การออกแบบข่ายงานเครื่องแลกเปลี่ยนความร้อนและโครงสร้างการควบคุมแบบแพลนไวท์ของโรงงานไอโซเมอร์ไรเซชันบิวเทน

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DESIGN OF HEAT EXCHANGER NETWORKS AND PLANTWIDE CONTROL STRUCTURE OF BUTANE ISOMERIZATION PLANT

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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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บุศรา คุณาจิตพิมล: การออกแบบข่ายงานเครื่องแลกเปลี่ยนความร้อนและโครงสร้างการควบคุมแบบแพลนท์ไวด์ของโรงงานไอโซเมอร์ไรเซชันบิวเทน. (DESIGN OF HEAT EXCHANGER NETWORKS AND PLANTWIDE CONTROL STRUCTURE OF BUTANE ISOMERIZATION PLANT) อ. ที่ปรึกษา: ผศ. ดร. มนตรี วงศ์ศรี, 226 หน้า.

ในงานวิจัยนี้ข่ายงานความร้อนแบบยืดหยุ่นซึ่งนำพลังงานกลับคืนสูงสุดทางพลวัตรเป็นผลสำเร็จและใช้กลยุทธ์การควบคุมแบบแพลนท์ไวด์ได้ถูกออกแบบสำหรับโรงงานไอโซเมอร์ไรเซชันบิวเทน ความยากในการควบคุมโรงงานที่มีการเบ็ดเสร็จของพลังงานถูกแก้ปัญหาโดยใช้หม้อต้มซ้ำช่วยซึ่งรักษาปริมาณการใช้ให้น้อยที่สุด 2 ทางเลือกของการออกแบบข่ายงานความร้อนของโรงงานไอโซเมอร์ไรเซชันถูกเสนอโดยทั้งสองข่ายงานใช้ความร้อนจากกระแสขาออกของถังปฏิกรณ์นำพลังงานความร้อนเหล่านั้นไปให้หม้อต้มซ้ำของหน่วยหอกลั่นซึ่งสามารถประหยัดพลังงานได้สูงถึง 24.88% เมื่อเทียบกับการออกแบบที่ไม่มีรูปแบบพลังงานเบ็ดเสร็จแต่ราคาการก่อสร้างเพิ่มขึ้นประมาณ 0.67% จากการติดตั้งเครื่องแลกเปลี่ยนความร้อนและหม้อต้มซ้ำช่วย 4 โครงสร้างควบคุมแบบแพลนท์ไวด์ของโรงงานที่มีการเบ็ดเสร็จของพลังงานถูกออกแบบ โดยใช้วิธีตามฮิวริสติกของลูเบน ผลการศึกษาชี้ให้เห็นว่าโครงสร้างการควบคุมที่4 สามารถปฏิเสธตัวรบกวนได้ดีกว่าโครงสร้างการควบคุมอื่น โดยทั่วไปแล้วผลการตอบสนองทางพลวัตรของระบบโครงสร้างการควบคุม CS1 ถึงCS4 ในโรงงานไอโซเมอร์ไรเซชันบิวเทนรูปแบบที่ 1 จะดีกว่ารูปแบบที่ 2 อย่างไรก็ตามผลการตอบสนองของระบบโครงสร้างการควบคุม CS1 ถึงCS4 ในโรงงานไอโซเมอร์ไรเซชันที่ไม่มีรูปแบบพลังงานเบ็ดเสร็จจะมีสมรรถนะการควบคุมที่ดีกว่ามีรูปแบบพลังงานเบ็ดเสร็จ สำหรับเส้นทางเดินความร้อนต่างๆในข่ายงานถูกออกแบบโดยใช้วิธีการส่งผ่านความแปรปรวนของวงศ์ศรี เพื่อที่จะได้พลังงานกลับคืนสูงสุดทางพลวัตรเป็นผลสำเร็จ โครงสร้างการควบคุมที่ออกแบบนี้ได้ถูกประเมินค่าอย่างเข้มงวดโดยใช้โปรแกรมจำลองกระบวน การทางการค้าไฮซิส (HYSYS)

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BUSARA KUNAJITPIMOL: DESIGN OF HEAT EXCHANGER NETWORKS AND PLANTWIDE CONTROL STRUCTURE OF BUTANE ISOMERIZATION PLANT. THESIS ADVISOR: ASST. PROF. MONTREE WONGSRI, D.Sc., 226 pp.

In this work, the resilient heat exchanger networks to achieve dynamic maximum energy recovery and plantwide control structures and strategies are designed for Butane Isomerization plant. The control difficulties associated with heat integration are solved by adding auxiliary utilities which is kept minimal. Two alternatives of heat exchanger networks (HEN) designs of the Butane Isomerization plant are proposed. Both used the heat from the reactor effluent stream to provide the heat for the column reboiler. The energy saved is 24.88% from the design without heat integration, but the capital cost raised is about 0.67% due to adding of a process to process exchanger and an auxiliary utility exchanger to the process. Four plantwide control configurations of heat-integrated plant are designed following Luyben's heuristic method. The result shows the fourth control structure can reject disturbances better than other control structures. In general, the control systems for CS1 to CS4 in the butane isomerization process alternative 1 are better than that in alternative 2. However, the control systems for CS1 to CS4 in the butane isomerization process without energy integration are the most effective one compared with the other two alternatives. Various heat pathways throughout the network designed using Wongsri's disturbance propagation method to achieve DMER. The designed control structure is evaluated based on the rigorous dynamic simulation using the commercial software HYSYS.

Department.......Chemical Engineering...... Student's signature Busara Kunajitpimol

Field of study......Chemical Engineering..... Advisor's signature M. Wongsri

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Finally, I would like to dedicate this dissertation to my family for their edification, support and endless love. Without them, I would not have been the person I am and certainly this work would never have reached completion.

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NOMENCLATURES

r	reaction rate of isomerization reaction
V_R	reactor volume
k_F	the kinetic expression for the isomerization reaction
nC_4	normal butane
iC_4	isobutene
C_3	propane
iC_5	isopentane
D	disturbance
T	temperature, ^{0}F
P	pressure, psia
W	the heat capacity flowrate units of Btu/hr-^{0}F
H_i	hot stream
C_i	cold stream
CS1	reference control structure I
CS2	reference control structure II
CS3	Design of control structure 1
CS4	Design of control structure 2
S1	the first control scheme of Poothanakul P.
S2	the second control scheme of Poothanakul P.
S3	the third control scheme of Poothanakul P.
MER	maximum energy recovery
DMER	dynamic maximum energy recovery
HPH	heat pathway heuristics
IAE	integral absolute error

ϵ	error
Alt1	alternative1
Alt2	alternative2
RHEN	Resilient heat exchanger network
HEN	Heat exchanger network

CHAPTER I

INTRODUCTION

This chapter is an introduction of this research. It consists of importance and reasons for research, research objectives, scope of research, procedure and method, contribution of research, and the research contents.

1.1 Importance and reasons for research

At present, the tendency of energy demands is rapidly increasing. With high fuel prices and the possibility of supplies in the years ahead, the importance of developing systems to use energy more efficiently is apparent. One of the major components in the chemical processing is the heat exchanger network, because it determines to a large extent the net energy consumption of the process. Tremendous efforts have been expanded to establish a series of systematic approaches toward conserving energy and also minimizing losses in the process industries.

Moreover, industries are very competitive both in quality and cost of production. Therefore, production process should have high quality and high efficiency. The process should always operate under the design condition, use little energy, low waste production and meet the required specification of the products. In the real situation, the process will not operate smoothly. All factors do not meet the design conditions. The process always changes due to disturbance from the external factors and the internal factor. It is necessary to have the control system to control the condition and compensate for any deviation occurred.

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 problem is extremely complex and is very much opened. There are a combinatorial number of possible choices and alternative strategies to control and manage the disturbance load entering the process.

In this research, the heuristic-based heat exchanger network of Butane isomerization process will be design using disturbance load propagation method (Wongsri, 1990) and design plantwide control structure using Luyben heuristic design method (1998).

The butane isomerization process is a complex plant consisting of many unit operations. At the preliminary stages of a process design with no energy integration, we are attempting to fix the structure of a flowsheet. It is well-established that savings in the operating costs (utilities) provide a large economic incentive for heat integration of processing streams. Consequently, more and more complex heat recovery networks are being utilized to transfer heat from parts of the process which need to be cooled to places where heat needs to be added.

The another important is a control strategy for process associate with energy integration, it is essential to study the heat pathway control in order to manage the disturbance load entering the process in such a way that the maximum energy recovery (MER) can always be achieved.

The goal of this study is to use plantwide control strategies to develop the new control structures for the butane isomerization process with energy integration schemes that are designed to achieve the control objective and reduce the cost of production. In this work, the commercial software HYSYS is chosen to carry out both steady state and dynamic simulations.

1.2 Research objectives

1. To design heat exchanger networks of the butane isomerization plant using disturbance load propagation method (Wongsri, 1990).

2. design control structures for energy-integrated butane isomerization plant.

3. To assess performance of the designed control structures for energy-integrated butane isomerization plant.

1.3 Scope of research

1. The target for design heat exchanger networks of the butane isomerization plant is to achieve possible maximum energy recovery or the minimum utility requirement (Wongsri, 1990).

2. To achieve the desired production rate and control the impurity of normal butane in isobutene product at 2 mol%.

3. Simulation of the butane isomerization plant is performed using a commercial process simulator-HYSYS.

4. Description and data of the butane isomerization plant is obtained from William L. Luyben, Bjorn D.Tyreus, and Michael L.Luyben (1998) and Poothanakul P.(2002).

5. The design control structures for energy-integrated butane isomerization plant are design using Luyben 's heuristics method.

6. The number of control structure design is 2 alternatives which are designed heat exchanger networks (not include Luyben's).

1.4 Contribution of Research

1. The new control structures of the butane isomerization plant with heat integration are designed and compared with the earlier work given by L.Luyben with no energy recovery.

2. New energy integrated designs of the butane isomerization plant.

1.5 Procedure Plan

1. Study of plantwide process control theory, the butane isomerization plant and concerned in formation.
2. Study and Design heat exchanger networks of the butane isomerization plant using HEN heuristics.
3. Steady state modeling and simulation of heat exchanger networks of the butane isomerization plant.
4. Study of dynamic modeling and simulation of the butane isomerization plant with no energy integration.
5. Design of control structures for the energy- integrated butane isomerization plant.
6. Dynamic Simulation for the energy- integrated butane isomerization plant 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 objective, 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 covers some background information of heat exchanger networks 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 compares with control structures of Luyben.

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

This is follow by:

References

Appendix A: Butane Isomerization Process Stream and Equipment Data

Appendix B: Parameter Tuning of Control Structures

Appendix C: Dynamic Responses Graph

Appendix D: Poothanakul's Control Structure

Appendix E: The Capital Cost Estimation

Appendix F: Design the Resilient HEN with three heat exchangers

CHAPTER II

LITERATURE REVIEW

The concept of plantwide control structure synthesis is not new to the chemical process industry. The research in this area grew, in part because of the number of heat management systems that were being installed. Before the details of the present study are given, a brief of the other previous work on heat exchanger networks design, and plantwide control design are reviewed first in this chapter.

2.1 Heat Exchanger Network (HEN)

A systematic procedure for calculating minimum heating and cooling requirements, as well as the minimum number of exchangers, for a heat-exchanger network (HEN) has been developed by Hohmann (1971), Umeda, et al., (1978), and Linnhoff and Flower (1978a,b). A thermodynamically orientated method is presented for the synthesis of heat exchanger networks. The network divided into several subnetworks (temperature intervals) according to supply and target temperatures. The matches in each subintervals are easy to find. The final combined network however, is not simple especially for large problems.

Linnhoff and Hindmarsh (1983) the pinch method utilizes design heuristics and insights derived from the previous work (Linnhoff and Flower 1978a). The problem first must be identified as to whether it is (1) a heating problem or, (2) a cooling problem or, (3) both, which divides the network at the pinch. If it is pinched, the heat must not be allowed to transfer across the pinch. The suggested matching heuristics are start matching from the pinch, do not transfer heat across the pinch, observe the heat capacity flow rate constraints, etc.

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

Cerda and Westerberg (1983) formulates the minimum utility calculation for a heat exchanger network synthesis as a ”transportation problem” from linear programming, allowing one to develop an effective interactive computing aid for this problem. To determine the optimum network for transporting a commodity (heat) from sources (hot streams) directly to destinations (cold stream) through temperature intervals accouting for thermodynamics constraints in the transfer of heat.

Papoulias and Grossmann(1983) use the transshipment model formulation which is a variation of the transportation problem to investigate the optimum network. The problem is formulated as a transportation problem, but instead of being sent directly to cold streams, the heat packets are sent from hot streams to intermediates nodes (i.e. temperature intervals) first and then to the cold streams. The models for the minimum utility cost target (linear programming or LP) and the minimum number of units target (mixed-integer linear programming or MILP) are developed.

Saboo and Morari (1984) 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 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 an explicit function for the minimum utility requirement valid over the whole disturbance range dose not exist, 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.

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 generate HEN design alternatives by the pinch method for the nominal (the base case designs) 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.

Calandranis and Stephanopoulos (1986) present an operability analysis for a HEN by exploring nonconvexity of a network. Several cases of HENs are investigated, e.g. pinch jump, temperature variation, etc. Their method is written in ZETALISP and the program is operated in interactively.

