24	0.96	0	0.17	0.62
Mole Frac (nC_4)	0.69	0.02	0.01	0.81	0.36
Mole Frac (iC_5)	0.05	0	0.99	0.02	0.02

Table A.3 Equipment data

Butane isomerization process (Base Case for reversible reaction case)

Kinetics	A_f [1/h]	4x10^8
	E_f [Btu/lb-mol]	3x10^4
K_{EQ}=$e^{(A+B/T)}$	A	-10
	B[^oR]	5100
Flooded Condenser	Holdup[ft^3]	340
Reactor	ID [ft]	7
	Length [ft]	50
	Holdup[ft^3]	1925
FEHE	UA (Btu/F-hr)	3.57E+04
	Shell holdup [ft^3]	21
	Tube hold[ft^3]	21

Butane isomerization process (RHEN-1)

Kinetics	A_f [1/h]	4x10^8
	E_f [Btu/lb-mol]	3x10^4
K_{EQ}=$e^{(A+B/T)}$	A	-10
	B[^oR]	5100
Flooded Condenser	Holdup[ft^3]	340
Reactor	ID [ft]	7
	Length [ft]	50
	Holdup[ft^3]	1925
FEHE	UA (Btu/F-hr)	1.27E+05
	Shell holdup [ft^3]	21
	Tube hold[ft^3]	21

Butane isomerization process (RHEN-2)

Kinetics	A_f [1/h]	4x10^8
	E_f [Btu/lb-mol]	3x10^4
K_{EQ}=$e^{(A+B/T)}$	A	-10
	B[^oR]	5100
Flooded Condenser	Holdup[ft^3]	340
Reactor	ID [ft]	7
	Length [ft]	50
	Holdup[ft^3]	1925
FEHE	UA (Btu/F-hr)	8.81E+05
	Shell holdup [ft^3]	21
	Tube hold[ft^3]	21

Butane isomerization process (RHEN-3)

Kinetics	A_f [1/h]	4x10^8
	E_f [Btu/lb-mol]	3x10^4
K_{EQ}=$e^{(A+B/T)}$	A	-10
	B[^oR]	5100
Flooded Condenser	Holdup[ft^3]	340
Reactor	ID [ft]	7
	Length [ft]	50
	Holdup[ft^3]	1925
FEHE	UA (Btu/F-hr)	1.58E+05
	Shell holdup [ft^3]	21
	Tube hold[ft^3]	21

Butane isomerization process (Base Case for irreversible reaction case)

Kinetics	A_f [1/h]	$4x10^8$
	E_f [Btu/lb-mol]	$3x10^4$
Flooded Condenser	Holdup[ft^3]	340
Reactor	ID [ft]	7
	Length [ft]	18
	Holdup[ft^3]	693
FEHE	UA (Btu/F-hr)	3.96E+04
	Shell holdup [ft^3]	21
	Tube hold[ft^3]	21

Table A.4 Column specifications for reversible reaction case

Column specifications	DIB column	Purge column
Total trays	50	20
Feed tray	20/30	11
Diameter (ft)	16	6
Reflux drum holdup(ft^3)	1700	370
Base holdup (ft^3)	2000	400
Reflux ratio	7.80	0.80

Table A.5 Column specifications for irreversible reaction case

Column specifications	DIB column	Purge column
Total trays	50	20
Feed tray	20/30	11
Diameter (ft)	16	6
Reflux drum holdup(ft^3)	1700	370
Base holdup (ft^3)	2000	400
Reflux ratio	7.30	0.80

APPENDIX B

PARAMETER TUNING OF CONTROL STRUCTURES

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

Flow Controllers

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

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

Level Controllers

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

Pressure Controllers

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

Temperature Controllers

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

B.2 Relay-Feedback Testing

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

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

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

$$\mathrm{K}_u = \frac{4h}{a\pi}$$

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

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

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

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

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

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

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

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

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

$$\tau_I=2.2P_u$$

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

Table B.1: Parameter tuning of Butane Isomerization process for reversible reaction case

Controller	Controlled variable	Manipulated variable		Control action	Set point		K$_C$	τ_I(min)	τ_d(min)
XC	product composition	CS1	DIB reboiler duty (qr1)	Reverse	0.02	-	0.502	103	7.4
	DIB column top stage composition	CS2,CS3	DIB product valve (V2)	Reverse	0.2596	-	30	25	0.1
TCR	reactor inlet temperature	furnace duty (E2)		Reverse	390.0	^oF	0.2	2.57	0.232
TC-COOL	cooler outlet temperature	cooler duty (E3)		Direct	125	^oF	10.7	0.303	0.245
LC12	DIB column base level	PFD feed valve (V1)		Reverse	50.00	%	2	-	-
LC11	DIB column reflux drum level	CS1	DIB product valve (V2)	Direct	50.00	%	2	-	-
		CS2,CS3	DIB column reflux valve (reflux)						
LC21	Purge column reflux drum level	Purge reboiler duty (qr2)		Reverse	50.00	%	2	-	-
LC22	Purge column base level	Purge feed valve (V3)		Reverse	50.00	%	2	-	-
PC1	DIB column pressure	DIB condenser duty (qc1)		Direct	100.0	psia	2	10	-
PC2	Purge column pressure	Purge condenser duty (qc2)		Direct	65.0	psia	2	10	-
PC3	FEHE1 hot stream outlet pressure	Recycle3 feed valve (V6)		Direct	620.0	psia	2	10	-
TC1	DIB column stage1 temperature	CS2, CS3	DIB reboiler duty (qr1)	Reverse	146.3	^oF	0.1	1	4.63
TC2	Purge column average temperature	CS3	Purge feed valve (V4)	Direct	173.5	^oF	0.1	2.57	-

Table B.2: Parameter tuning of Butane Isomerization process for irreversible reaction case

Controller	Controlled variable	Manipulated variable		Control action	Set point		K_C	τ_I(min)	τ_d(min)
XC	product composition	CS1	DIB reboiler duty (qr1)	Reverse	0.02	-	1	60	-
	DIB column top stage composition	CS2,CS3	DIB product valve (V2)	Reverse	0.2596	-	23	25	0.1
TCR	reactor inlet temperature	furnace duty (E2)		Reverse	390.1	^oF	0.5	0.215	0.049
TC-COOL	cooler outlet temperature	cooler duty (E3)		Direct	125	^oF	1	0.784	0.174
LC12	DIB column base level	PFD feed valve (V1)		Reverse	50.00	%	2	-	-
LC11	DIB column reflux drum level	CS1	DIB product valve (V2)	Direct	50.00	%	2	-	-
		CS2,CS3	DIB column reflux valve (reflux)						
LC21	Purge column reflux drum level	Purge reboiler duty (qr2)		Reverse	50.00	%	2	-	-
LC22	Purge column base level	Purge feed valve (V3)		Reverse	50.00	%	2	-	-
PC1	DIB column pressure	DIB condenser duty (qc1)		Direct	100.0	psia	2	2	-
PC2	Purge column pressure	Purge condenser duty (qc2)		Direct	65.0	psia	2	2	-
PC3	FEHE1 hot stream outlet pressure	Recycle3 feed valve (V6)		Direct	620.0	psia	1	2	-
TC1	DIB column stage1 temperature	CS2, CS3	DIB reboiler duty (qr1)	Reverse	142.7	^oF	14.5	0.88	0.196
TC2	Purge column average temperature	CS3	Purge feed valve (V4)	Direct	143.3	^oF	0.1	10	-

APPENDIX C

DYNAMIC RESPONSES

The dynamic responses and table of the IAE results of the control structures in the Butane Isomerization plant for Base Case and RHEN1-3 when changes in the reactor inlet and the recycle flowrates by decreasing are shown in this section.

These disturbances are made as follow:

- Step change of -10 ^oF decreasing at time 60 minute are made in the reactor inlet stream temperature.
- Step change of decreasing the recycle flowrates before entering the DIB column from 872.5 to 802.5 lb-mol/hr for reversible reaction case and 870.1 to 800.1 lb-mol/hr for irreversible reaction case

The disturbance testing is used to compare the dynamic response of heat integration processes (Base case, RHEN1-3) with control structures (CS1-3) because the responses of RHEN1-3 trend to similar Base case.

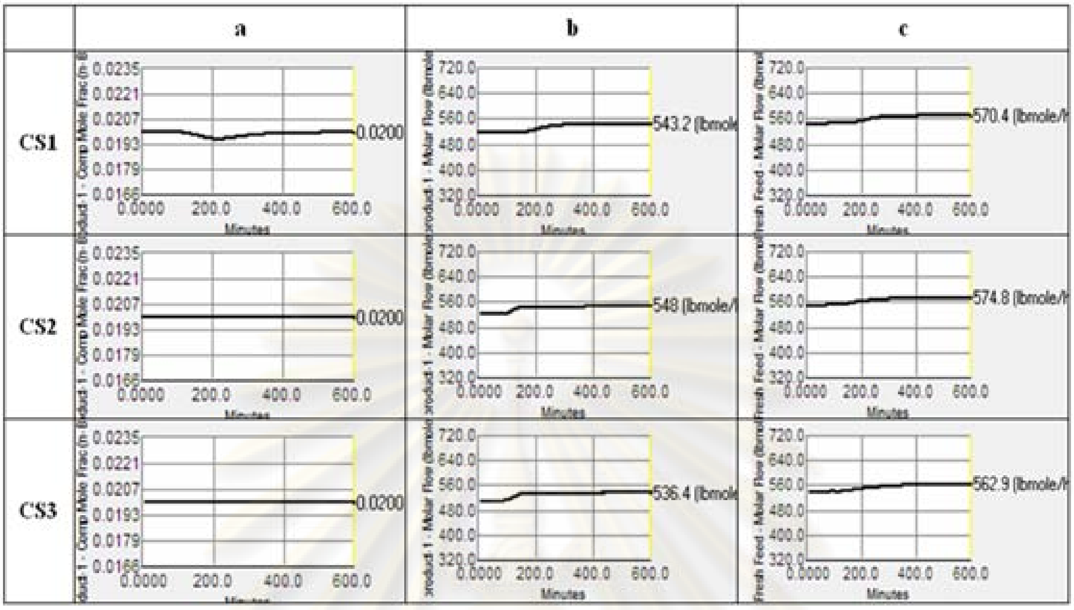

Figure C.1 Dynamic responses to 10 ^{o}F decrease in reactor inlet temperature of Base case (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

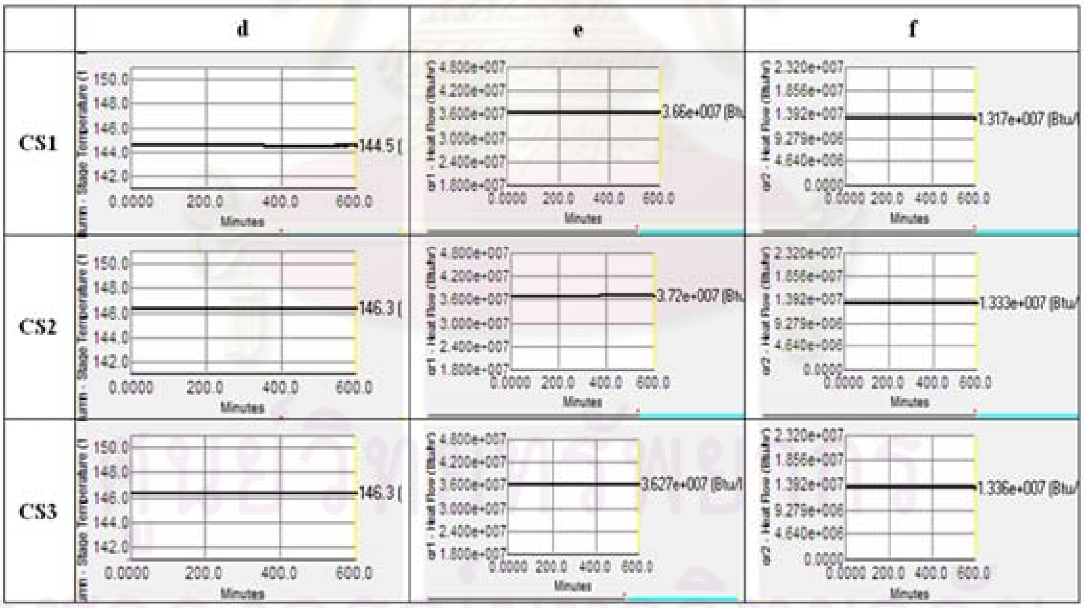

Figure C.1 Continued Dynamic responses to 10 ^{o}F decrease in reactor inlet temperature of Base Case (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