In a series papers, studies of the sensitivity of the total processing cost to heat exchanger network alternatives and steady state operability evaluation were undertaken by D.L.Terrill and J. M. Douglas (1987a,b,c). They considered a heat exchanger network for HDA process. The T-H (temperature-enthalpy) diagram was considered and obtained six alternative heat exchanger networks, all of which had close to maximum energy recovery. Most of the alternatives include a pressure shifting of the recycle column, and the other distinguishing feature is the number of column reboilers that are driven by the hot reactor products. The benefit obtained from energy integration with the base-case flow rates for the six alternatives, the energy saving from the energy integration fall between 29 and 43 % but cost savings were in the range from -1 to 5%. The cost savings were not as dramatic because the raw material costs dominate the process economics

Worravitudomsuk(1989) studied energy system design using pinch technology . An optimal energy system design approach base on the first law and second law of thermodynamics was applied too a selected large scale process, the refinery plant of Bangchak Petroleum Industry. In pinch design method, a maximum energy recovery (MER) design was obtained after the pinch point and minimum energy targets had been identified with the computer software. The present application results showed that the MER design could significantly reduce the utility consumption of the existing plant (base case) by 25% and 22% off hot and could utility requirement, respectively. The payback period for MER design war estimated to be 1.58 years.

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

Ploypaisansang A. (2003) designed resilient network for the Hydrodealkylation process (HDA Process). The match pattern heuristic, shift approach and the heat load propagation technique were essential approach. Six alternatives for the HDA process were redesign to be the resiliency networks for maintain target temperature and also reached maximum energy recovery (MER). The Resiliency Parameters of resilient networks were required to compare and selected the best resilient network. In order to receive resilient network, a trade-off between cost and resilient may be needed. The auxiliary unit should be added in the network for cope safely with variations and easy to design control structure to the networ

2.2 Design and Control of Energy-Integrated Plants

Renanto Handogo and W. L. Luyben (1987) studied the dynamics and control of heat-integrated reactor/column system. An exothermic reactor was the heat source, and a distillation column reboiler was the heat sink. Two types of heat-integration systems were examined: indirect and direct heat integration. Both indirect and direct heat integration systems are found in industry. In the indirect heat-integration system, steam generation was used as the heating medium for the reboiler. The direct heat-integration system used the reactor fluid to directly heat the column. The indirect heat-integration system was found to have several advantages over the direct heat-integration system in term of its dynamic performance. Both systems were operable for both large and small temperature differences between the reactor and column base.

M.L. Luyben, and W.L. Luyben (1995) examines the plantwide design and control of a complex process. The plant contains two reaction steps, three distillation columns; two recycle streams, and six chemical components. Two methods, a heuristic design procedure and a nonlinear optimization, have been used to determine an approximate economically optimal steady-state design. The designs differ substantially in terms of the purities and flow rates of the recycle streams. The total annual cost of the nonlinear optimization design is about 20 %less than the cost of the heuristic design. An analysis has also been done to examine the sensitivity to design parameters and specifications. Two effective 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.

M.L. Luyben, B.D. Tyreus, and W.L. Luyben (1997) presented A general heuristic design procedure is presented that generates an effective plantwide control structure for an entire complex process flowsheet and not simply individual units. The nine steps of the proposed procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental and safety constraints; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization. Application of the procedure is illustrated with three industrial examples: the vinyl acetate monomer process, the Eastman plantwide-control process, and the 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.

Calandranis,J. and Stephanopoulos,G.,(1988) A new approach to address the following problems: (a) design the configuration of control loops in a network of heat exchangers; (b) sequence the control action of loops, the accommodate set-point changes and reject load disturbances. The approach proposed exploits the structure characteristic of heat exchanger network (HEN) by identifying routes through the HEN structure that can allocate loads to available sinks. Several design issues such as the placement of bypass lines, the restrictions imposed by the existence of a "process pinch". The plan of control actions is generated by an "expert" controller, which selects what path(s) through the HEN is to be used for each entering disturbance or set-point change, and what loops should be activated to carry the associated load to a utility unit.

Luyben (2000) studied process which had exothermic, irreversible, gas phase reaction A + B C occurring in an adiabatic tubular reactor. A gas recycle returned unconverted reactants from the separation section. Four alternative plantwide control structures for achieving reactor exit temperature control were explored. 1 the set point of the reactor inlet temperature controller was changed (CS1), 2 the recycle flow rate was changed, 3 the flow rate of one of the reactant fresh feeds was changed (CS3) and 4 used an "on-demand" structure. Manipulation of inlet reactor temperature appeared to be the last attractive scheme. Manipulation of recycle flow rate gave the best control but may be undesirable in some system because of compressor limitations. The on demand structure provided effective control in the face of feed composition disturbances. And in the same year he considered the design and control aspects of a ternary system with the gas phase reversible, exothermic reaction A + B C occurring in an adiabatic tubular reactor packed with solid catalyst. He designed different control structure by fresh feed control pressure. The inlet reactor temperature is fixed. The recycle flowrate is used to indirectly set the production rate (CS1). Pressure was controlled by recycle flowrate and the production rate was directly set by the fresh feed flowrate (CS2). Given a control structure where the recycle flowrate was fixed (CS3). If process had inerts, the additional control loop added is the control of composition of the inert component in recycle and purge gas. Effective control was obtained in the face of quite large disturbances.

Wongsri and Kunlawaniteewat (2002) presented rules and procedure for design control structure of heat exchanger network using heuristic approach. The rules devised in this work were categorized as following: generals, match pattern, loop placement, bypass placement, and split fraction rules. In this research, 6 alternative control structures of 3 networks were designed. It shown that the network with control structure designed using their procedure gave minimum the integral time absolute error, compared to the other network found in the literature, while maintained maximum energy recovery and achieved outlet temperature targets.

Wongsri and Poothanakul (2002) used plantwide control strategies for designed control structures of butane isomerization process to achieved impurity of normal butane in product and desired production rate. First control structure controlled quality of product by fix product flow, second control structure concerned about reduction of effected of recycle by controlled temperature inside the distillation which could be controlled by adjusted distillate rate of column. And the last wanted to reduce effect of recycle indirectly by controlled temperature inside the distillation with outlet flow of bottom.

Distillation columns which large temperature differences between the condenser and reboiler; the base temperature of this type of column was often quite high. It required the use of expensive high-pressure steam. Luyben L (2004) presented method to reduce energy costs by using two reboilers. One at the base of the column used high-pressure steam. A second was at an intermediate tray in the stripping section. His paper compared the steady-state design and the dynamic control of a conventional single-reboiler distillation column with a column having both intermediate and base reboilers. Result shown consumption of high-pressure heat could be reduced, and the column diameter was also reduced. The economic effect is a reduction in both energy and capital costs. Dynamic controllability is just as good in the intermediate reboiler column as it is in the standard column. Average temperature control should be used in both because of the very sharp temperature profile.

Wongsri and Thaicharoen (2004) presented the new control structures for the hydrodealkylation of toluene (HDA) process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben's structure (CS1). The result shows that hydrodealkylation of toluene 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 dynamic 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 disturbance. 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. 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 Y.D. (2004) studied the control strategies for energy-integrated HDA plant (i.e. alternatives 1 and 6) based on the heat pathway heuristics (HPH), i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the dynamic MER can be achieved with some trade-off. In they work, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network. The new control structure with the LSS has been applied in the HDA plant alternatives 1 and 6. The designed control structure is evaluated based on the rigorous dynamic simulation using the commercial software HYSYS. The study reveals that, by selecting an appropriate heat pathway through the network, the utility consumptions can be reduced according to the input heat load disturbances; hence the dynamic MER can be achieved.

CHAPTER III

THEORIES

The starting point for an energy integration analysis is the calculation of the minimum heating and cooling requirement for a heat exchanger network. These calculations can be performed without having to specify any heat-exchanger network. Similarly, we can calculate the minimum number of exchangers required to obtain the minimum energy requirements without having to specify a network. Then the minimum energy requirements and minimum number of exchanger provide targets for the subsequent design of a heat-exchanger network.

3.1 Minimum Heating and Cooling Requirements

3.1.1 First law Analysis

Suppose we consider a very simple problem where we have two streams that need to be heated and two streams that need to be cooled (see the data in Table 3.1). If we simply calculate the heat available in the hot streams and heat required for the cold streams, the difference between these two values is the net amount of heat that we would have to remove or supply to satisfy the first law. The results are also shown in the Table 3.1, and the first two entries are determined as follows:

Table 3.1: First-law calculation

stream	Condition	mC_p	T_{in}	T_{out}	ΔH_t
1	Hot	1000	250	120	130
2	Hot	4000	200	100	400
3	Cold	3000	90	150	-180
4	Cold	6000	130	190	-360
					-10

NOTE $mCp = FCp$ is the heat capacity flowrate units of Btu/hr-^{0}F

$Q = \Delta H_t = FCp(T_{in} - T_{out})$is the heat available for each stream 10^3 Btu/hr

$$Q_1 = F_1Cp_1\ T_1 = [1000 \text{ Btu} / (\text{hr.}^0\text{F})]\ (250\text{-}120)$$

$$= 130 \times 10^3 \text{ Btu/hr}$$

$$Q_2 = F_2Cp_2\ T_2 = [4000 \text{ Btu} / (\text{hr.}^0\text{F})]\ (200\text{-}100)$$

$$= 400 \times 10^3 \text{ Btu/hr}$$

Thus, 10 x 10^3 Btu/hr must be supplied from utilities if there are no restrictions on temperature-driving forces.

3.1.2 Temperature Intervals

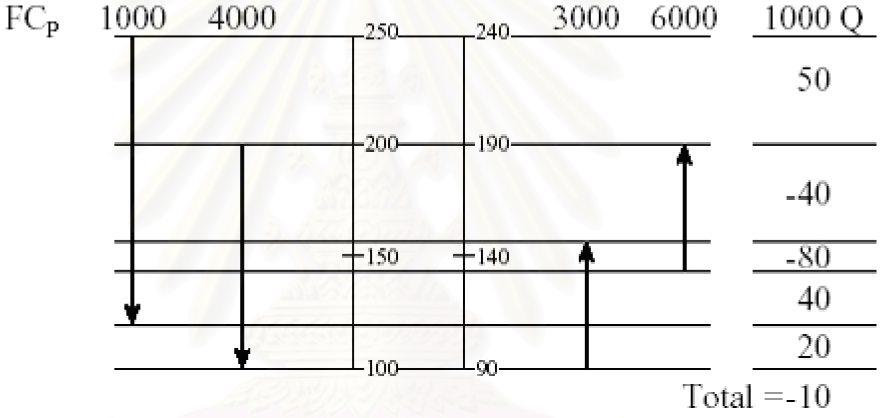


Figure 3.1: Net energy required at each interval

A very simple way of incorporating second-law considerations into the energy analysis was presented by Hohman, Umeda et al., and Linoff and Flower. Referring to the data giving in Table 3.1, if we choose a minimum driving force of 10 ^{0}C between the hot and cold streams, we can establish two temperature scales on a graph, one for the hot streams and the other for the cold streams, which are shifted by 10 ^{0}C. Next we establish a series of temperature intervals that correspond to the heads and tails of the arrows on the graph, i.e., the inlet and outlet temperatures of the hot and cold streams given in the Table 3.1 (see Figure 3.1).

In each temperature interval we can transfer heat from the hot streams to the cold streams because we are guaranteed that the temperature driving force is adequate. Of course, we can also transfer heat form any of the hot streams in the high temperature intervals to any of the cold streams at lower-temperature intervals. Knowing the stream population in each interval (form Figure 3.1), enthalpy balance can easily be calculated according to

$$Qi = [(\sum FCp)hot,i - (\sum FCp)cold,i] \Delta Ti$$

for each interval. The results are shown in the right-hand-side column of Figure 3.1. We also note that the summation of the heat available in all the intervals is -10 x 10^3 Btu/hr, which is identical to the result obtained for the first law calculation, i.e., the net difference between the heat available in the hot streams and in cold streams.

3.1.3 Cascade Diagram

As key feature of the temperature intervals, any heat available in interval is hot enough to supply any duty in interval i+1. This is shown in Figure 3.2 where heats cascading of each interval are illustrated. Instead of sending the 50 x 10^3 Btu/hr of surplus heat form interval 1 into cold utility, it can be sent down into interval 2. There it joins the 40 x 10^3 Btu/hr deficit in interval 2, making 10 x 10^3 Btu/hr to cascade into interval 3. Interval 3 has a 80 x 10^3 Btu/hr deficit, hence after accepting the 10 x 10^3 Btu/hr we must supply other 70 x 10^3 Btu/hr form a hot utility to satisfy the heat requirement.

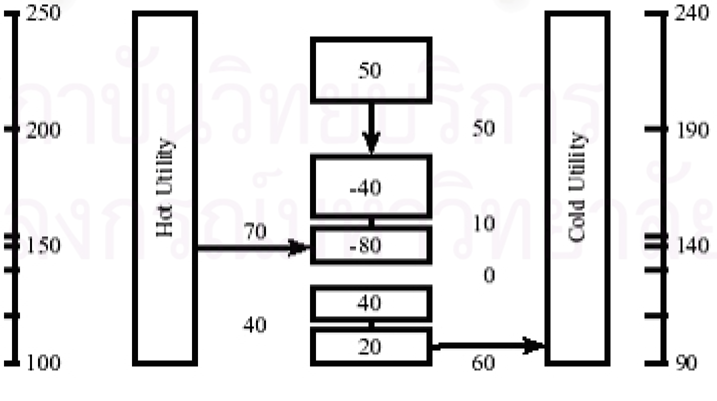


Figure 3.2: Cascade Diagram

Then,there would be no transfer of heat between the third and fourth temperature intervals. Interval 4 has a 40 x 10^3 Btu/hr surplus passing to interval

5. Finally, the 20 x 10^3 Btu/hr surplus in interval 5 means that 60 x 10^3 Btu/hr is the final cascade energy to cold utility.

3.1.4 Minimum Utility Loads

The net result of the operation is that the minimum utility requirements have been predicted, i.e., 70 x 10^3 Btu/hr of hot utilities and 60 x 10^3 Btu/hr cold utilities.

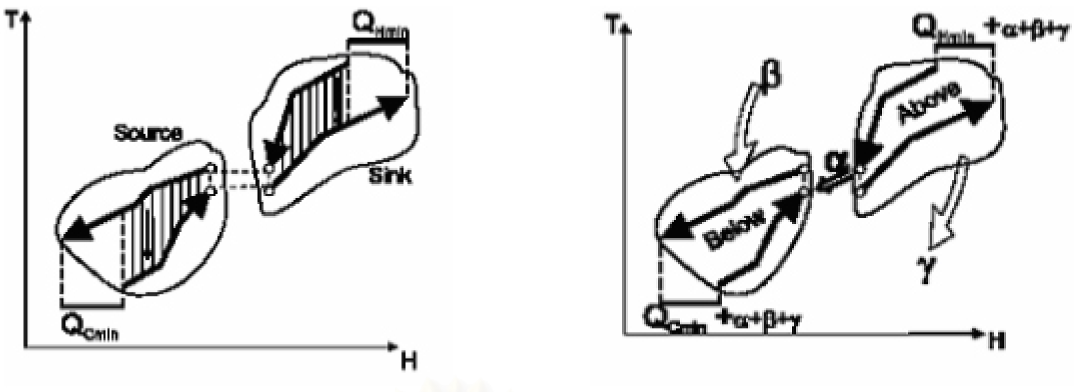
3.1.5 Pinch Temperature

At the third and fourth temperature intervals, there is no energy transfer. We call this the *pinch temperature*(130 ^{0}C for the cold streams or 140 ^{0}C for the hot streams) Thus, the pinch temperature provides a decomposition of the design problem. That is, above the pinch temperature we only supply heat, whereas below the pinch temperature we only reject heat to a cold utility.

3.1.6 The Pinch Principle

The point where Δ Tmin is observed is known as the "Pinch" and recognizing its implications allows energy targets to be realized in practice. Once the pinch has been identified, it is possible to consider the process as two separate systems: one above and one below the pinch, as shown in Figure 3.3(a). The system above the pinch requires a heat input and is therefore a net heat sink. Below the pinch, the system rejects heat and so is a net heat source.

In Figure 3.3(b) α amount of heat is transferred from above the pinch to below the pinch. The system above the pinch, which was before in heat balance with Q_{Hmin},now loses α units of heat to the system below the pinch. To restore the heat balance, the hot utility must be increased by the same amount that is units. Below the pinch,α units of heat are added to the system that had an excess of heat, therefore the cold utility requirement also increases by α units. In conclusion, the consequence of *a cross-pinch heat transfer*(α) is that both the hot and cold utility will increase by the cross-pinch duty (α).



(a) (b)

Figure 3.3: The Pinch Principle

Figure 3.3(b) also shows γ amount of external cooling above the pinch and β amount of external heating below the pinch. The external cooling above the pinch of γ amount increases the hot utility demand by the same amount. Therefore on an overall basis both the hot and cold utilities are increased by γ amount. Similarly external heating below the pinch of β amount increases the overall hot and cold utility requirement by the same amount (i.e. β).

To summarize, the understanding of the pinch gives three rules that must be obeyed in order to achieve the minimum energy targets for a process:

- *Heat must not be transferred across the pinch*
- *There must be no external cooling above the pinch*
- *There must be no external heating below the pinch*

Violating any of these rules will lead to cross-pinch heat transfer resulting in an increase in the energy requirement beyond the target. The rules form the basis for the network design procedure which is described in "Heat Exchanger Network Design". The design procedure for heat exchanger networks ensures that there is no cross pinch heat transfer. For retrofit applications the design procedure "corrects" the exchangers that re passing the heat across the pinch.

3.1.7 Design of minimum-Energy Heat-Exchanger Networks

There is design heuristic for feasible matches at the pinch condition

$$\textit{Above the pinch}: (\mathrm{FCp})_{hotstreams} \leq (\mathrm{FCp})_{coldstreams}$$
$$\textit{Below the pinch}: (\mathrm{FCp})_{hotstreams} \geq (\mathrm{FCp})_{coldstreams}$$

Violating any of these rules will lead to violate the minimum approach temperature.

3.1.8 Problem Table

For more complication problems, it would be a lengthy procedure to evaluate possible designs for each subnetwork. Fortunately, a for more rapid procedure can adopted (Linnhoff and Flower, 1978)

NOTE mCp = heat capacity flowrate units of kW/C

Heat load = mCp (Ts-Tt) unit

Table 3.2: Data for test case

stream	condition	mCp	T(supply)	T(target)	Heat Load
1	cold	3	60	180	-360
2	hot	2	180	40	280
3	cold	2.6	30	105	-195
4	hot	4	150	40	140
					Total =165

Table 3.3: Problem table for test case Table 3.2

			COLUMNS				1	2	3	4	5
	Stream and Temperature									Maximum	
SN	Hot				Cold		Deficit	Accumulate		permissible	
	(2)	(4)		180	(1)	(3)		input	output	input	output
SN(1)			180	170	↑		+30	0	-30	**+60**	+30
SN(2)	│		150	140	│		+30	-30	-60	+30	0
SN(3)	│	│	115	105	│		-105	-60	+45	0	+105
SN(4)	│	│	70	60	│	↑	-18	+45	+63	+105	+123
SN(5)	↓	↓	40	30		│	-102	+63	**+165**	+123	**+225**

In Table 3.3, the search for the upper limits to the loads of heaters and coolers in the subnetworks is carried out in a systematic way. The data used refer to test case Table 3.2, and Table 3.3 represents what will be referred to as a problem table. In column1, the values are given of net heat requirement for each subnetwork. This deficit D_k is difference between the heat input I_k, which correspond to the heat supplied by the heater(s), and the heat output O_k, that is, the heat removed by the cooler(s). For the $K^t h$ subnetwork, the D_k may be calculated by means of Equation (3.1)

$$D_k = I_k - O_k = (T_k - T_{k+1})(\sum Cp_{cold} - \sum Cp_{hot}) \qquad (3.1)$$

The summations only include the streams present in SN(K). Since Equation (1) is just an enthalpy balance, the results will be independent of any subnetwork design subsequently adopted. D_k will be positive or negative, depending on whether the heat capacity flow rates of the hot streams are less or greater than those of the cold streams. If D_k is positive, more heating than cooling is required.

Consider, now, the output form SN(K) is passed to SN(K+1) to satisfy any requirements for heat in SN(K+1). If there is no separate connection to a process utility heat source in (K+1), Equation (3.2) can be used to calculate the maximum amount of heat made available to SN(K+1):

$$I_{k+1} = O_k \qquad (3.2)$$

Form SN(K+1):

$$O_{k+1} = O_k - D_{k+1} \qquad (3.3)$$

Thus, assuming no heat supply to SN(1), the Table 3.3 for the inputs and outputs for each subnetwork are found in columns 2 and 3.

The physical significance of these tables is as follows. If no process utility heat is supplied to any of the subnetworks, and all surplus heat form the matches between the streams in one subnetwork is passed to the next, the heat inputs to each subnetwork would be given as the values in column 2 and the heat outputs in column 3. If any of the values in column 3 are negative, as is the case here for SN(1) and SN(2), process utility heat must be introduced to these subnetworks to increase these outputs to zero. It follows that if one must use process utility heat anywhere in the system, it may as well be introduced at its highest available temperature, that is, into SN(1) and then passed through the sequence of subnetworks. In this way, the amount of heat available in the intervening subnetwork designs. Accordingly, columns 4 and 5 in Table 3.3 have been drawn up. They are base on exactly the same sequence of calculations as column2 and 3, with the single difference that the minimum heat requirement for the whole network (the most negative Table in column 3) is introduced as the input to SN(1) from process utility heat sources. As result, the Table 3.3 in columns 4 and 5 represent the heat flows into and out of the subnetworks for the case where the necessary minimum process utility heat is received at highest possible temperature.

The transfer of this heat form one subnetwork to the next creates the maximum degree of choice for subnetwork design without any adverse effect on consumption of resources. Any further increase of a subnetwork's heat input must be provided by additional heat form process utilities. Thus , the Table 3.3 in column 4 and 5 represent the upper limits for the heater and cooler loads in the subnetworks which must not be exceed if subnetworks are to be designed which do not prevent maximum energy recovery. In these sense, they are maximum permissible values (see Table 3.3). Comparing the limits obtained in Table 3.3 for SN(3), SN(4), and SN(5) with the alternative designs for these subnetworks, it could be adopted for SN(4) and SN(5), but not for SN(3).

Owing to the logic on which the problem table is based, three values in columns 3, 4 and 5 will have a significance not just for the subnetwork to which they belong, but also for whole problem.

In Table 3.3, these figures are shown boxed:

1. The bottom Table3.3 in column 3 denotes the net cooling requirement for the whole problem as found by an overall enthalpy balance (see Table 3.2).

2. The top Table 3.3 in column 4 is the minimum process utility heat requirement for the whole problem.

3. The bottom Table 3.3 in column 5 is the corresponding cooling requirement for the whole problem.

In summary, the following procedure is used:

1. The temperature T_1, T_2.. $T_n + 1$ are identified.

2. An enthalpy balance, that is Equation (3.1), must be solved for each subnetwork, giving Table 3.3 for net heat requirements, column1.

3. Columns 2and 3 are calculated by means of Equation (3) and Equation (4), assuming $I_1 = 0$.

4. Columns 4 and 5 are produced by adding the value of the most negative entry in columns 3 to each entry in columns 2 and 3, if there is no negative entry in column 3.

The problem table will then show:

1. Values for the total process heat and cooling loads which will be required if maximum energy recovery is achieved.

2. Maximum permissible Table 3.3 for the heater and cooler loads of each subnetwork which must not be exceeded if the final network is to be optimum form an energy recovery point of view.

3.2 Rule-Based Heat Exchanger Network Synthesis

3.2.1 Problem Definition

The problem of heat exchanger network synthesis can be described as follows:

A set of a cold streams (i =1, n_c) initially at supply temperature T_{i^s} and at heat capacity flowrate W_i is to be heated to target T_{i^t}. Concurrently, a set of hot streams (j =1, n_h) initially at supply temperature Tis and at heat capacity flow rate W_j is to be cooled to target temperature T_{j^t}. Variations in these temperatures and heat capacity flow rates may arise due to real world situations. Hot and cold utilities are available for use. The enthalpy versus temperature relationship is known for all streams. The appropriate physical properties for determining heat transfer characteristics are also given. The objective is to design the optimal network of heat exchangers, coolers and heaters to accomplish the desired temperature changes. Optimal usually means most economic for the capital and utility costs available.

Three major properties of a HEN may be:

1. The maximum energy recovery (MER) or minimum utility usage.
2. The number of heat exchanger units (N_{min}).
3. The minimum approach temperature difference between hot process and cold process streams which is a bottleneck in a design.

3.2.2 Preanalysis

This step determines targets for a network to be designed. The design targets of a network are the maximum energy (MER) and the minimum number of matches. Other targets proposed in replacing the minimum number of units are (1) heat transfer area, (2) capital cost, and (3) number of shells.

The Maximum Energy Recovery (MER). MER can be determined by using the temperature-enthalpy diagram (Hohmann, 1971) or by the problem table (Hohmann, 1971; Linnhoff et al., 1982) or by mathematical programming techniques, i.e. the northwest corner algorithm, (Cerda and Westerberg, 1983a). The idea of the first two merges all hot streams into a single composite hot stream and all cold into a single composite cold stream. By shifting the position of the composite cold stream curve along the enthalpy axis to produce a separation between these two curves equal to the specified minimum approach temperature in the temperature-enthalpy diagram, the pinch temperature and the MER can be the obtained.

The Pinch Temperature. The pinch temperature arises in heat exchanger network which require both heating and cooling utilities. It is the point of closest approach, on the temperature scale, of the composite heating and cooling curves as dictated by the network ΔT_{min} or the minimum approach temperature between hot process streams and cold process streams. The pinch temperature divides the network into subnetworks with the requirement that no heat is allowed to transmit through that point in order to achieve MER. In each subnetwork, only one utility (heating or cooling) is required.