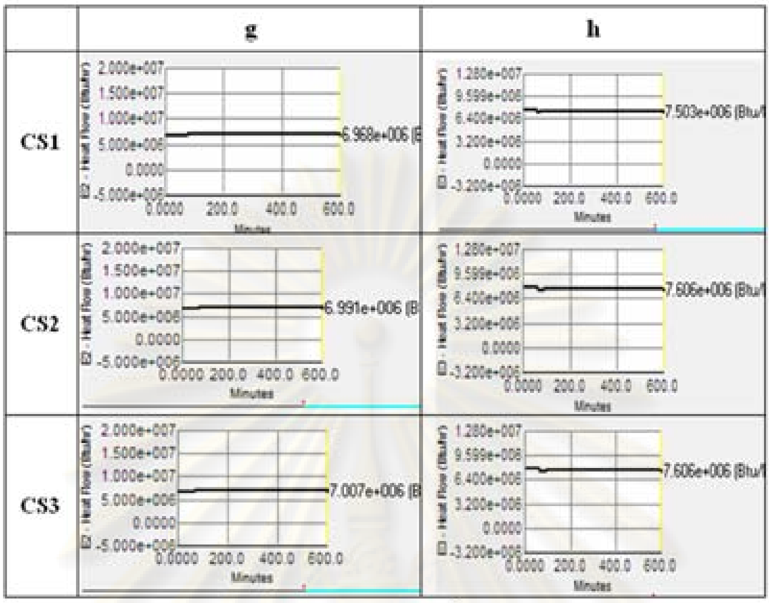

Figure C.1 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of Base Case (reversible), where (g) furnace duty and (h) cooler duty

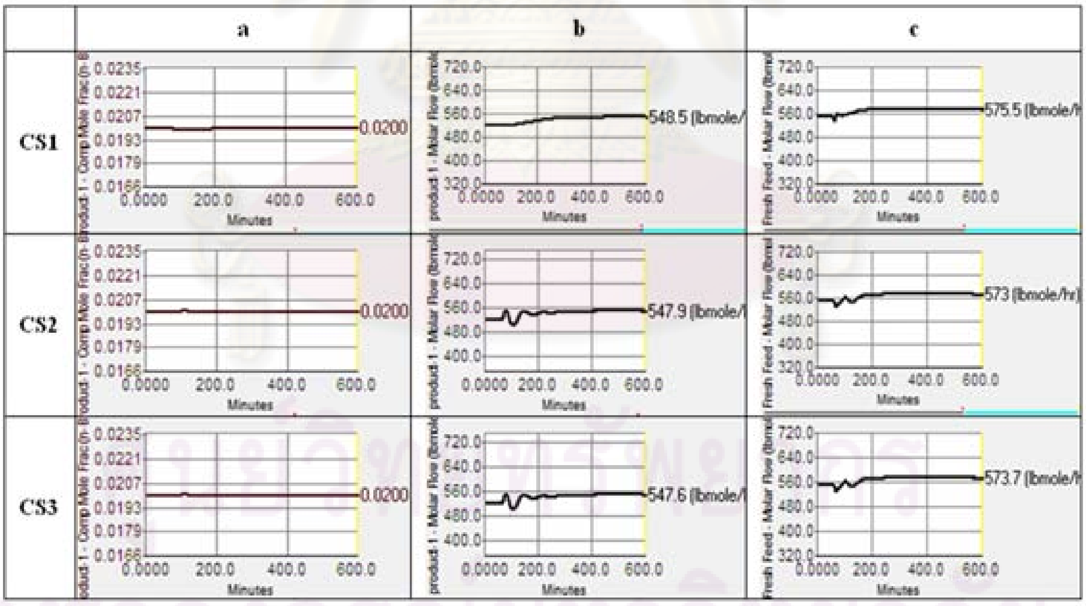

Figure C.2 Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-1 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

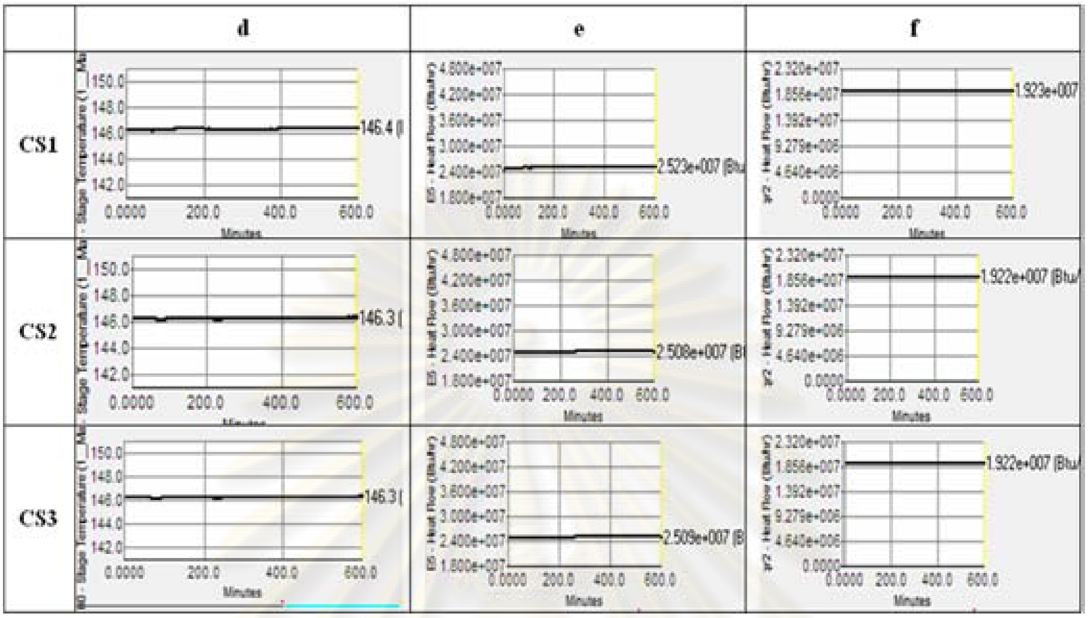

Figure C.2 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-1 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

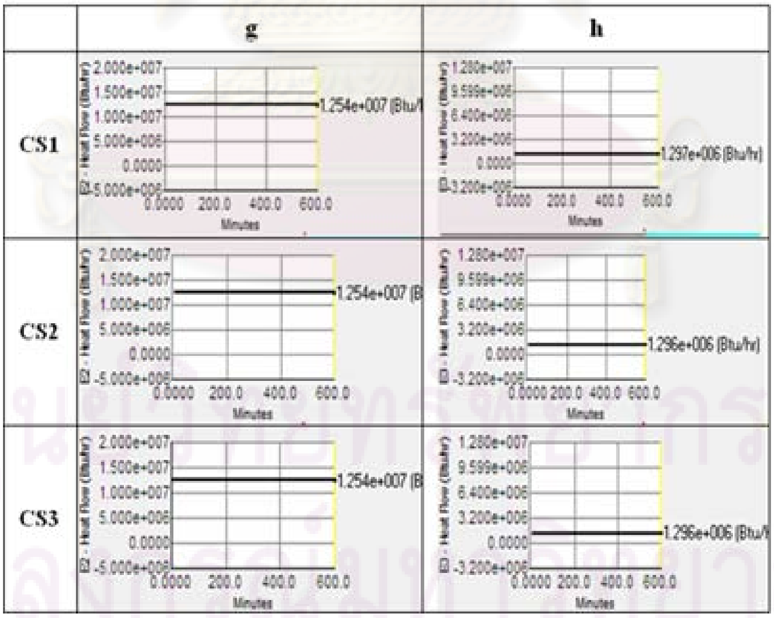

Figure C.2 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-1 (reversible), where (g) furnace duty and (h) cooler duty

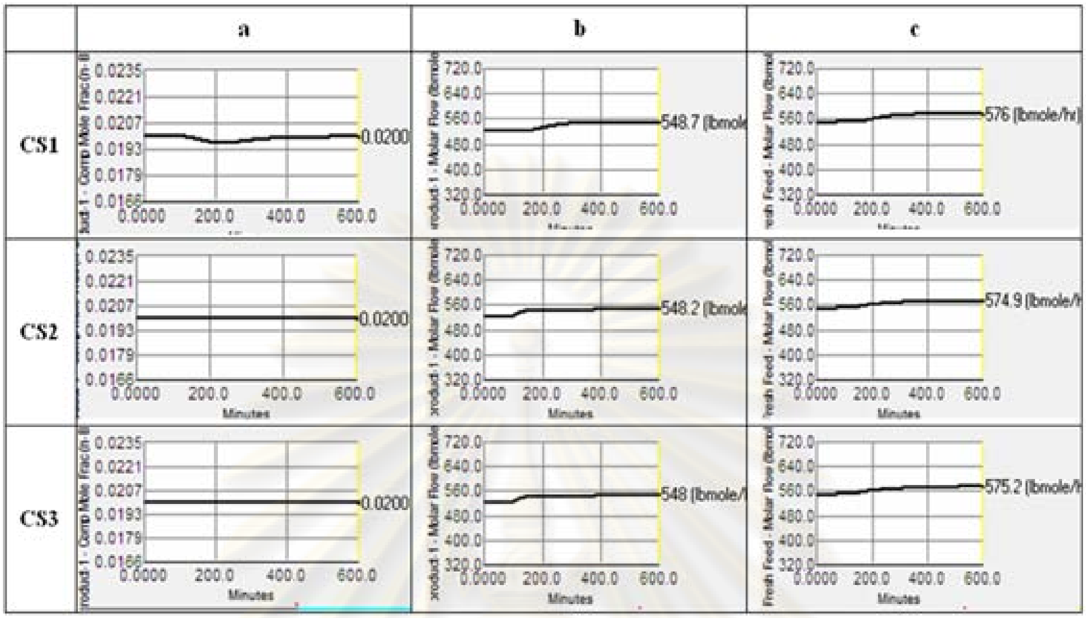

Figure C.3 Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-2 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

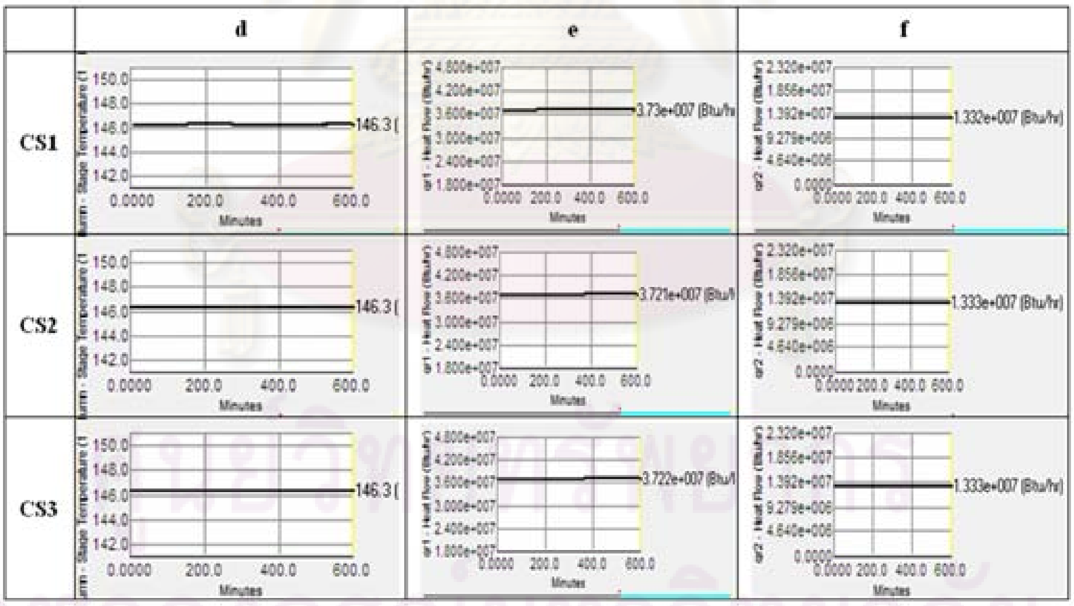

Figure C.3 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-2 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