The Minimum Number of Matches. The probable minimum number of matches (heat exchangers, heaters and coolers) can be predicted by the following equation (Hohmann, 1971),

$$N_{min} = N_h + N_c + N_{hu} + N_{cu} - 1$$

Where N_h and N_{hu} are the numbers of hot process and utility streams; N_c and N_{hu} are the numbers of process and utility streams. For problems with a pinch this equation should be applied separately to the subnetworks above and below the pinch (Linnhoff et al., 1982).

3.2.3 Heat Exchanger Network Synthesis

Usually, heat exchanger network synthesis is divided into 2 steps:

3.2.3.1. Network targeting.

In the targeting step, the following important properties are determined before the actual network is designed. They are used as the targets for a design.

(1) The maximum energy (or the minimum utilities). The minimum utilities can be calculated by constructing the problem table (Linnhoff and Flower, 1978a). The values depend on the minimum approach temperature; ΔT_{min} on the generation of network configurations is such that, at its higher value, some configuration will be prohibited from appearing.

(2) The minimum number of matches (or units). The minimum number of matches is calculated from

$$N_{match,min} = N_{HotStream} + N_{ColdStream} - 1$$

If a problem is separated by pinch, this equation must be applied separately to each separated problem. If a matching procedure follows the 'tick-off 'heuristics, a solution obtained will feature the minimum matches predicted by the above equation. In general, the cost of a minimum matches network solution is close to the minimum capital cost network (Nishida et al., 1997)

3.2.3.2. Network Synthesis

The heuristic approach finds a HEN solution in a sequence of steps. This can be viewed a math operator to map one design state to another. There can be many match operators or in contrast just one operator. Mehta and Fan (1987) use the following condition in testing a math:

For a math at hot end position,

$$\Delta T_{he} \geq \Delta T_{min}$$

where $\Delta T_{he} = T_h^{supply} - T_c^{target}$, h = hot stream , c = cold stream

For a math at cold end position,

$$\Delta T_{ce} \geq \Delta T_{min}$$

where $\Delta T_{ce} = T_h^{target} - T_c^{supply}$

Using one operator does not use any heuristic knowledge at all. To make use of heuristics we must discriminate among matches according to criteria or preferences. We can classify matches into several categories and give them different priorities. In this way, heuristics are used.

The HEN heuristics have appeared in the literature over two decades. The following is a summary of published HENS heuristics. The best known one is to make use of the pinch temperature which is called *pinch* heuristics (see Linnhoff and Hindmarsh, 1983). However, it alone cannot solve difficult problems.

3.2.4 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 Hahne, 1986; 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 Δ T$_{min}$ or more and the heat capacity flowrate of a hot stream is less than or equal to the heat capacity flowrate of a cold stream, the match between these two streams is feasible. (Immediately above the pinch temperature, the heat capacity flowrate 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 Δ T$_{min}$ or more and the heat capacity flowrate of a hot stream is greater than equal to the heat capacity flowrate of a cold stream, the mach between these two streams is feasible. (Immediately below the pinch temperature, the heat capacity flowrate 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 fesibility must be determined by checking whether the minimum temperature difference of a match violates the minimum approach, ΔT$_{min}$, specific by the design.

3.2.5 Math Classification

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

3.2.5.1. 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)

3.2.5.2. Heat capacity flowrate (between hot and cold stream)
See Heuristic T.1 and T.2.

3.2.5.3. 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).

3.2.5.4. 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 reasoning 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.

3.2.6 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 Figures 3.4, 3.5, 3.6 and 3.7 respectively. Any eligible match must belong to one of the four match pattern classes.

Definition 3.1 Class A Match Pattern: The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the cold end of the cold stream. The residual heat load is on the hot portion of the cold stream. (See Figure 3.4)

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 an 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 3.4)

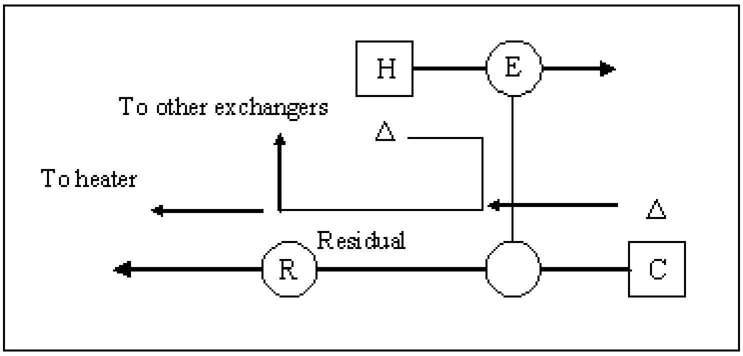


Figure 3.4: Class A Match Pattern

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 3.5)

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 3.4)

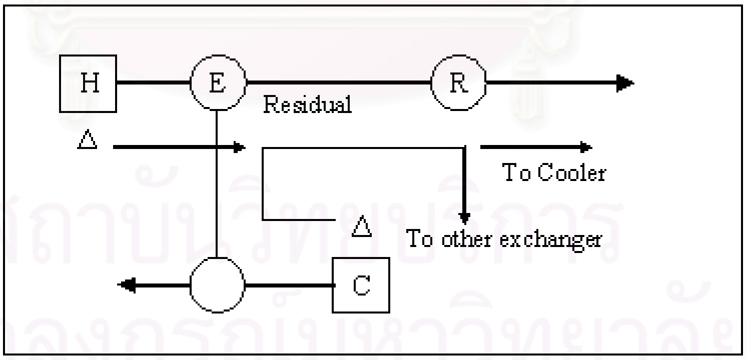


Figure 3.5: Class B Match Pattern

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 3.6)

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 3.5)

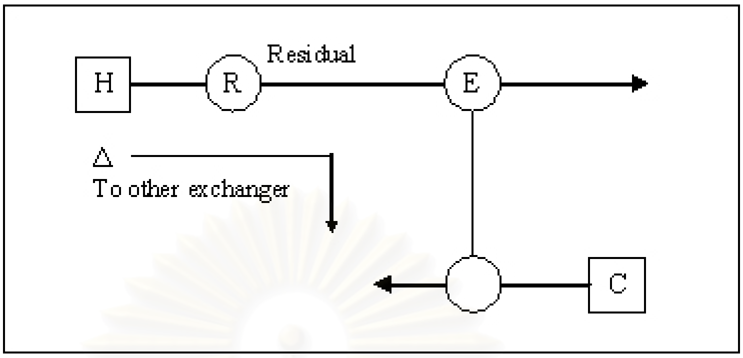


Figure 3.6: Class C Match Pattern

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 3.7)

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 3.5)

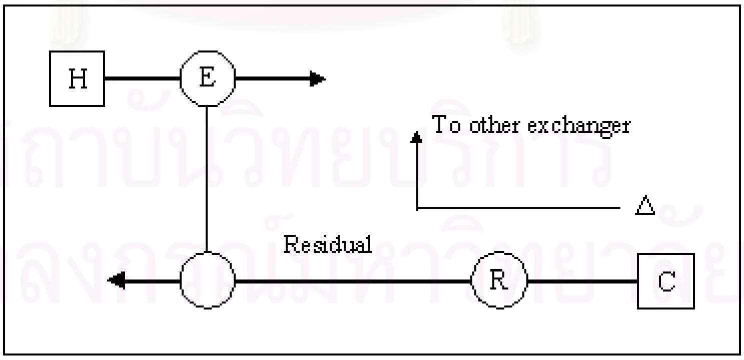
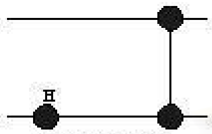
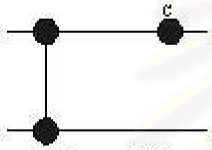
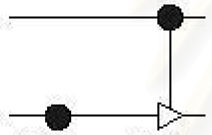
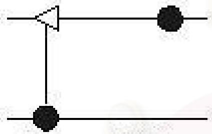
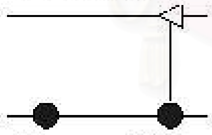
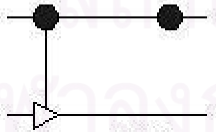


Figure 3.7: Class D Match Pattern

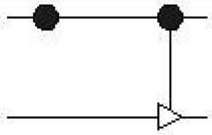
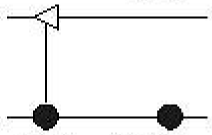
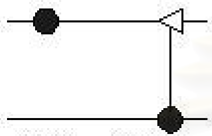
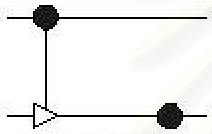
When the residual heat load in a match pattern is matched to a utility stream, it is closed or completed pattern. Otherwise, it is an open or incomplete pattern. It can be seen that if the heat load of the residual stream is less than the minimum heating or cooling requirement then the chances that the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

Table 3.4: Match Pattern Operators of Class A andB

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 $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$

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 3.5: Match Pattern Operators of Class C and D

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

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

** Cold stream temperatures are shifted up by ΔTmin.

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

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

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

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

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

We further discriminate match pattern according to heat capacity flowrate. By following pinch heuristic, in a heating problem, we prefer a match where the heat capacity flowrate of a cold stream is greater or equal to that of a hot stream.

For example, A[H]H is a match in which the heat capacity flow rate of the cold stream is matched to the heating utility.

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

In summary, the ranking of the match patterns in a heating problem are AH, A[H], B[H], C[H], D[C], C[C], and D[H]. For a cooling problem, BK, B[C], A[H], B[H], A[C] ,D[C] ,C[H] ,D[H] and C[C].(Wongsri, 1990)

3.2.7 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 Figures 3.8 and 3.9.

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).

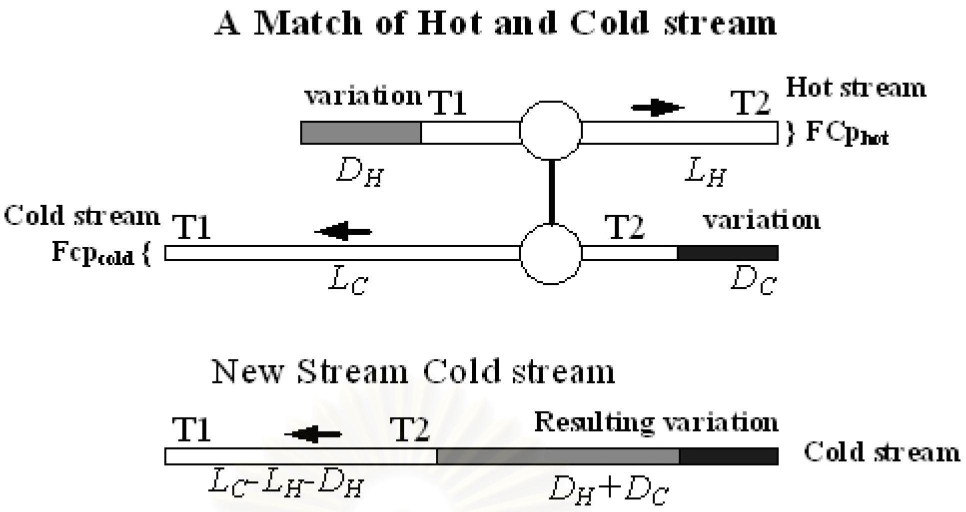


Figure 3.8: A Concept of Propagated Disturbance

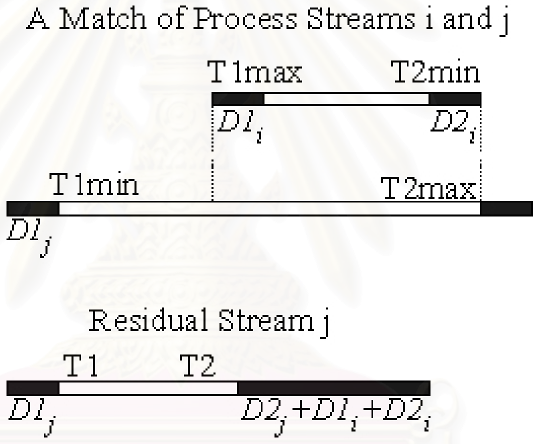


Figure 3.9: A General Concept of Propagated Disturbance

3.2.8 Synthesis Procedure

The synthesis of a resilient heat exchanger network by using (1) match patterns as operators in mapping one design state to the next and (2) heat load propagation technique can be done by the following systematic sequence:

1. Pop a match pattern operator from the ordered stack of match patterns. If all the patterns are chosen backtrack to the parent designed state and repeat the procedure. If the current state is the starting state and all patterns have been tried without success the problem cannot be solved with the current knowledge in the rule -based system. A trade-off between cost and resiliency may be needed.

2. Choose a pair of hot and cold streams from the set of unmatched process

streams. If all the streams have been chosen and none were satisfied, go back to the first step to try a new pattern.

3. Apply the match pattern to the selected pair of streams. If the streams satisfy the pattern test and the resiliency requirement, go to the next step. Otherwise go back to the previous step to select a new pair of streams.

Match pattern test: Check whether the heat load, input temperatures and heat flowrate capacity satisfy the match pattern description.

Resiliency test: Check whether the disturbance load of the smaller heat load stream can be shifted to the larger heat load stream.

4. Create a new state to support the new fact. A new state is a descendant of a current one. Change the parameters of the larger heat load stream: the supply or target temperature, the heat load the disturbance load

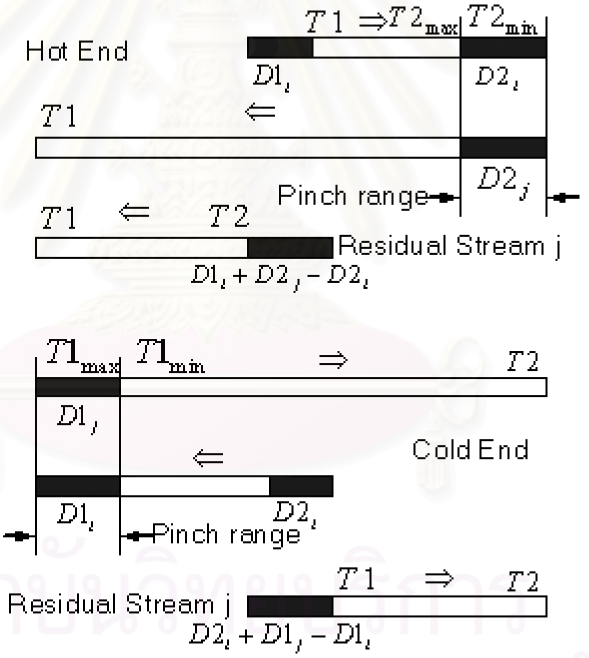


Figure 3.10: A Pinch Match on the Propagated Disturbance Concept

The new supply or target temperature will be adjusted according to the regular heat load and the disturbance heat load of the matched stream. The new heat load of the residual streams is the value between the supply and target temperatures at the design condition.

The new disturbance load is the sum of the disturbance load of both matched streams. A special treatment is needed for a pinch match or the match starts off from the pinch point. The new disturbance will be the sum of the upstream disturbance of a stream in the match pair and the difference between the pinch included disturbance of the two streams. See Figure 3.10.

For a pinch match of streams i and j for which $W_j > W_i$ and $L_j > L_i$ the disturbance of a residual stream:

$$D_j = D_i + (D_{jpinch} - D_{ipinch})$$

The disturbance at the pinch of the two streams must be deductive instead of being additive as in general case. Since the variations of the inlet temperature of stream j and outlet temperature of stream I are not independently varied but tied to the pinch temperature.

5. If there are unmatched hot and cold streams, go to the second step. Otherwise go to the next step.

6. Match the only hot or cold streams with the utility streams.

7. If there are other unused match patterns go to the first step. This is equivalent to saying that there might be other solutions available, continue.

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

3.3.1 Integrated Process

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

3.3.1.1 Material recycle

Material is recycled for six basic and important reasons.

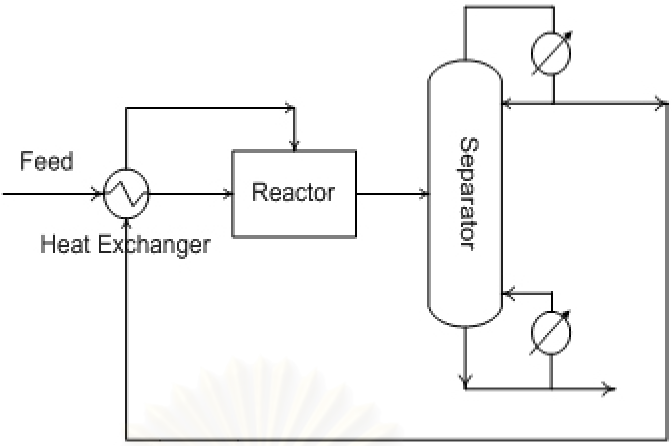


Figure 3.11: Integrated Process flowsheet

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 $A \rightarrow B \rightarrow C$, 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 inerts. 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 units, chemical component balancing is not a problem because exit streams from the unit automatically adjust their flows and composition. However, when 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 Procedure

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

The goals for an effective plantwide process control system include

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

3.3.3.1 Basic Concepts of Plantwide Control

1. *Buckley Basic*

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

(1.) Material balance control.

(2.) Production quality control.

He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loop is established, using the flowrates of liquid and gas process streams. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated as small as possible. The most level controllers should be proportional-only (P) to achieve flow smoothing. The time constants of the liquid level loops are a factor of 10 larger than the product-quality time constants.

2. *Douglas doctrines*

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

(1.) Minimize losses of reactants and products.

(2.) Maximize flowrates through gas recycle systems.

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

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

3. *Downs drill*

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

4. *Luyben laws*

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

(1.) All recycle loops should be flow controlled.

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

(3.) If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). Even if steady-state economics favor a liquid feed stream, the profitability of an operating plant with a product leaving the bottom of a column may be much better if the feed to column is vaporized.

5. *Richardson rule*

Bob Richardson suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense because it provides more muscle to achieve the desired control objective.

6. *Shinskey schemes*

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

7. *Tyreus tuning*

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

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

$$K_{ZN} = K_u/2.2 \qquad \tau_{ZN} = P_u/1.2$$
$$K_{TL} = K_u/3.2 \qquad \tau_{TL} = 2.2P_u$$

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

3.3.3.2 Step of Plantwide Process Control Design Procedure

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.

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

Count the number of control valves available.

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to setpoint. 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. minimize 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 function

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 transfer between process streams can create significant interaction. In the case of reactor feed/effluent heat exchangers it can lead to positive feedback and even instability.

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

Step 4: Set production rate

Establish the variable that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate.

To obtain higher production rate, we must increase overall reaction rates. This can be accomplished by raising temperature, increasing reactant concentrations, increasing reactor holdup, or increasing reactor pressure. The variable we select must be dominant for the reactor.

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

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

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

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

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

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

Fix a flow in every recycle loop and then select the best manipulated variables to control inventories.

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

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

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

Step 7: Check component balances

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

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

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

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations.

A tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor.

Step 9: Optimize economics or improve dynamic controllability

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

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

3.4 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provided we can independently manipulate the two inlet flowrates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom for temperature control. We can restore one of these degrees of freedom fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Fig.3.12.a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig 3.12.b.

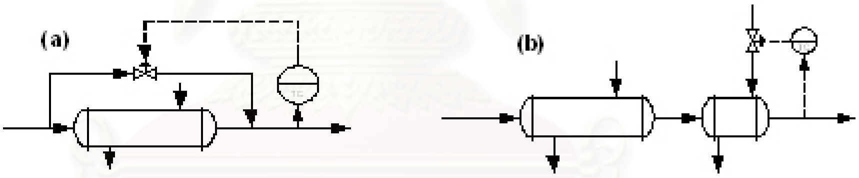


Figure 3.12: Control of P/P heat exchangers: (a) Use of bypass; (b) use of auxiliary utility exchanger.

3.4.1 Use of Bypass Control

When the bypass method is used for unit operation control, we have several choices about the bypass location and the control point. Figure 3.13 shows the most common alternatives. We may ask "Which option is the best? It depends on how we define "best". As with many other examples, it boils down to a trade-off between design and control. Design considerations might suggest we measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high-temperature service. Cost considerations would also suggest a small bypass flow to minimize the exchanger and control valve sizes. From a control standpoint we should measure the most important stream, regardless of temperature, and bypass on the same side as we control. This minimizes the effects of exchanger dynamics in the loop. We should also want to bypass a large fraction of the controlled stream since it improves the control range. This requires a large heat exchanger.

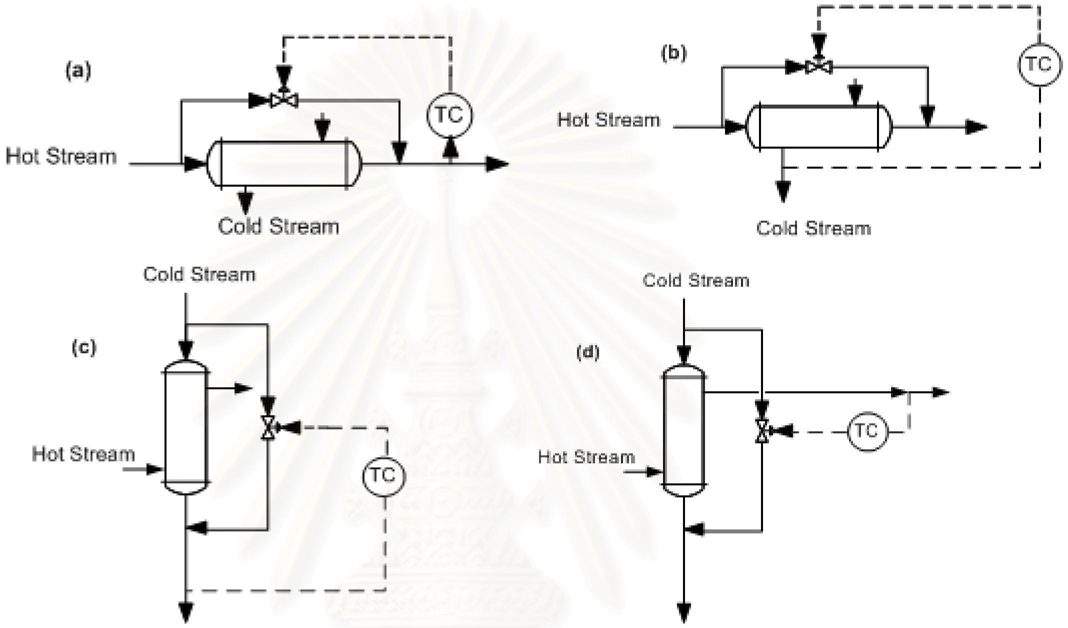


Figure 3.13: Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

3.4.2 Use of auxiliary utility exchangers

When the P/P exchanger is combined with a utility exchanger, we also have a few design decisions to make. We must first establish the relative sizes between the recovery and the utility exchangers. From a design standpoint we would like to make the recovery exchanger large and the utility exchanger small. This gives us the most heat recovery, and it is also the least expensive alternative from an investment standpoint. However, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control standpoint.

Next, we must decide how to combine the utility exchanger with the P/P exchanger. This could be done either in a series or parallel arrangement. Physical implementation issues may dictate this choice but it could affect controllability. Finally, we have to decide hoe to control the utility exchanger for best overall control performance. Consider a distillation column that uses a large amount of high-pressure stream in its thermo siphon reboiler. To reduce operating costs we would like to heat-integrate this column with the reactor. A practical way of doing this is to generate stream in a waste heat boiler connected to the reactor as suggested. We can then use some or all of this steam to help reboil the column by condensing the stream in the tubes of a stab-in reboiler. However, the total heat from the reactor may not be enough to reboil the column, so the remaining heat must come from the thermo siphon reboiler that now serves as an auxiliary reboiler. The column tray temperature controller would manipulate the stream to the thermo siphon reboiler.

3.5 Cascade Control

One of the most useful concepts in advanced control is cascade control. A cascade control structure has two feedback controllers with the output of the primary (or master) controller changing the setpoint of the secondary (or slave) controller. The output of the secondary goes to the slave.

There are two purposes for cascade control: (1) to eliminate the effects of some disturbances, and (2) to improve the dynamic performance of the control loop.

To illustrate the disturbance rejection effect, consider the distillation column reboiler. Suppose the steam supply pressure increases. The pressure drop over the control valve will be larger, so the steam flow rate will increase. With the single-loop temperature controller, no correction will be made until the higher steam flow rate increases the vapor boilup and the higher vapor rate begins to rise the temperature on tray. Thus the whole system is disturbed by a supply-steam pressure change

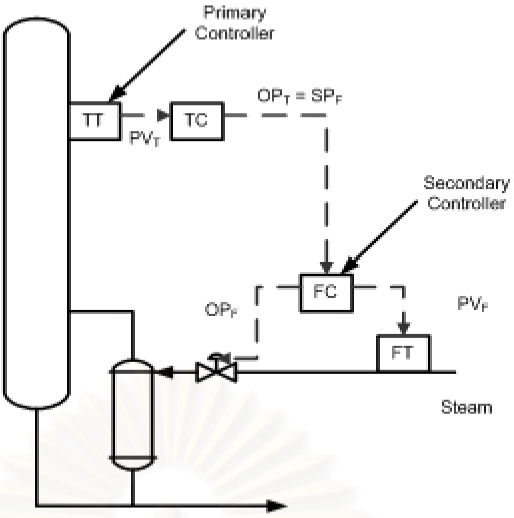


Figure 3.14: Cascade control in distillation-column-reboiler.

With the cascade control system, the steam flow controller will immediately see the increase in steam flow and will pinch back on the steam valve to return the steam flow rate to its setpoint. Thus the reboiler and the column are only slightly affected by the steam supply-pressure disturbance.

Figure 3.14 shows another common system where cascade control is used. The reactor temperature controller is the primary controller; the jacket temperature controller is the secondary controller. The reactor temperature control is isolated by the cascade system from disturbances in cooling-water inlet temperature and supply pressure.