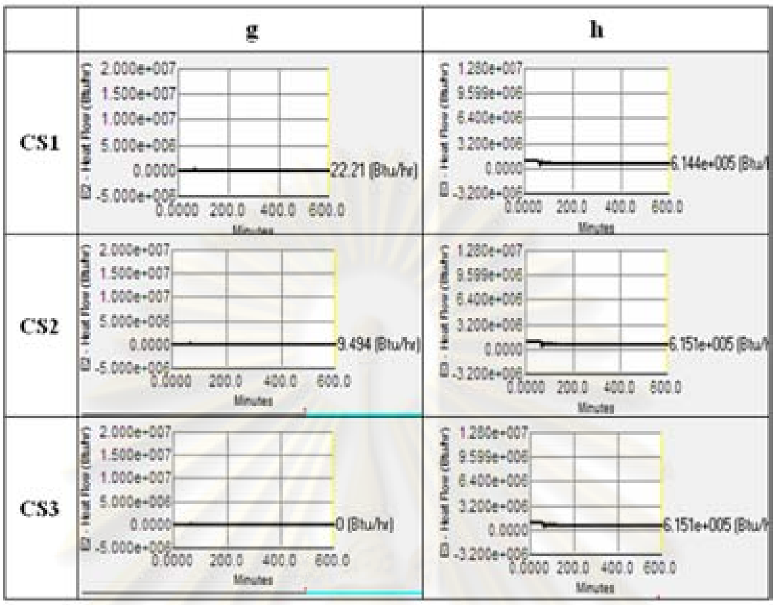

Figure C.3 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-2 (reversible), where (g) furnace duty and (h) cooler duty

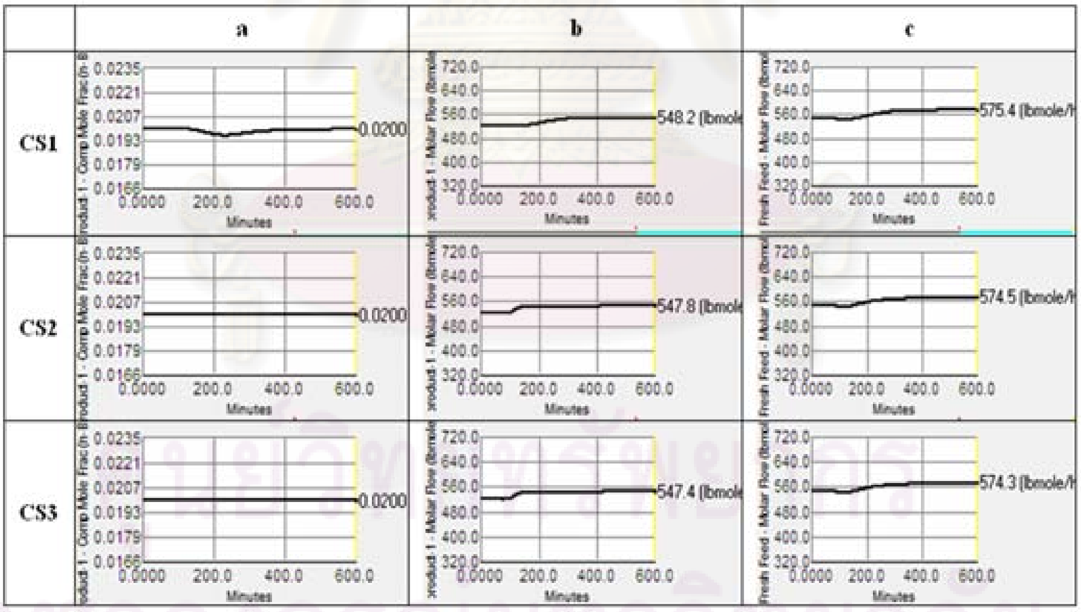

Figure C.4 Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-3 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

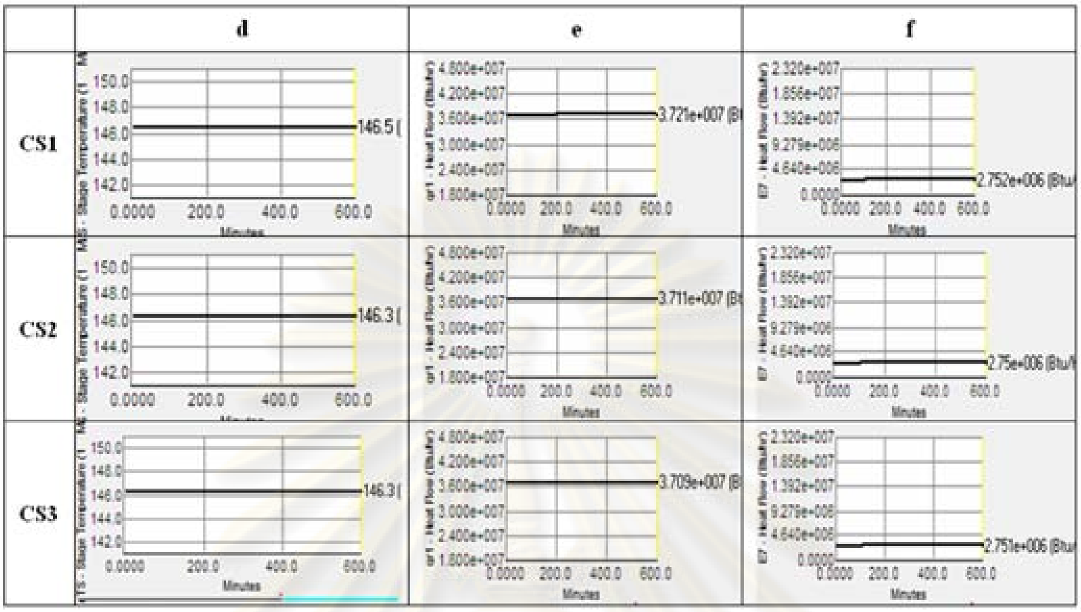

Figure C.4 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-3 (reversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty

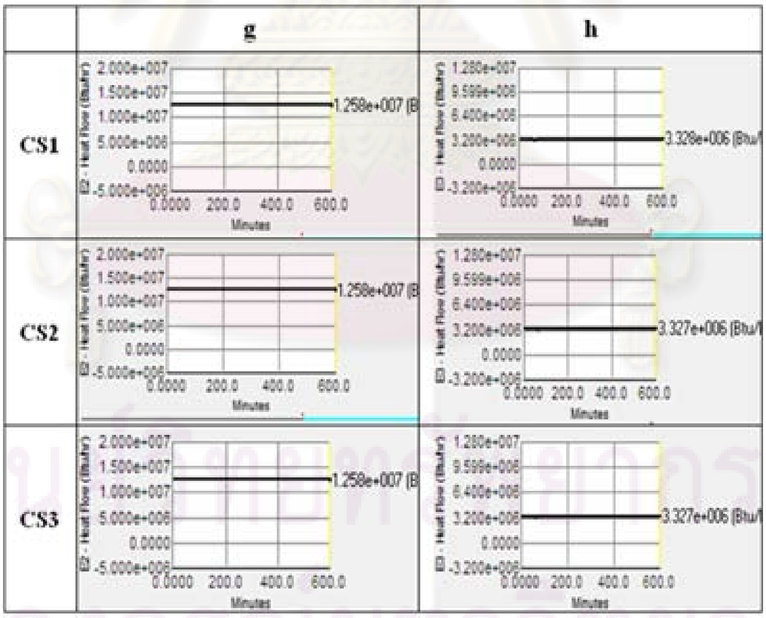

Figure C.4 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of RHEN-3 (reversible), where (g) furnace duty and (h) cooler duty

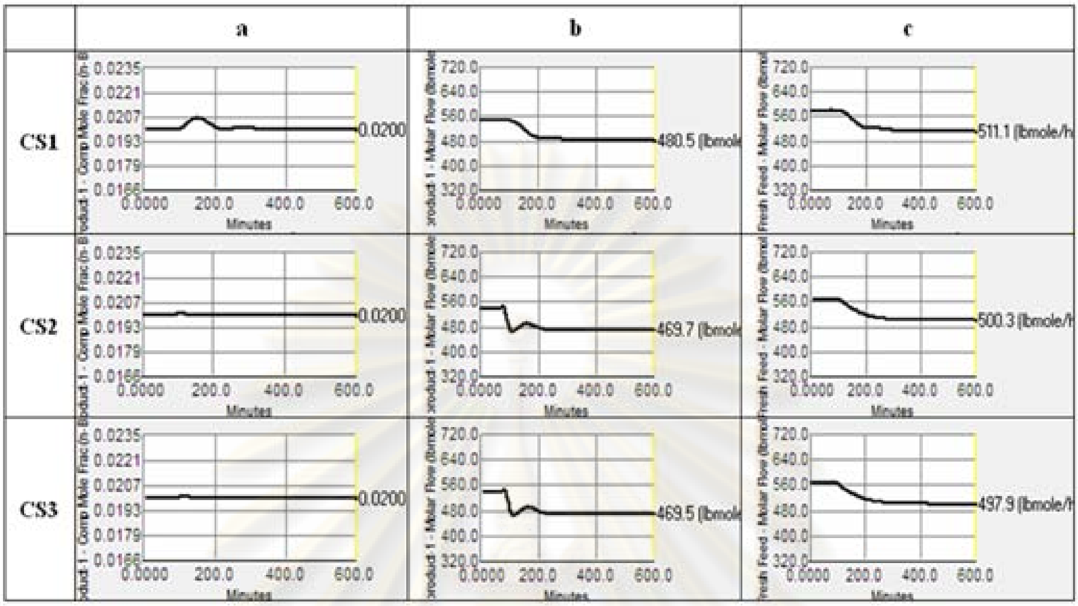

Figure C.5 Dynamic responses to 10 ^oF decrease in reactor inlet temperature of Base case (irreversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

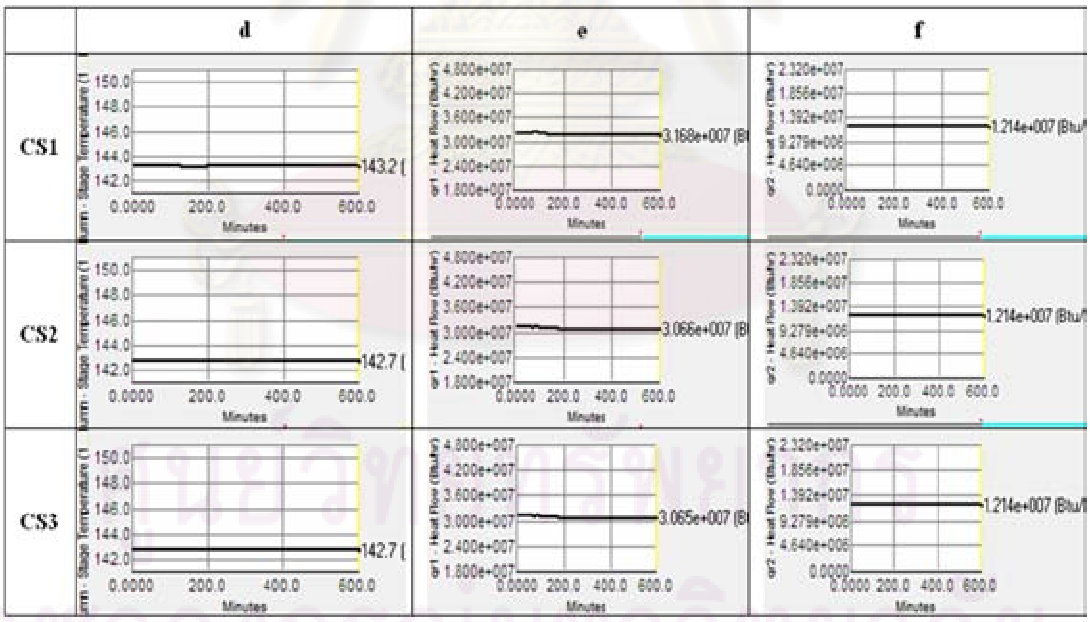

Figure C.5 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of Base Case (irreversible), where (d) tray 1 temperature of DIB column (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