CHAPTER IV

ISOMERIZATION PROCESS

4.1 Process Description

The isomerization 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 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 isobutene 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 isobutene (iC_4).

$$\text{nC4} \longrightarrow \text{iC4}$$

The reaction of nC_4 to iC_4 occurs in the vapor phase and is run at elevated temperatures (400 ^{0}F) 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 a high reflux ratio (7) are required. For the design case considered, this column ends up being16 feet in diameter. This column is called a deisobutanizer (DIB)

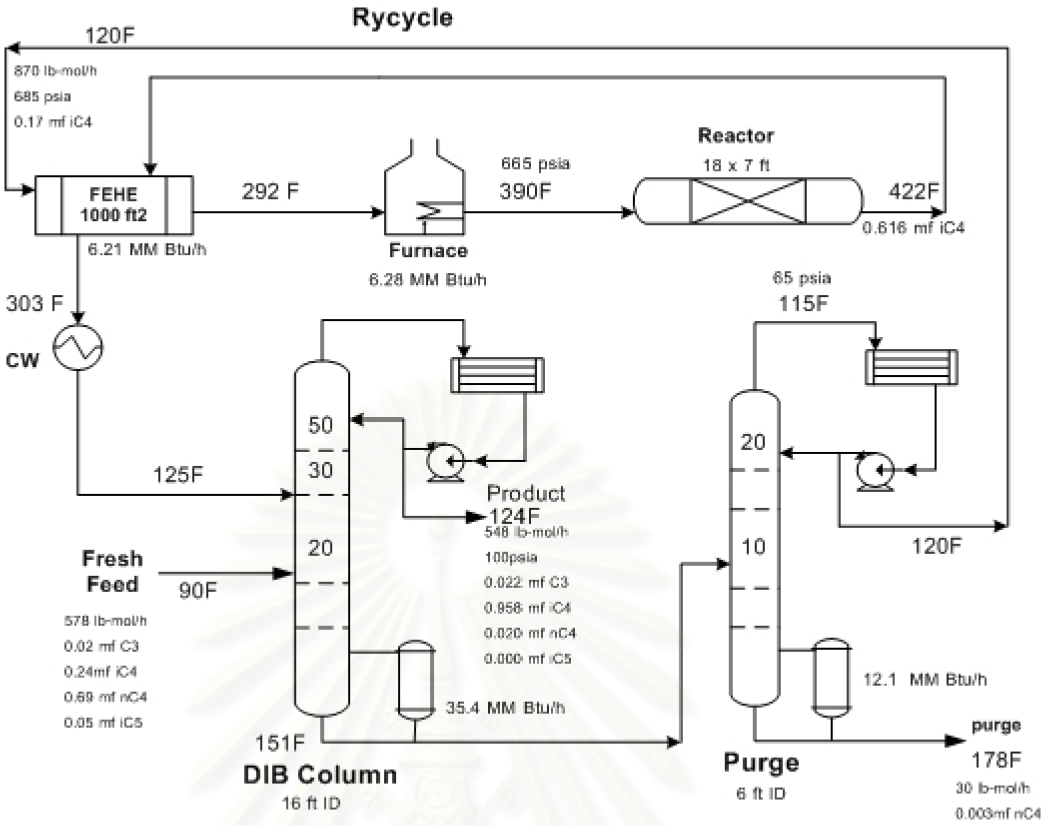


Figure 4.1: The butane isomerization process (Plantwide Process Control, 1998)

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 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 ^{0}F). The base temperature is 150 ^{0}F, so low-pressure stream can be used.

The distillate product from the DIB is the isobutene 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.

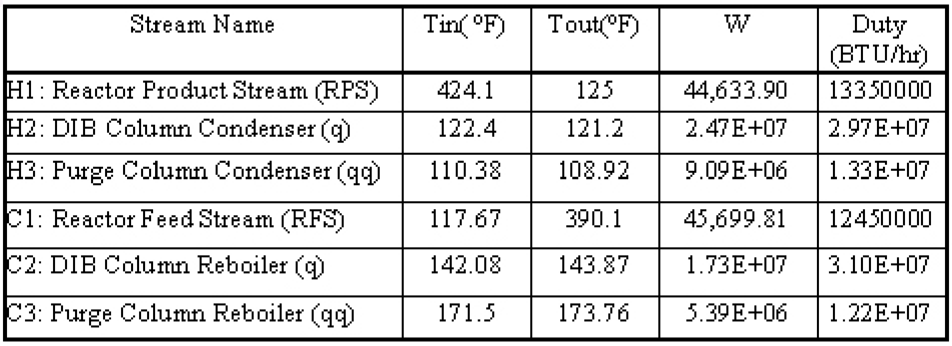
The bottoms from the DIB contains most of the nC_4, along with some iC_4 impurity and all of the heavy isopentane impurity. Since this heavy component will build up in the process unless it is removed, a second distillation column is used to purge out a small stream that contains the isopentane. Some 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 report, only reactor inlet and exit conditions. We consider that the reaction is irreversible. An activation energy of 30,000Btu/lb.mol is used, and the preexponential factor is adjusted to give the same conversation reported in the SRI report. Table A.1 gives stream data for the butane isomerization process. Table A.5 and Table A.6 list the process parameter value

4.2 Design of heat exchanger networks

At this point, the heat exchanger network design method provided 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



Stream Name	Tin(°F)	Tout(°F)	W	Duty (BTU/hr)
H1 : Reactor Product Stream (RPS)	424.1	125	44,633.90	13350000
H2: DIB Column Condenser (q)	122.4	121.2	2.47E+07	2.97E+07
H3: Purge Column Condenser (qq)	110.38	108.92	9.09E+06	1.33E+07
C1: Reactor Feed Stream (RFS)	117.67	390.1	45,699.81	12450000
C2: DIB Column Reboiler (q)	142.08	143.87	1.73E+07	3.10E+07
C3: Purge Column Reboiler (qq)	171.5	173.76	5.39E+06	1.22E+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 only two streams in the network. We can not find Pinch temperature using Problem table method, because no heat integration.

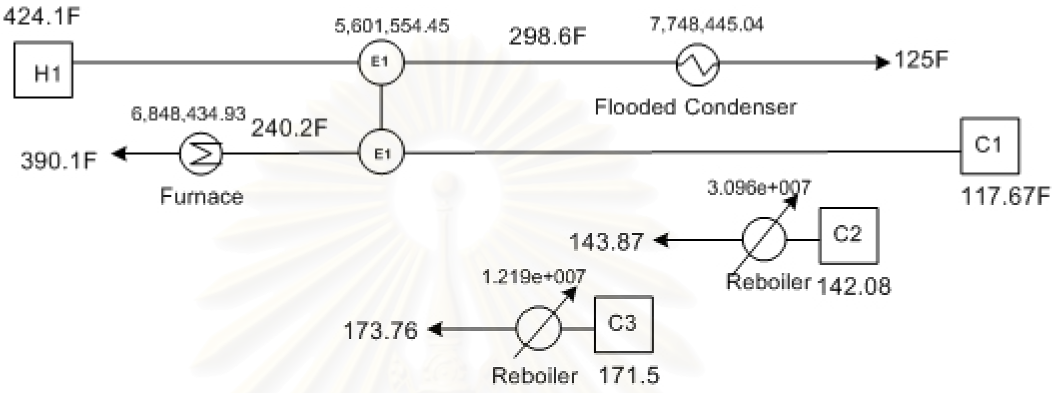


Figure 4.2: The heat exchanger network, Base Case

4.2.2 RHEN Alternative 1

There are three streams in the network. So we can find Pinch temperature using Problem table method as shown in Table 4.4. At the minimum heat load condition, the pinch temperature occurs at 137.67/117.67 ^{0}F. The minimum utility requirements have been predicted 30.626x 10^6 Btu/hr of hot utilities and 5.655 x 10^5 Btu/hr of cold utilities.

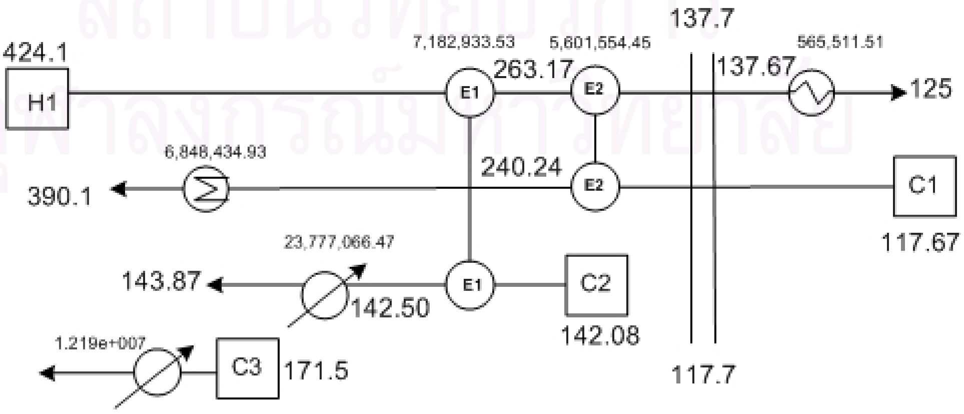


Figure 4.3: The resilient heat exchanger network, alternative 1

The synthesis procedure using the disturbance propagation method and math pattern is shown in Table 4.3. Figure 4.3 shows a design of resilient heat exchanger network for Butane Isomerization process alternative 1. In our case as shown in Fig.4.3, the minimum temperature difference in the process-to-process-heat-exchangers, ΔT_{min} is set to 20 ^{0}F.

Table 4.2:Process stream data for alternative 1

Alt 2	Pinch at 137.7/117.7(°F)				
		Tsupply (°F)			Ttarget (°F)
stream	W (Btu/hr-°F)	Nominal	Max	Min	Nominal
H1	44,633.90	424.1	444.1	404.1	125
C1	45,699.80	117.67	137.67	117.67	390.1
C2	17,296,089.39	142.08	143.08	141.08	143.87

Synthesis Table For Cold End Of Alternative 1							
Stream	Load	W	T1	T2	D1	D2	Action
a) State 1							
H1	565,511.51	44,633.90	137.67	125	892,678	0	Selected B[H]
C1	0	45,699.80	117.67	117.67	0	913,996	Selected
b) State 2							
H1	565,511.51	44,633.90	137.67	125	21,318	0	To Cooler
C1							

Synthesis Table For Hot End Of Alternative 1							
Stream	Load	W	T1	T2	D1	D2	Action
a) State 1							
H1	11,891,809.98	44,633.90	404.10	137.67	892,678	892,678	Selected C[H]
C1	11,536,000.51	45,699.80	137.67	390.1	913,996	0	Selected
C2	13,663,910.62	17,296,089.39	143.08	143.87	17,296,089.39	0	
b) State 2							
H1	6,290,255.53	44,633.90	404.10	263.17	892,678	0	Selected AH
C1	5,934,446.06	45,699.80	260.24	390.10	0	21,318	To Heater
C2	13,663,910.62	17,296,089.39	143.08	143.87	17,296,089.39	0	Selected
c) State 3							
H1							Matched To C2
C2	7,373,655.09	17,296,089.39	143.51	143.87	18,188,767.39	0	To Heater

Table 4.4:Problem table for alternative 1

W			T hot	T cold	ΔT	Sum W	Require	Interval (H)	Cascade	Sum Interval
h1	c1	c2								
0	0	0	424.1	404.1			Qh			
44,633.90	0.00	0	410.1	390.1	14	44,633.90	0.00	624,874.60	624,874.60	624,874.60
44,633.90	45,699.80	0	298.6	278.6	111.5	-1,065.90	31,250,383.14	-118,847.85	31,131,535.29	506,026.75
44,633.90	45,699.80	0	284	264	14.6	-1,065.90	31,131,535.29	-15,562.14	31,115,973.15	490,464.61
44,633.90	45,699.80	0	163.87	143.87	120.13	-1,065.90	31,115,973.15	-128,046.57	30,987,926.58	362,418.04
44,633.90	45,699.80	1.73 E+07	162.43	142.43	1.44	-17,297,155	30,987,926.58	-24,907,903.61	6,080,022.97	-24,545,485.57
44,633.90	45,699.80	1.73 E+07	162.08	142.08	0.35	-17,297,155	6,080,022.97	-6,054,004.35	26,018.62	-30,599,489.92
44,633.90	45,699.80	0	161.43	141.43	0.65	-1,065.90	26,018.62	-692.84	25,325.78	-30,600,182.75
44,633.90	45,699.80	0	137.67	117.67	23.76	-1,065.90	25,325.78	-25,325.78	0.00	**-30,625,508.54**
44,633.90	0	0	125	105	12.67	44,633.90	0.00	565,511.51	565,511.51	-30,059,997.02
									Qc	

4.2.3 RHEN Alternative 2

There are three streams in the network. So we can find Pinch temperature using Problem table method as shown in Table 4.7. At the minimum heat load condition the pinch temperature occurs at 137.67/117.67 ^{0}F. The minimum utility requirements have been predicted 11.856 x 10^6 Btu/hr of hot utilities and 5.655 x 10^5 Btu/hr of cold utilities.

The synthesis procedure using the disturbance propagation method and math patterns is shown in Table 4.6. Figure 4.4 shows a design of resilient heat exchanger network for Butane Isomerization Process alternative 2. In our case as shown in Fig.4.4, the minimum temperature difference in the process-to-process-heat-exchangers, ΔT_{min} is set to 20 ^{0}F.