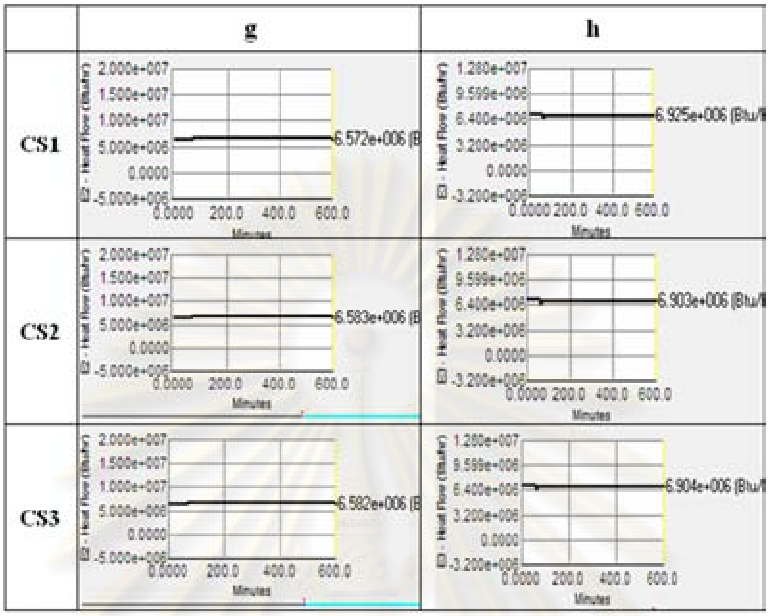

Figure C.5 Continued Dynamic responses to 10 ^oF decrease in reactor inlet temperature of Base Case (irreversible), where (g) furnace duty and (h) cooler duty

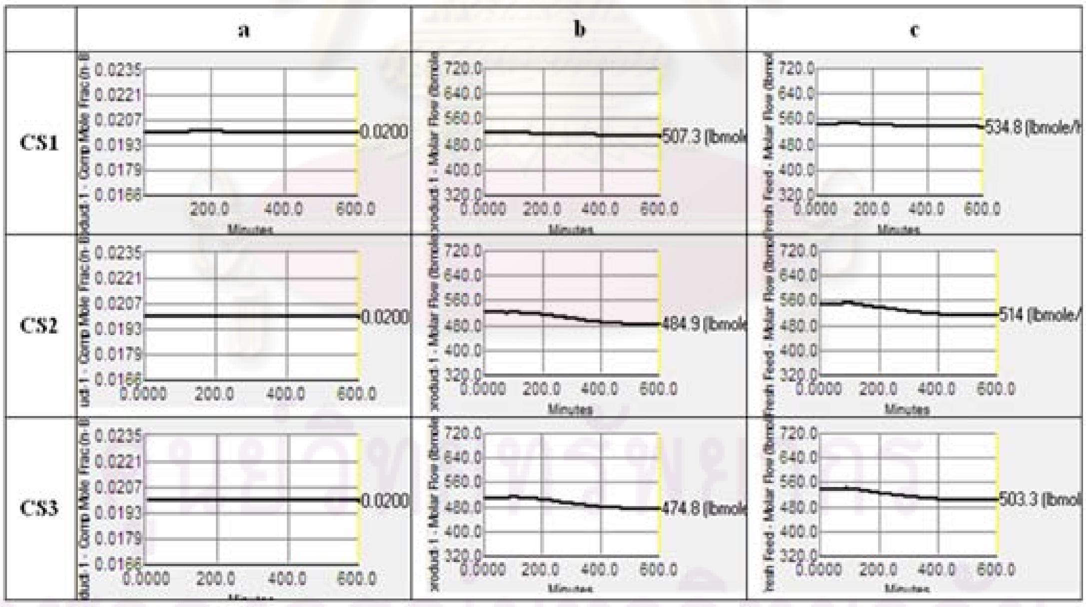

Figure C.6 Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of Base Case (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

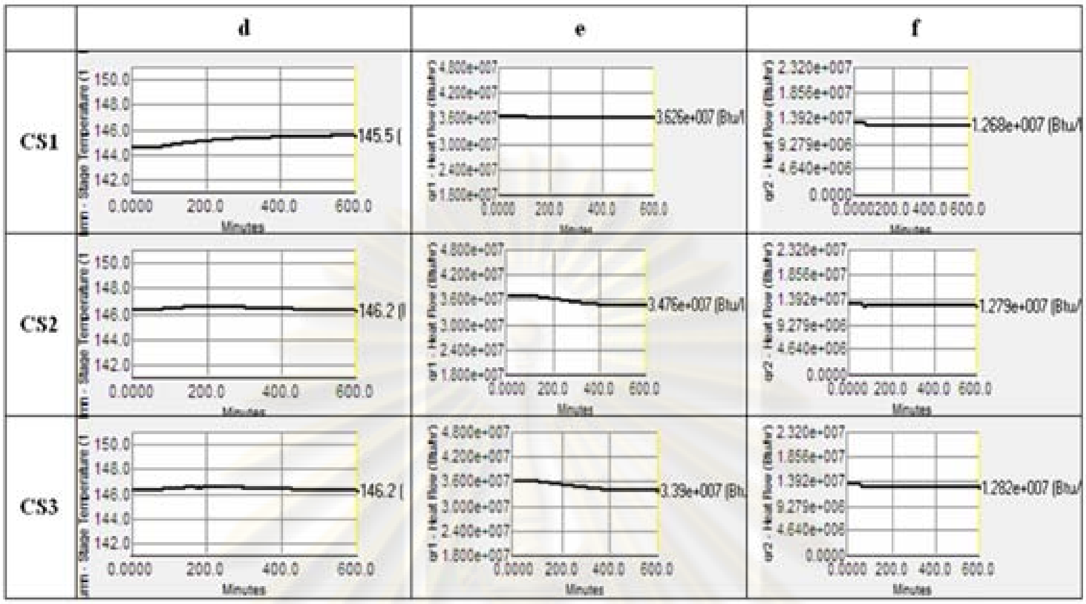

Figure C.6 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of Base Case (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

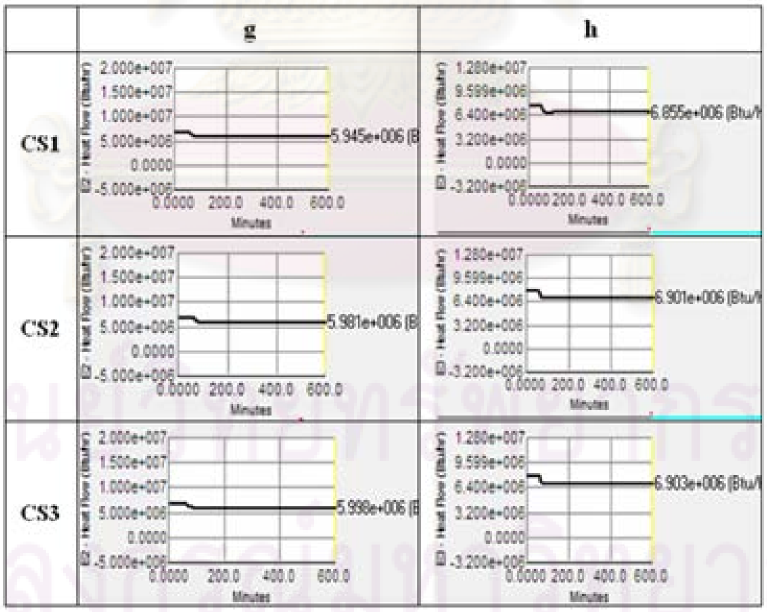

Figure C.6 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of Base Case (reversible), where (g) furnace duty and (h) cooler duty

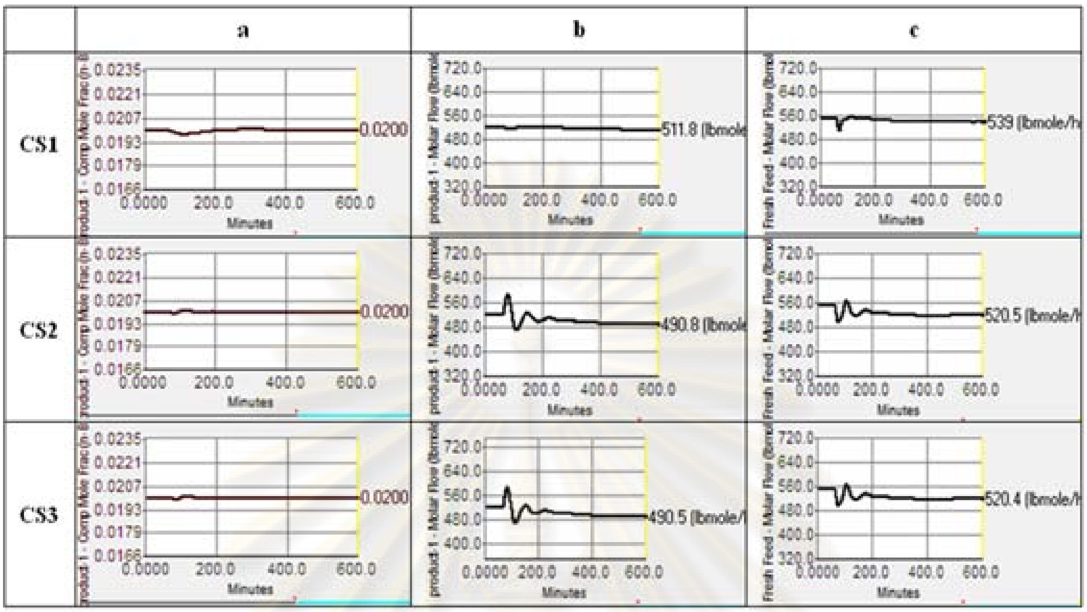

Figure C.7 Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-1 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

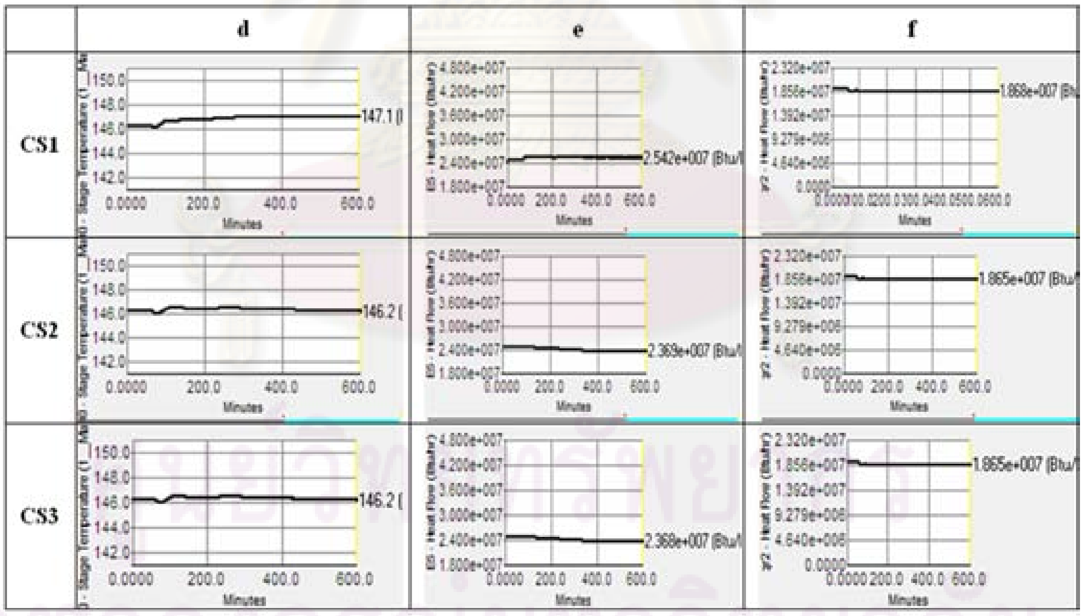

Figure C.7 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-1 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