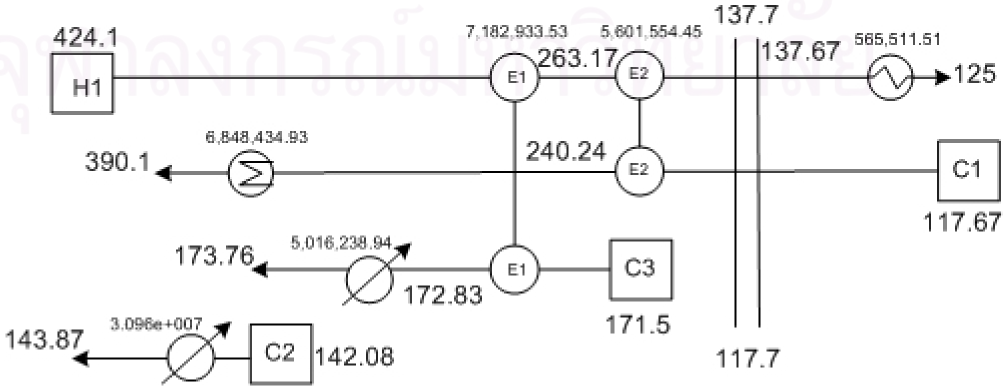


Figure 4.4: The resilient heat exchanger network, alternative 2

Table 4.5:Process stream data for alternative 2

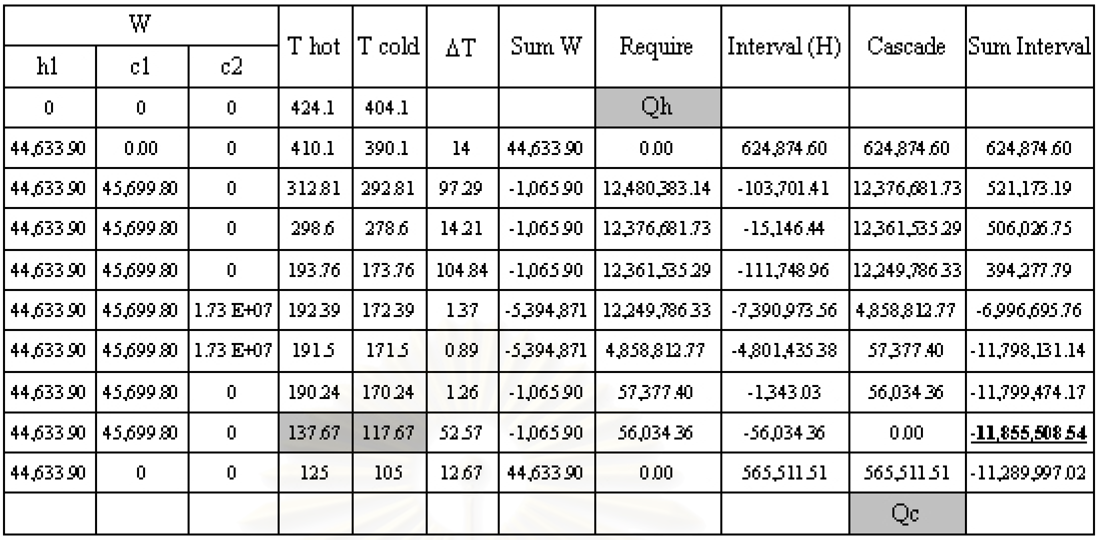
Alt 3	Pinch at 137.7/117.7(°F)				
		Tsupply (°F)			Ttarget (°F)
stream	W (Btu/hr-°F)	Nominal	Max	Min	Nominal
H1	44,633.90	424.1	444.1	404.1	125
C1	45,699.80	117.67	137.67	117.67	390.1
C3	5,393,805.31	171.5	172.5	170.5	173.76

T

Synthesis Table For Cold End Of Alternative 2							
Stream	Load	W	T1	T2	D1	D2	Action
a) State 1							
H1	565,511.51	44,633.90	137.67	125	892,678	0	Selected [BH]
C1	0	45,699.80	117.67	117.67	0	913,996	Selected
b) State 2							
H1	565,511.51	44,633.90	137.67	125	21,318	0	To Cooler
C1							

Synthesis Table For Hot End Of Alternative 2							
Stream	Load	W	T1	T2	D1	D2	Action
a) State 1							
H1	11,891,809.98	44,633.90	404.10	137.67	892,678	892,678	Selected C[H]
C1	11,536,000.51	45,699.80	137.67	390.1	913,996	0	Selected
C3	6,796,194.69	5,393,805.31	172.5	173.76	5,393,805.31		
b) State2							
H1	6,290,255.53	44,633.90	404.10	263.17	892,678	0	Selected AH
C1	5,934,446.06	45,699.80	260.24	390.10	0	21,318	To Heater
C3	6,796,194.69	5,393,805.31	172.50	173.76	5,393,805.31	0	Selected
c) State 3							
H1							Matched To C3
C3	505,939.16	5,393,805.31	172.59	173.76	6,286,483.31	0	To Heater

Table 4.7:Problem table for alternative 2



W			T hot	T cold	ΔT	Sum W	Require	Interval (H)	Cascade	Sum Interval
h1	c1	c2								
0	0	0	424.1	404.1			Qh			
44,633.90	0.00	0	410.1	390.1	14	44,633.90	0.00	624,874.60	624,874.60	624,874.60
44,633.90	45,699.80	0	312.81	292.81	97.29	-1,065.90	12,480,383.14	-103,701.41	12,376,681.73	521,173.19
44,633.90	45,699.80	0	298.6	278.6	14.21	-1,065.90	12,376,681.73	-15,146.44	12,361,535.29	506,026.75
44,633.90	45,699.80	0	193.76	173.76	104.84	-1,065.90	12,361,535.29	-111,748.96	12,249,786.33	394,277.79
44,633.90	45,699.80	1.73 E+07	192.39	172.39	1.37	-5,394,871	12,249,786.33	-7,390,973.56	4,858,812.77	-6,996,695.76
44,633.90	45,699.80	1.73 E+07	191.5	171.5	0.89	-5,394,871	4,858,812.77	-4,801,435.38	57,377.40	-11,798,131.14
44,633.90	45,699.80	0	190.24	170.24	1.26	-1,065.90	57,377.40	-1,343.03	56,034.36	-11,799,474.17
44,633.90	45,699.80	0	137.67	117.67	52.57	-1,065.90	56,034.36	-56,034.36	0.00	**-11,855,508.54**
44,633.90	0	0	125	105	12.67	44,633.90	0.00	565,511.51	565,511.51	-11,289,997.02
									Qc	

4.3 The Butane Isomerization Alternatives

Two alternatives of heat exchanger networks (HEN) designs of the Butane Isomerization plant are proposed both, used the heat from the reactor effluent stream to provide the heat for the column reboiler.

In Butane Isomerization process (Figure 4.5) with no energy integration, we use 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.

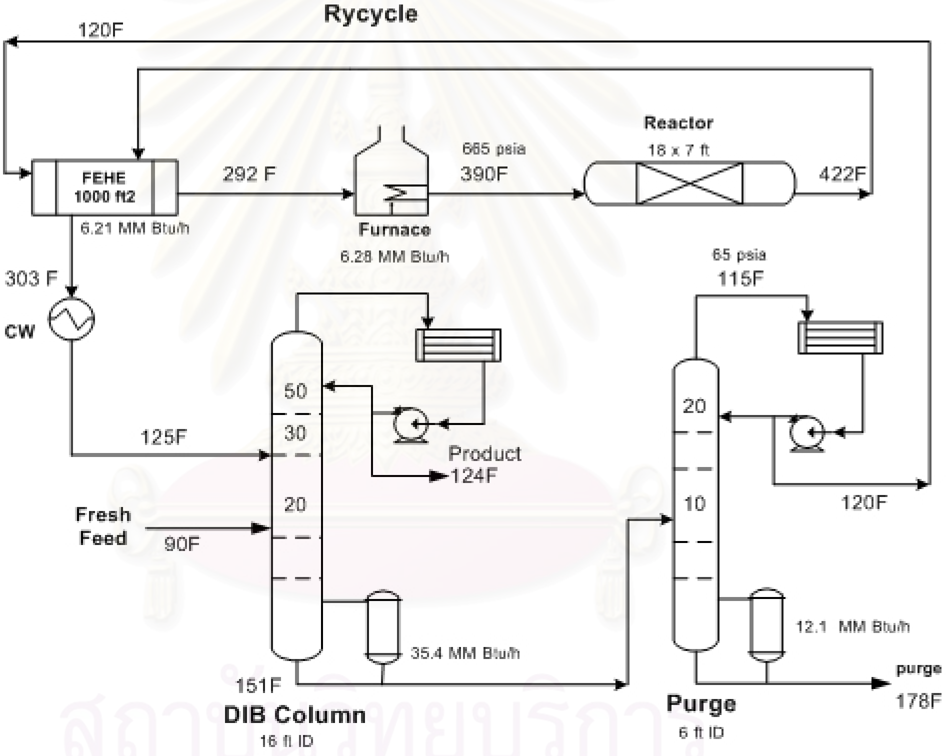


Figure 4.5: Butane Isomerization process-Base Case

In alternative 1 has two heat exchangers for preheat feed and the reboiler in the DIB column is driven by the reactor effluent stream. In this work, the DIB column is added an auxiliary reboiler to supply the heat, because the total heat from the reactor isn't enough to reboil the column as in Figure 4.6.

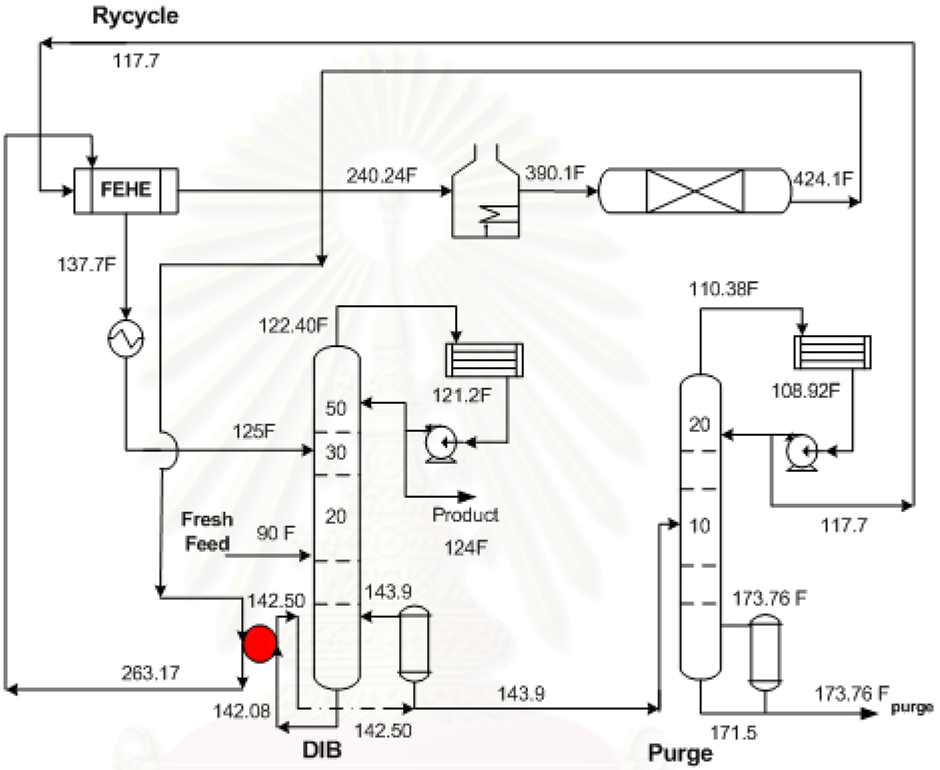


Figure 4.6: Butane Isomerization process-alternative 1

In alternative 2 has two heat exchangers for preheat feed and the reboiler in the Purge column is driven by the reactor effluent stream. In this work, the Purge column is added an auxiliary reboiler to supply the heat, because the total heat from the reactor isn't enough to reboil the column as in Figure 4.7.