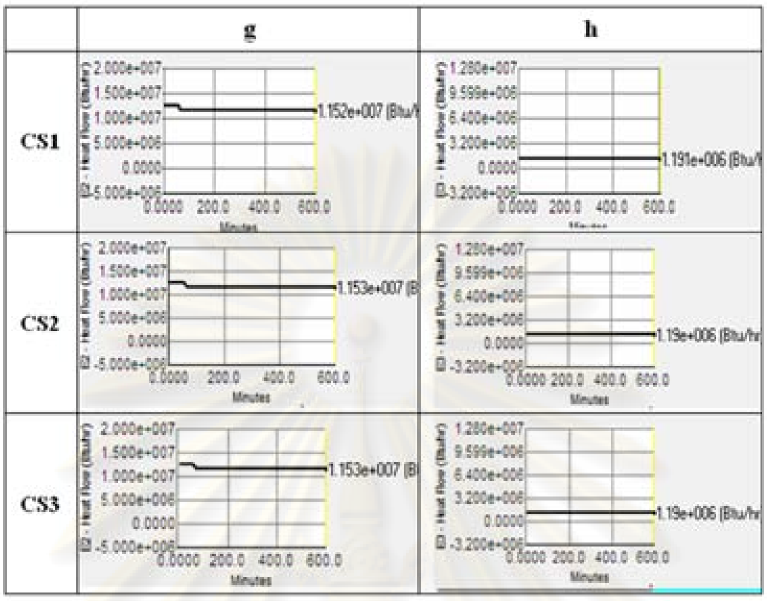

Figure C.7 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-1 (reversible), where (g) furnace duty and (h) cooler duty

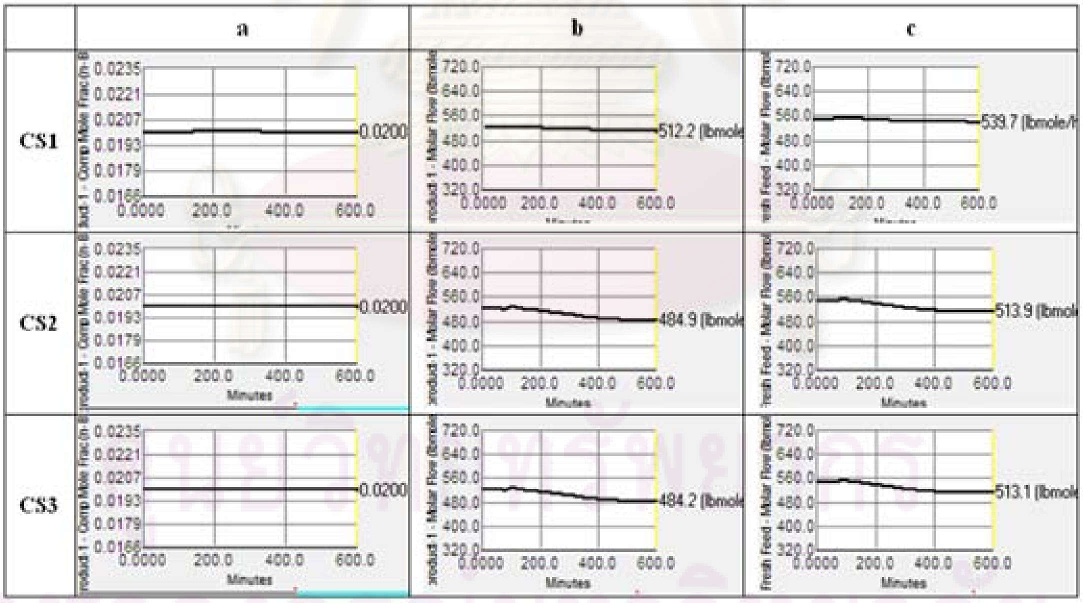

Figure C.8 Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-2 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

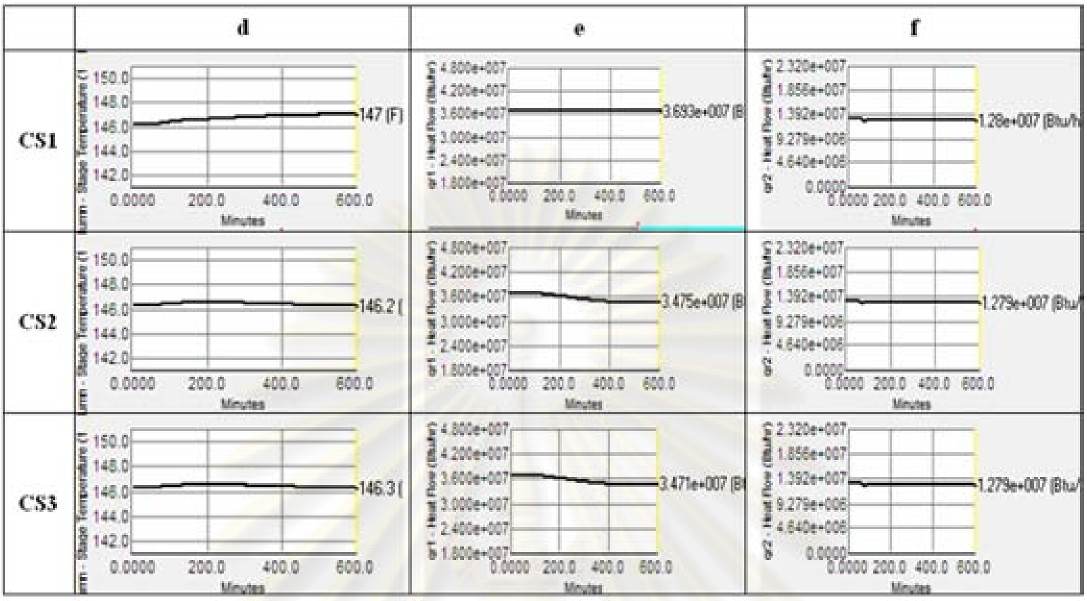

Figure C.8 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-2 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

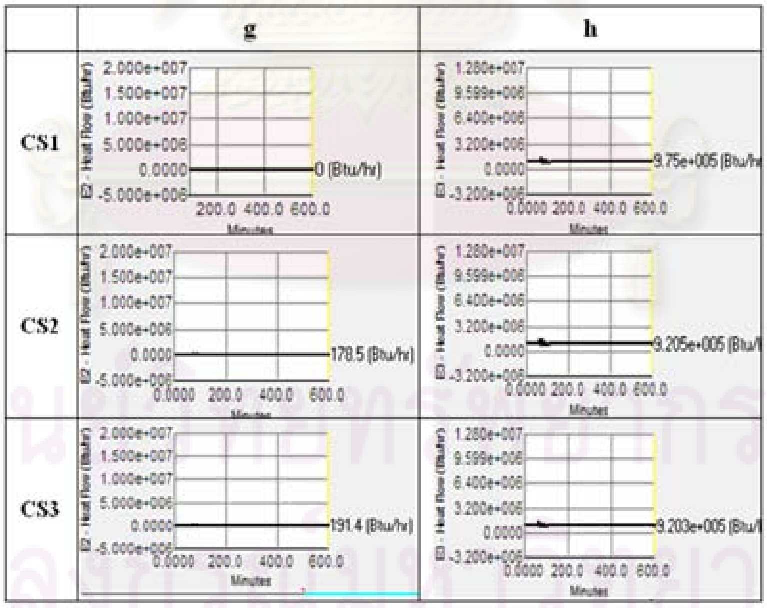

Figure C.8 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-2 (reversible), where (g) furnace duty and (h) cooler duty

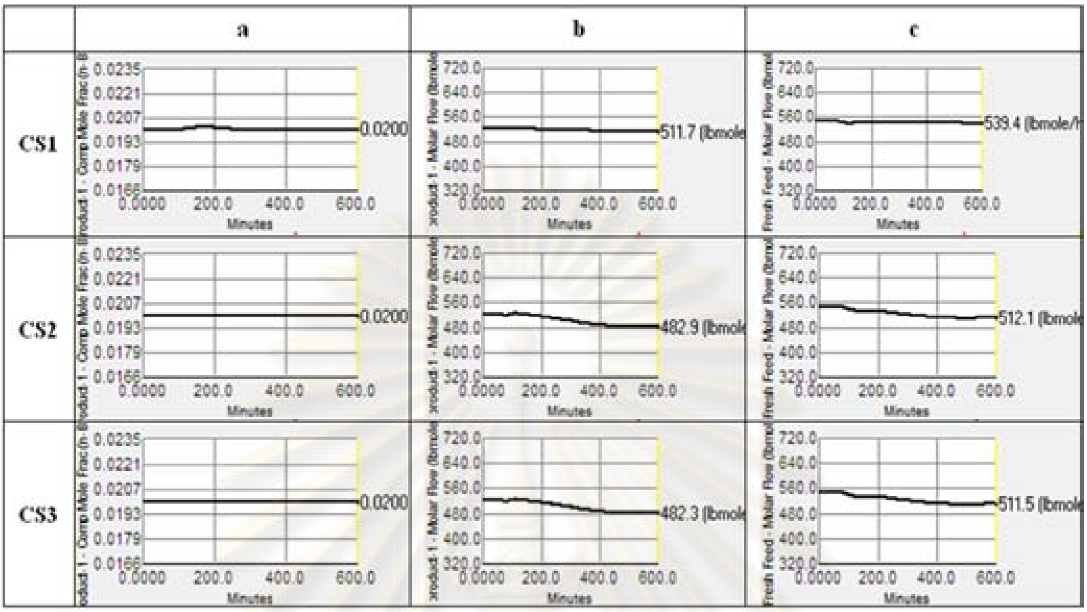

Figure C.9 Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-3 (reversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

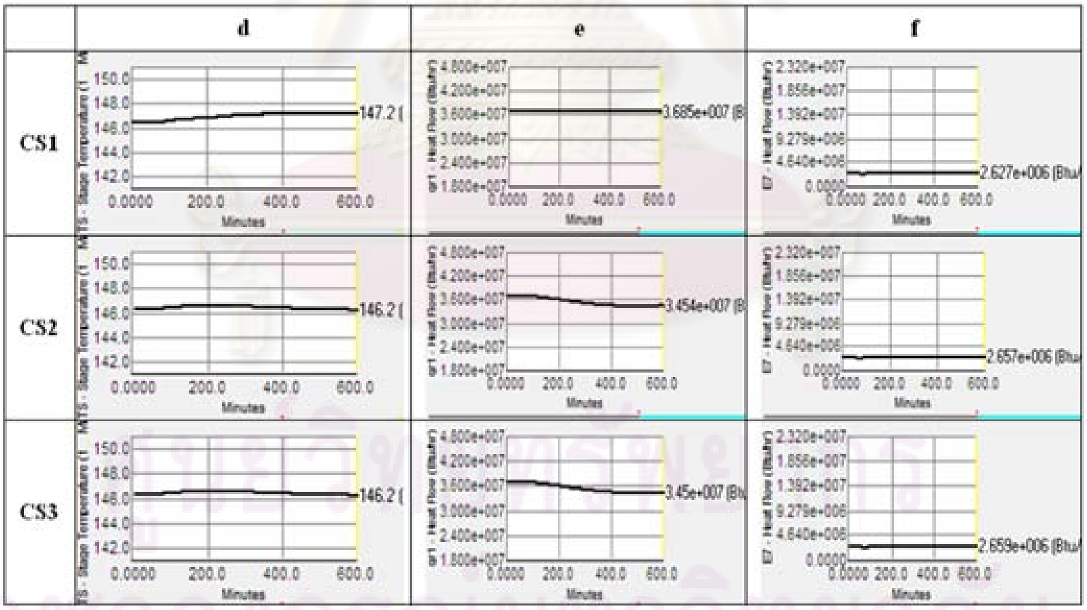

Figure C.9 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-3 (reversible), where (d) tray 1 temperatureof DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

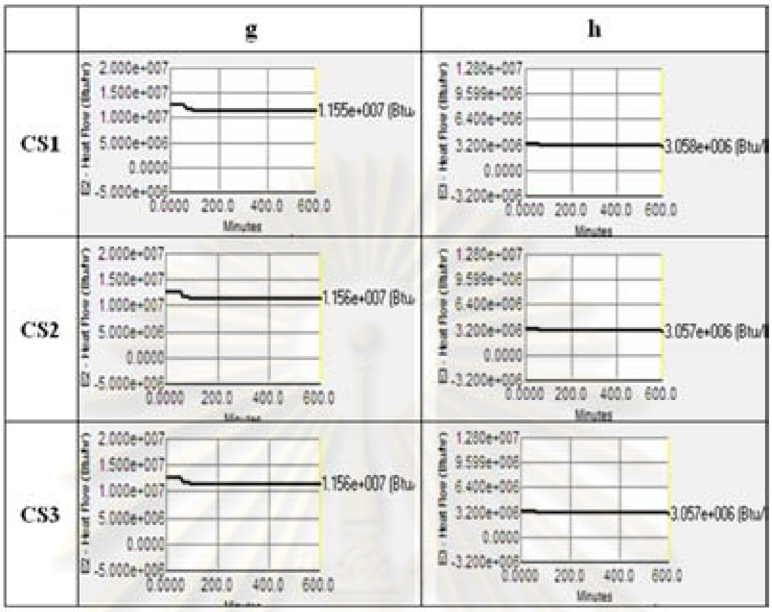

Figure C.9 Continued Dynamic responses to decrease in recycle flows from 872.5 to 802.5 lb-mol/hr of RHEN-3 (reversible), where (g) furnace duty and (h) cooler duty

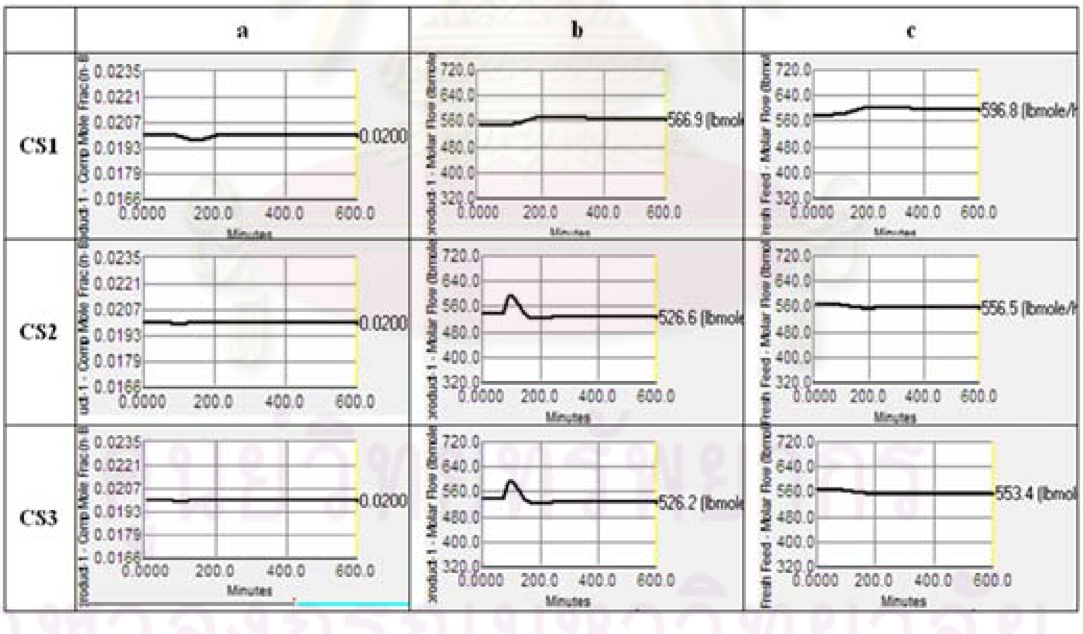

Figure C.10 Dynamic responses to decrease in recycle flows from 870.1 to 800.1 lb-mol/hr of Base case (irreversible), where (a) product composition, (b) product flowrate and (c) fresh feed flowrate

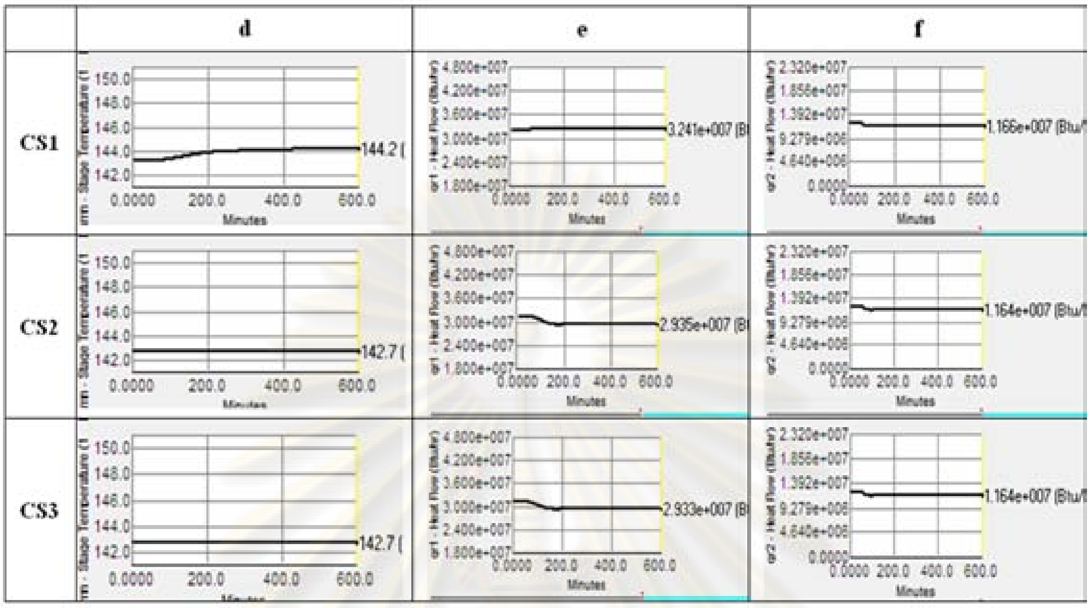

Figure C.10 Continued Dynamic responses to decrease in recycle flows from 870.1 to 800.1 lb-mol/hr of Base case (irreversible), where (d) tray 1 temperature of DIB column, (e) reboiler duty of DIB column and (f) reboiler duty of Purge column

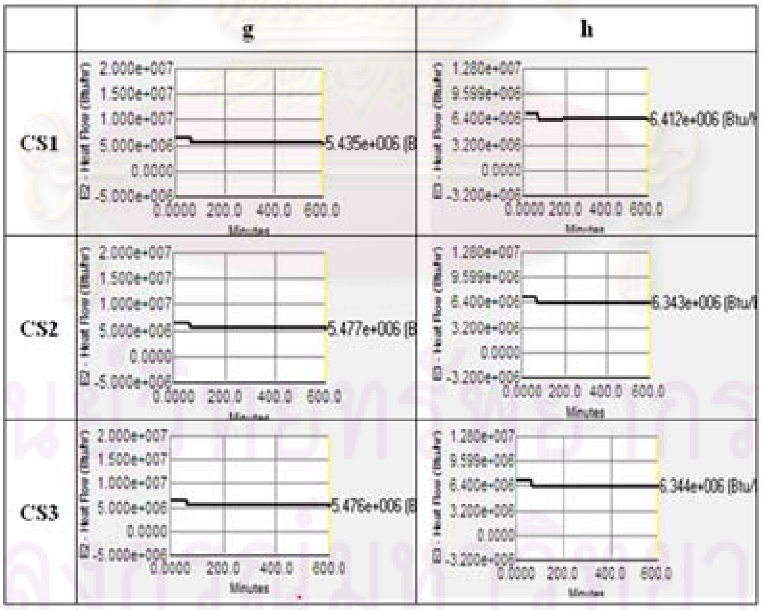

Figure C.10 Continued Dynamic responses to decrease in recycle flows from 870.1 to 800.1 lb-mol/hr of Base case (irreversible), where (g) furnace duty and (h) cooler duty

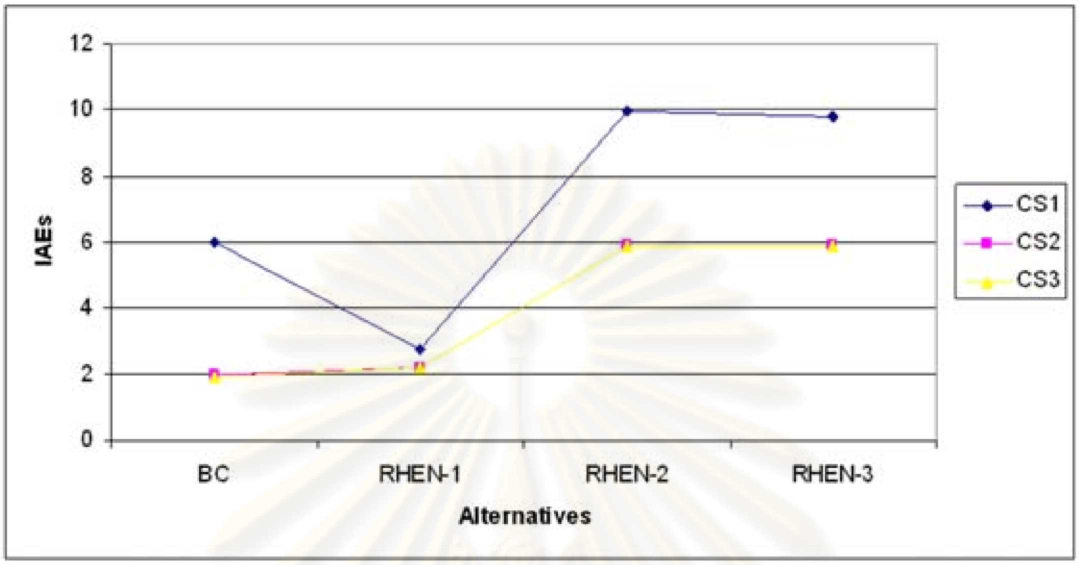

Figure C.11 The IAE re1sults of the control systems to 10 ^oF decrease in the setpoint of the reactor inlet temperature

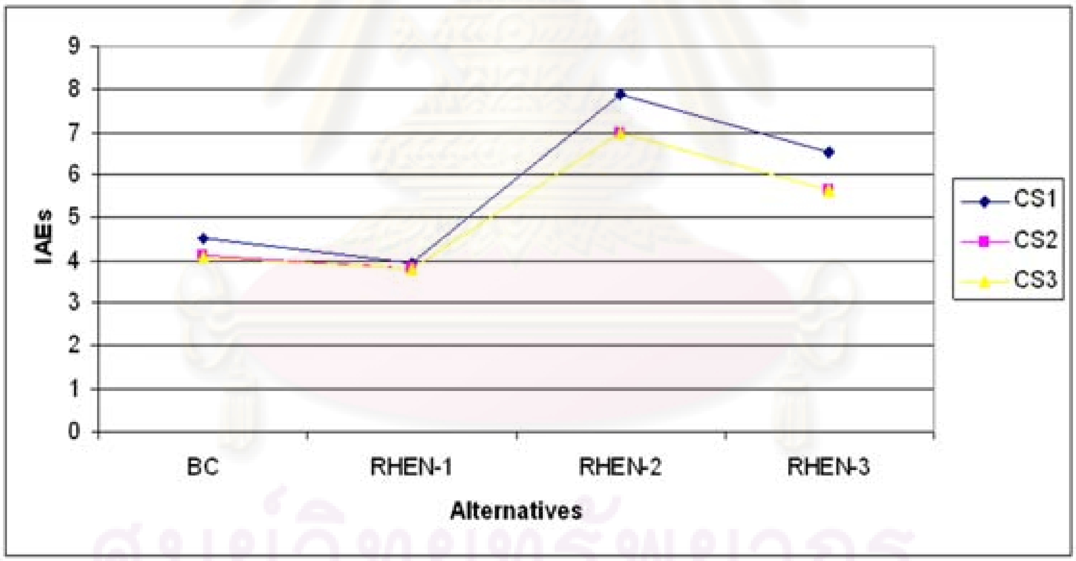

Figure C.12 The IAE results of the control systems to decrease in recycle flowrates from 872.5 to 802.5 lb-mol/h.

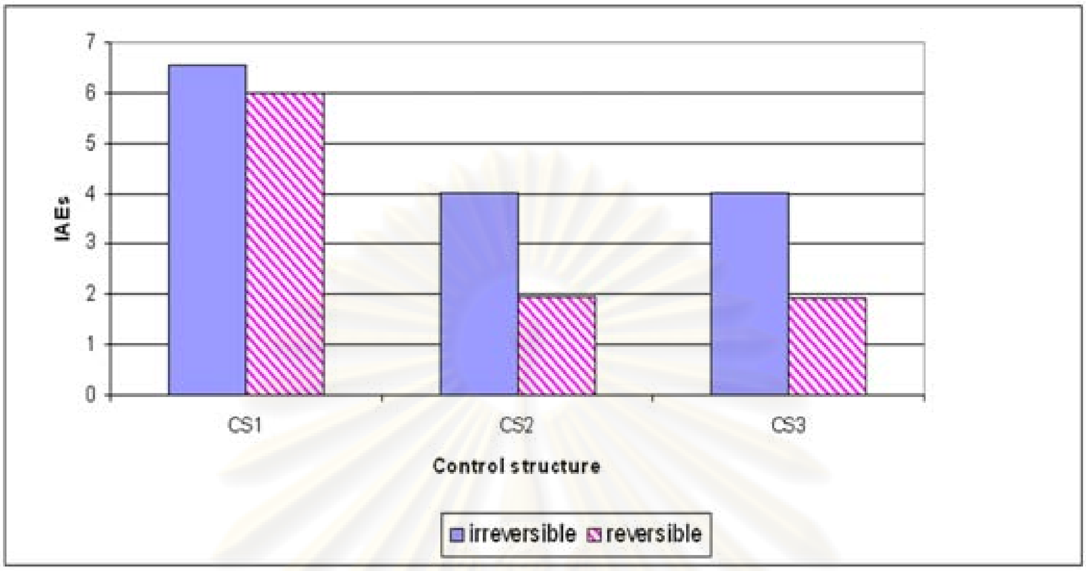

Figure C.13 The IAE results of the control systems to 10 ^oF decrease in the setpoint of the reactor inlet temperature: irreversible and reversible reaction case

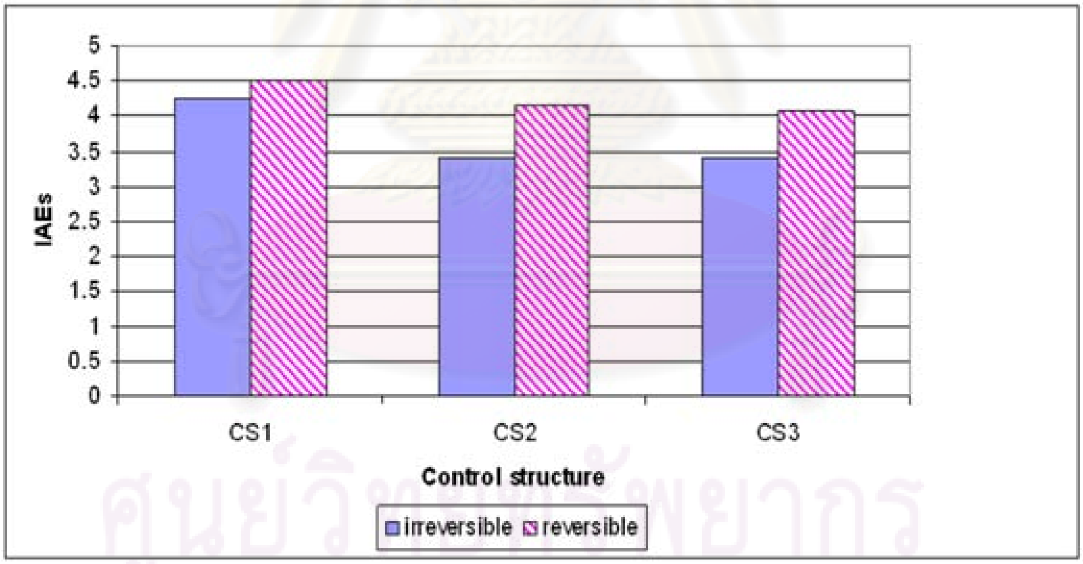

Figure C.14 The IAE results of the control systems to decrease in recycle flowrates : irreversible and reversible reaction case

APPENDIX D

FIXTURE POINT THEOREM DATA

Table D.1: List of Manipulated Variables for the Butane Isomerization Process

Manipulated Variable	Description
V1	Fresh feed valve
V2	DIB column distillate valve
V3	Purge column feed valve
V4	Purge column bottom valve
V5	Purge column distillate valve
V6	DIB column feed recycle valve
qc1	DIB column condenser duty
qr1	DIB column reboiler duty
qc2	Purge column condenser duty
qr2	Purge column reboiler duty
E2	Heat duty of furnace
E3	Heat duty of cooler

Table D.2: IAE Results of Flow Rate Deviation for the Process Stream

Stream	V1	V2	V3	V4	V5	V6	qc1	qr1	qc2	qr2	E2	E3	Sum IAE
Fresh Feed	6.748897	0.489411	0.20824	0.022619	0.25612	0.297402	0.520112	0.040664	0.405059	0.366746	0.748963	0.736367	10.8406
2	6.748897	0.489411	0.20824	0.022619	0.25612	0.297402	0.520112	0.040664	0.405059	0.366746	0.748963	0.736367	10.8406
product	0.412751	4.026131	0.343789	0.039247	0.428059	0.498566	0.88887	0.061073	0.674851	0.598055	1.225243	1.257105	10.45374
product-1	0.412751	4.026131	0.343789	0.039247	0.428059	0.498566	0.88887	0.061073	0.674851	0.598055	1.225243	1.257105	10.45374
bot1	0.703719	1.396	7.798671	0.062289	0.734134	0.858011	1.479102	0.145677	1.156747	2.588636	1.752008	2.149451	20.82445
bot-1	0.703719	1.396	7.798671	0.062289	0.734134	0.858011	1.479102	0.145677	1.156747	2.588636	1.752008	2.149451	20.82445
distil2	0.198227	0.395168	0.190867	0.023194	1.902251	1.795985	0.249075	0.037814	0.878772	0.732646	0.968709	0.741876	8.114584
bot2	0.059781	0.124751	0.109282	5.168038	0.075927	0.065532	0.081278	0.007632	0.203127	0.192402	0.184802	0.166098	6.43865
bot2-1	0.059781	0.124751	0.109282	5.168038	0.075927	0.065532	0.081278	0.007632	0.203127	0.192402	0.184802	0.166098	6.43865
p1	0.198227	0.395168	0.190867	0.023194	1.902251	5.42E-05	0.249075	0.037814	0.878772	0.732646	0.968709	0.741876	6.318654
p1-1	0.198227	0.395168	0.190867	0.023194	1.902251	1.795985	0.249075	0.037814	0.878772	0.732646	0.968709	0.741876	8.114584
furnace-in	0.195402	0.389968	0.188831	0.02321	1.885289	1.795985	0.246641	0.037576	0.867971	0.731174	0.941203	0.734677	8.037926
reac-in	0.195611	0.389783	0.188787	0.023155	1.883636	1.78284	0.24656	0.037571	0.867588	0.731106	0.941457	0.73436	8.022455
reac-out	0.177982	0.345616	0.195507	0.025791	1.489081	1.784966	0.232899	0.036823	0.945634	0.756472	0.696869	0.724695	7.412335
liq	1E-12	1.32E-12	1.34E-12	5.59E-12	1.84E-12	1.38E-12	1.45E-12	3.47E-14	3.43E-12	2.52E-12	1.43E-12	2.07E-12	2.34E-11
liq-1	1E-12	1.32E-12	1.34E-12	5.59E-127	1.84E-12	1.38E-12	1.45E-12	3.47E-14	3.43E-12	2.52E-12	1.43E-12	2.07E-12	2.34E-11
recycle2	0.177982	0.345616	0.195507	0.025791	1.489081	1.784966	0.232899	0.036823	0.945634	0.756472	0.696869	0.724695	7.412335
cooler-in	0.175081	0.338627	0.186075	0.030236	1.513906	1.683649	0.230279	0.036645	0.801173	0.772829	0.730966	0.654259	7.153725
cooler-out	0.16144	0.309164	0.175836	0.020721	1.544284	1.764099	0.218325	0.03559	0.909127	0.786961	0.875031	0.625218	7.425795
cooler-out1	0.16144	0.309164	0.175836	0.020721	1.544284	1.764099	0.218325	0.03559	0.909127	0.786961	0.875031	0.625218	7.425795
recycle3	0.16144	0.309164	0.175836	0.020721	1.544284	1.764099	0.218325	0.03559	0.909127	0.786961	0.875031	0.625218	7.425795
To CondenserDIB	0.606471	3.720553	0.417963	1.896134	0.467229	0.539571	7.024778	0.064956	0.721979	0.612602	1.355202	1.351398	18.77883
RefluxDIB	0	0	0	0	0	0	0	0	0	0	0	0	0
BoilupDIB	1.057873	1.870963	1.439584	12.81679	1.018379	1.561551	3.892027	0.23364	1.262822	1.128427	3.386637	3.08033	32.74902
To ReboilerDIB	7.452819	2.871011	0.429567	0.262725	1.737381	1.841415	6.804564	0.204086	1.443576	1.093414	1.472282	1.634626	27.24747
To CondenserPurge	0.143763	0.367243	0.178458	1.327835	1.701393	1.690059	0.284541	0.035208	5.124351	0.854249	0.813453	0.634728	13.15528
RefluxPurge	0	0	0	0	0	0	0	0	0	0	0	0	0
BoilupPurge	0.589091	1.364041	0.732557	1.716286	0.820139	0.760629	0.821445	13.86649	0	5.686407	1.396074	2.025855	29.77901
To ReboilerPurge	1.298627	2.810999	6.827092	0.13592	1.666399	1.451026	1.642443	13.67988	5.776009	3.826349	3.215736	3.981054	46.31153

Table D.3: IAE Results of Pressure Deviation for the Process Stream

Stream	V1	V2	V3	V4	V5	V6	qc1	qr1	qc2	qr2	E2	E3	Sum IAE
Fresh Feed	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0.971284	0.950872	0.780055	0.868768	0.001218	0.288422	1.306642	0.94860	0.483243	0.519475	0.768873	0.839561	8.727025
product	0.975141	0.953786	0.782741	0.811913	0.475295	0.289233	1.31050	0.950987	0.484309	0.521207	0.771442	0.842371	9.16893
product-1	0	0	0	0	0.017988	0	0	0	0	0	0	0	0.017988
bot1	0.970575	0.94886	0.778736	0.835856	0.497386	0.287975	1.305074	0.947284	0.481969	0.51853	0.767427	0.837784	9.177476
bot-1	1.588335	1.654437	1.875183	1.739288	1.332816	0.431422	1.390689	1.222786	1.667166	1.772196	1.252591	1.268162	17.1950
distil2	1.589191	1.655416	1.875977	1.751385	1.327369	0.431671	1.39143	1.222763	1.668138	1.772787	1.253004	1.269078	17.20822
bot2	1.587295	1.65336	1.871845	1.720176	1.190879	0.431100	1.38969	1.257560	1.66627	1.772480	1.251980	1.26734	17.05999
bot2-1	0	0	0	0	0.166373	0	0	0	0	0	0	0	0.166373
p1	0.970361	0.948098	0.966514	1.06050	1.365515	6.65192E-05	0.806130	1.143863	1.248626	1.150423	1.232936	1.041660	11.93469
p1-1	1.088785	1.055821	1.062465	1.152949	1.354880	2.05922	0.88938	1.357857	1.493243	1.33832	1.577422	1.406354	15.8367
furnace-in	1.095953	1.062089	1.068402	1.196074	1.23666	2.905249	0.894276	1.371069	1.508716	1.353968	1.600774	1.429730	16.722974
reac-in	1.054884	1.021800	1.025752	1.092616	2.628134	2.970628	0.856125	1.334919	1.474772	1.331043	1.551970	1.42584	17.76849
reac-out	1.054884	1.021800	1.025752	1.092616	2.044748	2.970628	0.856125	1.334919	1.474772	1.331043	1.551970	1.42584655	17.18510
liq	1.054884	1.021800	1.025752	1.092616	2.044749	2.970628	0.856125	1.334919	1.474772	1.331043	1.551970	1.42584	17.185109
liq-1	0	0	0	0	0	0	0	0	0	0	0	0	0
recycle2	1.054884	1.021800	1.025752	1.092616	2.044506	2.970628	0.856125	1.334919	1.474772	1.331043	1.551970	1.425846	17.18486
cooler-in	1.061379	1.031277	1.025595	1.064428	0.653323	3.130200	0.847707	1.374513	1.522996	1.383062	1.527550	1.486266	16.10830
cooler-out	0.691938	0.672537	0.628260	0.623510	1.315038	3.40564	0.635737	1.206981	1.306819	1.363081	1.160477	1.494134	14.50416
cooler-out1	0.972904	0.951681	0.781305	0.783008	1.275181	0.288654	1.307399	0.949427	0.483077	0.520130	0.769963	0.840493	9.923229
recycle3	0.972904	0.951681	0.781305	0.783008	1.275181	0.288654	1.307399	0.949427	0.483077	0.520130	0.769963	0.840493	9.923229
To CondenserDIB	0.975141	0.953786	0.782741	0.811913	0.472415	0.289233	1.31050	0.950987	0.484309	0.521207	0.771442	0.842371	9.166055
RefluxDIB	0.975141	0.953786	0.782741	0.811913	0.475295	0.289233	1.31050	0.950987	0.484309	0.521207	0.771442	0.842371	9.16893
BoilupDIB	0.970575	0.94886	0.778736	0.835856	0.497379	0.28797	1.305074	0.947284	0.481969	0.518534	0.767427	0.837784	9.177469
To ReboilerDIB	0.970575	0.94886	0.778736	0.835856	0.510886	0.287975	1.305074	0.947284	0.481969	0.51853	0.767427	0.837784	9.190976
To CondenserPurge	1.589191	1.655416	1.875977	1.751385	1.290897	0.431671	1.39143	1.222763	1.668138	1.772787	1.253004	1.269078	17.17175
RefluxPurge	1.589191	1.655416	1.875977	1.751385	1.327369	0.431671	1.39143	1.222763	1.668138	1.772787	1.253004	1.269078	17.20822
BoilupPurge	1.587295	1.65336	1.871845	1.720176	1.190876	0.431100	1.38969	1.257560	1.668138	1.7724802	1.251980	1.267349	17.061854
To ReboilerPurge	1.587295	1.653360	1.871845	1.720176	0.987624	0.431100	1.389690	1.257560	1.666273	1.772480	1.251980	1.267349	16.856736

Table D.4: IAE Results of Temperature Deviation for the Process Stream

Stream	V1	V2	V3	V4	V5	V6	qc1	qr1	qc2	qr2	E2	E3	Sum IAE
Fresh Feed	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0.001812	0.001773	0.001191	0	0.001219	0.001188	0.002572	0.002368	0.000932	0.001006	0.0012663	0.0018194	0.017145
product	0.711264	0.680367	0.447698	0.531622	0.475295	0.455933	0.892063	0.835671	0.365106	0.383733	0.4791962	0.711619	6.969568
product-1	0.042805	0.029913	0.015584	0.052106	0.017989	0.015259	0.041719	0.04041	0.013455	0.021298	0.0214263	0.0226152	0.334581
bot1	0.72026	0.663794	0.435239	0.965228	0.497387	0.448645	0.801263	0.884712	0.375085	0.519801	0.5164807	0.701919	7.529814
bot-1	1.601901	1.649711	1.440348	1.561045	1.332817	0.984909	1.491333	1.43733	1.689494	1.58465	1.0774209	1.5390145	17.38997
distil2	1.586154	1.628372	1.440607	1.320873	1.32737	0.985727	1.485771	1.404589	1.667676	1.681775	1.0736515	1.5123458	17.11491
bot2	1.426005	1.609371	1.685299	1.40505	1.190879	0.883616	1.315427	1.094582	1.601394	1.838431	0.7398024	1.5507106	16.34057
bot2-1	0.206186	0.142231	1.720804	0.117998	0.166374	0.104964	0.180755	0.274638	0.191166	0.068074	0.2710983	0.086216	3.530504
p1	1.634281	1.676685	1.48162	1.582047	1.365516	0.000221	1.52807	1.454144	1.720583	1.735514	1.1042242	1.5527713	16.83568
p1-1	1.623172	1.664894	1.470777	1.611789	1.354881	1.012288	1.517788	1.443597	1.70818	1.72322	1.096464	1.5421799	17.76923
furnace-in	0.979944	0.94642	0.814034	1.083615	1.236668	1.005498	0.951878	1.11511	1.036067	1.027297	1.0809052	0.8011671	12.0786
reac-in	1.518234	1.48564	1.256246	1.460164	2.628134	3.593815	1.412197	1.890441	1.730322	1.707398	3.2895795	1.2396349	23.21181
reac-out	1.337532	1.222412	1.125218	1.396795	2.044748	2.751641	1.36823	1.627453	1.348216	1.268531	2.6027258	1.0609268	19.15443
liq	1.337532	1.222402	1.125215	1.396795	2.044749	2.751636	1.368225	1.627428	1.348229	1.26852	2.602725	1.0609212	19.15438
liq-1	0	0	0	0	0	0	0	0	0	0	0	0	0
recycle2	1.337151	1.221951	1.124943	1.396504	2.044506	2.75147	1.367965	1.627081	1.347994	1.268514	2.6024973	1.0605219	19.1511
cooler-in	0.571227	0.544335	0.457512	0.636752	0.653323	1.113758	0.551284	0.796221	0.629531	0.689673	0.6984411	0.4559938	7.798052
cooler-out	1.28337	1.247003	1.161851	1.388006	1.315039	1.620251	1.362337	1.068325	1.497994	1.177939	1.5165616	1.8465834	16.48526
cooler-out1	1.244057	1.208771	1.124492	1.356783	1.275181	1.566514	1.319915	0.991722	1.451334	1.078617	1.4667562	1.7400872	15.82423
recycle3	1.244057	1.208771	1.124492	1.356783	1.275181	1.566514	1.319915	0.991722	1.451334	1.078617	1.4667562	1.7400872	15.82423
To CondenserDIB	0.703478	0.675517	0.446078	0.426905	0.472415	0.451543	0.904219	0.835928	0.362364	0.384433	0.4781917	0.706357	6.847429
RefluxDIB	0.711264	0.680367	0.447698	0.531622	0.475295	0.455933	0.892063	0.835671	0.365106	0.383733	0.4791962	0.711619	6.969568
BoilupDIB	0.720253	0.663788	0.435235	0.964791	0.49738	0.44864	0.801258	0.884707	0.375082	0.519798	0.5164776	0.7019125	7.529323
To ReboilerDIB	0.73335	0.674324	0.45437	0.627575	0.510887	0.454655	0.791073	0.885915	0.382558	0.50564	0.5281468	0.7154474	7.26394
To CondenserPurge	1.547209	1.584673	1.394565	1.644955	1.290898	0.948129	1.442688	1.430959	1.646702	1.731181	1.0524869	1.433373	17.14782
RefluxPurge	1.586154	1.628372	1.440607	1.320873	1.32737	0.985727	1.485771	1.404589	1.667676	1.681775	1.0736515	1.5123458	17.11491
BoilupPurge	1.426	1.609367	1.685293	1.40505	1.190876	0.883616	1.315425	1.094577	1.667676	1.838428	0.7398004	1.5507072	16.40682
To ReboilerPurge	1.165349	1.428775	3.242983	1.458271	0.987624	0.757906	1.088797	1.020111	1.358744	1.832403	0.4240701	1.441104	16.20614

Table D.5: IAE Results of n-Butane Deviation for the Process Stream

Stream	V1	V2	V3	V4	V5	V6	qc1	qr1	qc2	qr2	E2	E3	Sum IAE
Fresh Feed	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0
product	0.251640489	0.314915479	0.084685	0.152716	0.198006	0.137217	0.297059	0.60884	0.200979	0.405421	0.20563	0.306709	3.163818369
product-1	0	0	0	0	0	0	0	0	0	0	0	0	0
bot1	1.493963993	1.450482015	0.345082	1.620737	0.896259	0.830194	1.875124	0.777991	0.702185	1.001545	0.749038	1.035821	12.77842515
bot-1	0	0	0	0	0	0	0	0	0	0	0	0	0
distil2	1.24993535	1.455272531	1.020887	1.631248	0.882054	0.848727	1.975704	0.685084	0.796328	1.566466	0.706012	1.207978	14.0256958
bot2	1.30716615	0.949752613	5.545833	0.457608	1.008308	0.505593	0.768439	2.087884	1.610629	0.559034	1.332543	0.792259	16.92504982
bot2-1	0	0	0	0	0	0	0	0	0	0	0	0	0
p1	0	0	0	0	0	0	0	0	0	0	0	0	0
p1-1	0	0	0	0	0	0	0	0	0	0	0	0	0
furnace-in	0	0	0	0	0	0	0	0	0	0	0	0	0
reac-in	1.247244636	1.450700367	1.019918	1.56435	0.880805	0.848597	1.974705	0.68246	0.794058	1.563921	0.70561	1.20267	13.93504014
reac-out	1.17677E-07	2.93185E-08	1.06E-08	2.35E-08	2.13E-08	1.83E-08	7.71E-08	2.42E-08	1.15E-08	1.34E-08	5.79E-09	2.28E-08	3.75264E-07
liq	1.537559644	1.525059949	0.679975	1.566746	2.142427	2.326783	1.059615	1.764195	2.032418	1.64718	2.170022	1.906643	20.35862384
liq-1	0	0	0	0	0	0	0	0	0	0	0	0	0
recycle2	0	0	0	0	0	0	0	0	0	0	0	0	0
cooler-in	0	0	0	0	0	0	0	0	0	0	0	0	0
cooler-out	0	0	0	0	0	0	0	0	0	0	0	0	0
cooler-out1	1.45624481	1.426908508	0.65181	1.503298	1.99607	2.251444	1.024676	1.696773	1.931701	1.628216	2.065572	1.773959	19.40667326
recycle3	1.45624481	1.426908508	0.65181	1.503298	1.99607	2.251444	1.024676	1.696773	1.931701	1.628216	2.065572	1.773959	19.40667326

Table D.6: IAE Results of level Deviation for the Process Stream

Stream	V1	V2	V3	V4	V5	V6	qc1	qr1	qc2	qr2	E2	E3	Sum IAE
DIB condenser	0.043532491	0.117415896	0.015382	0.006945	0.05608	0.079731	0.982339	0.116468	0.029138	0.035276	0.063187	0.070465	1.615958734
DIB reboiler	2.023175955	1.018284484	0.728874	0.025391	0.818848	0.631799	1.193149	1.330421	0.373107	0.347339	1.091498	1.0176	10.59948638
Purge condenser	0.126446518	0.205466414	0.058457	0.006961	0.308552	0.34315	0.108865	0.256487	1.623568	0.238681	0.176441	0.19182	3.644895875
Purge reboiler	1.806845036	2.658833207	3.197287	3.960703	2.81652	2.945319	1.715647	2.296623	1.974187	3.378705	2.668874	2.720116	32.13965901

VITA

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