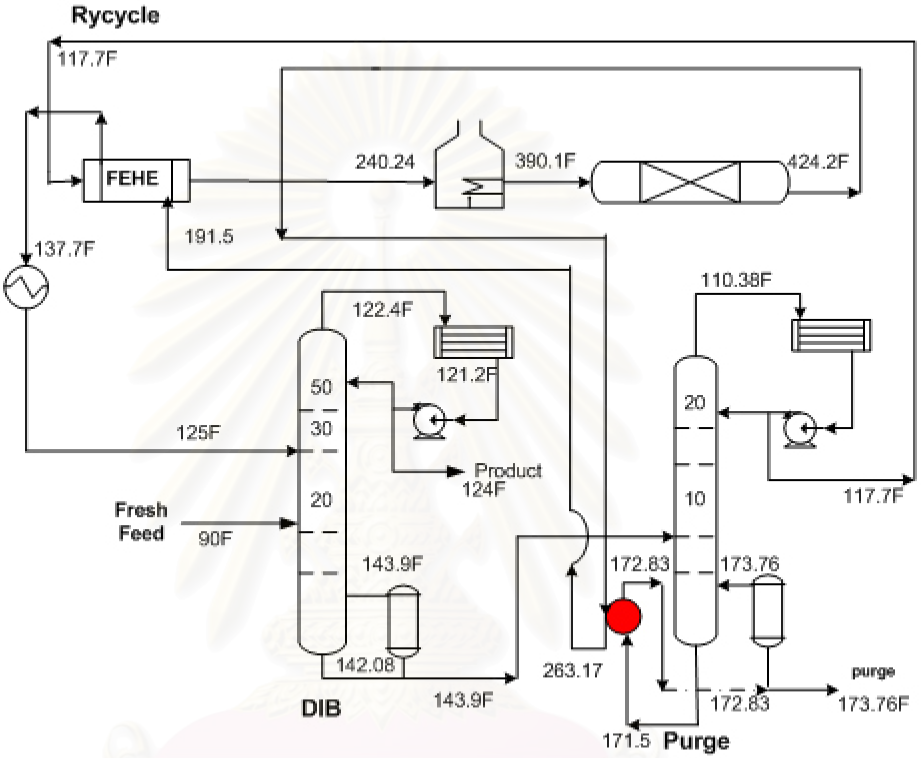
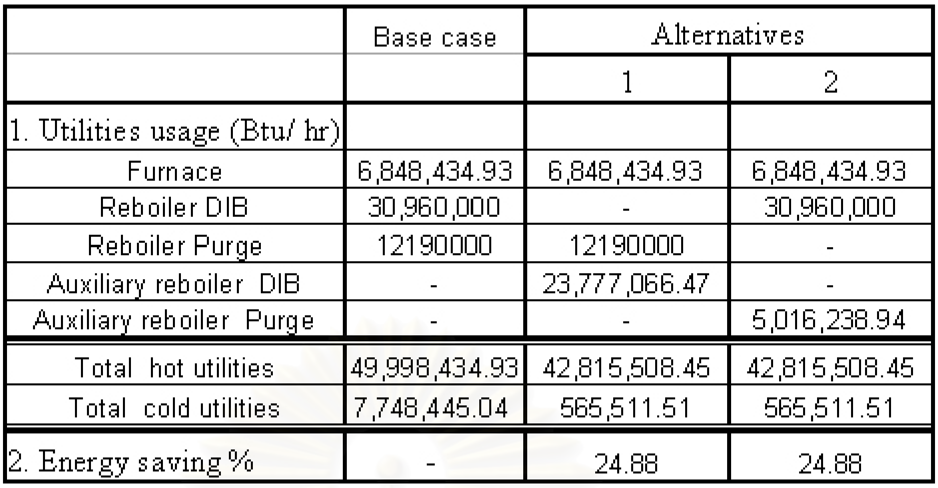


Figure 4.7: Butane Isomerization process-alternative 2

From Tables 4.8, we see that when we install the various heat-exchanger network alternatives on the base-case design for the Butane Isomerization processes, the energy saved is 24.88% from the design without heat integration.

Table 4.8:Energy integration for Butane Isomerization process



	Base case	Alternatives	
		1	2
1. Utilities usage (Btu/ hr)			
Furnace	6,848,434.93	6,848,434.93	6,848,434.93
Reboiler DIB	30,960,000	-	30,960,000
Reboiler Purge	12190000	12190000	-
Auxiliary reboiler DIB	-	23,777,066.47	-
Auxiliary reboiler Purge	-	-	5,016,238.94
Total hot utilities	49,998,434.93	42,815,508.45	42,815,508.45
Total cold utilities	7,748,445.04	565,511.51	565,511.51
2. Energy saving %	-	24.88	24.88

4.4 Steady-State Modeling

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Luyben et al. (1998) and Poothanakul P. (2002). 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 4.8 shows the HYSYS flowsheet of Butane Isomerization process (Base Case). The steady state simulation results are summarized in Table A.1 and Figure 4.9. For the comparison, the steady state simulation results given by Poothanakul P. (2002) are also listed in Table A.2.

Since there are three material recycle streams in Butane isomerization process alternative1, three recycle modules are inserted in the streams: hot stream to FEHE, the recycle stream to the reactor and DIB-Feed. Proper initial values should be chosen for these streams; otherwise the iterative calculations might converge to another steady state due to the non-linearity and unstable characteristics of the process.

All of the three columns are simulated using the "distillation column" module. When columns are modeled in steady state, besides the specification of inlet streams, pressure profiles, number of trays and feed tray, two additional variables should be additionally specified for columns with condenser or reboiler. These could be the duties, reflux rate, draw stream rates, composition fraction, etc. We chose to specify a priori overhead and bottom component mole fraction for all columns. These mole fractions are specified to meet the required purity of product given in Luyben et al. (1998) and Poothanakul P. (2002). The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on sieve trays. The column specifications of Butane Isomeriazation process (Base Case) are given in Table A.5. Although the tray diameter and spacing, weir length and height are not required for steady state modeling, they are required for dynamic simulation.

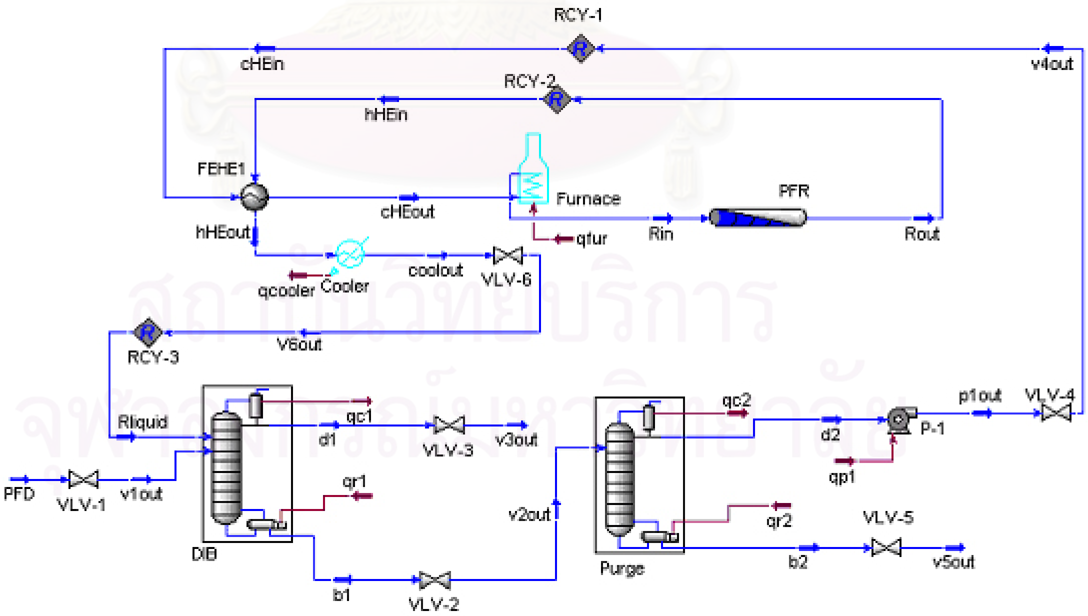


Figure 4.8: The simulated Butane isomerization process (Base Case) at steady-state by HYSYS

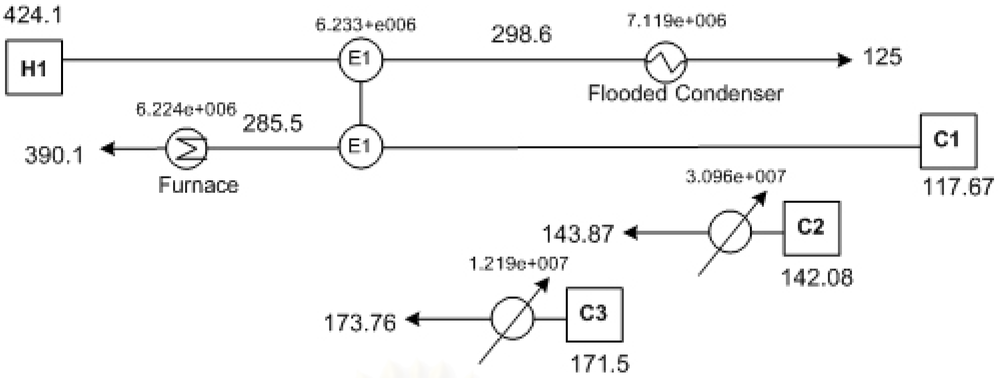


Figure 4.9: The steady state simulation results of heat exchanger network, Base Case

4.4.2 Steady State Simulation of Butane Isomerization Process Alternatives 1 and 2

The steady state simulation results of Butane Isomerization process (Base Case) have been compared with the earlier study by Poothanakul P. (2002) and the results are found consistent with those in the earlier study. Then, considering the consistency of the simulation results of the butane isomerization process (Base Case) with respect to the previous work, the other alternatives considered in this work, i.e. alternatives 1 and 2 are also developed in the HYSYS software environment. Figures 4.12 and 4.13 show the HYSYS flowsheets of the butane isomerization process with energy integration schemes for alternatives 1 and 2. The selected process streams data for these alternatives are not included in this chapter but listed in Appendix A. The steady state simulation results are shown in Figures 4.10 and 4.11.

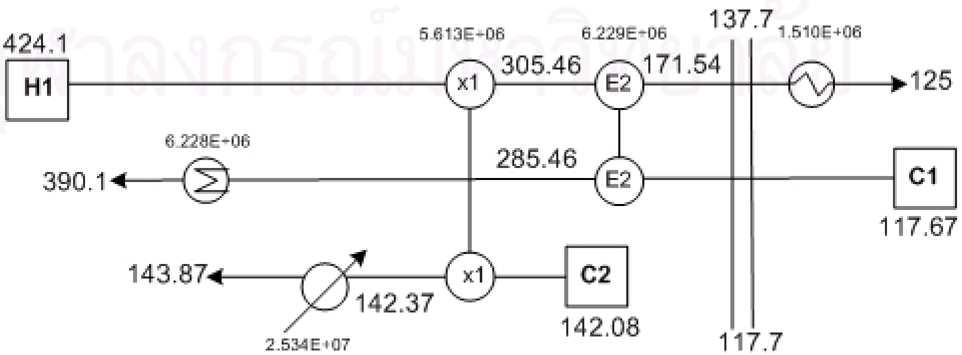


Figure 4.10: The steady state simulation results of resilient heat exchanger network, alternative 1

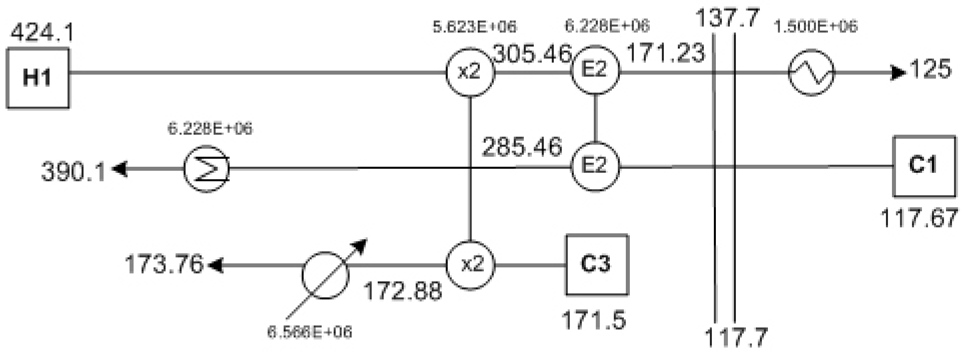


Figure 4.11: The steady state simulation results of resilient heat exchanger network, alternative 2

In alternative 1, there are two FEHEs and additionally the reboiler in the DIB column is driven by the reactor effluent stream, whereas in alternative 2, the reboiler in the purge column is driven by the reactor effluent stream.

Several RECYCLE modules should be inserted in the streams for these alternatives in the simulations. The numbers of RECYCLE modules are 6 for alternatives 1 and 2. As the earlier explanation, proper initial values should be chosen for these streams; otherwise the iterative calculations might converge to another steady state due to the non-linearity and unstable characteristics of the process.

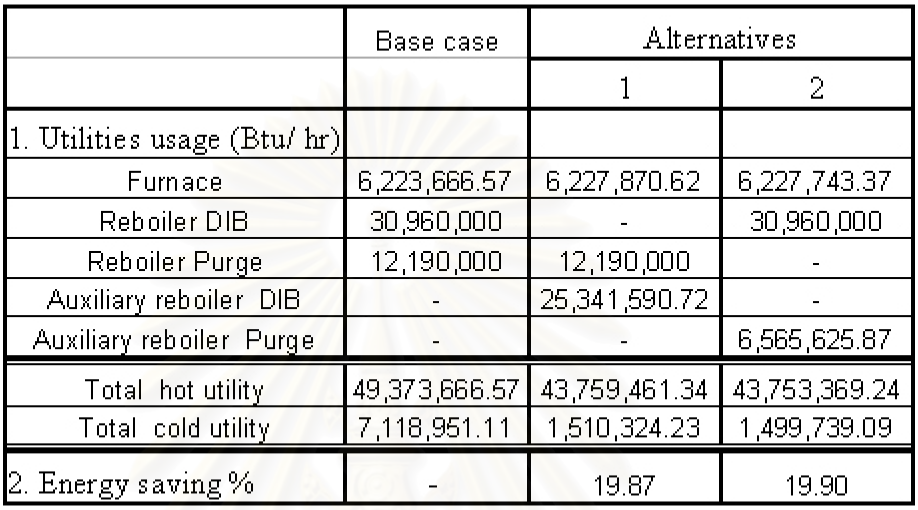
All process-to-process heat exchangers are simulated using a heat exchanger with a hot stream on the shell side and a cold stream on the tube side. Note that, a minimum ΔT of about 20 ^{0}F is assumed for all process-to-process heat exchangers.

The DIB column for alternative 1 is simulated using a "refluxed absorber" that it does not include a reboiler, and for alternative 2, it is simulated using the "distillation column" module. Purge column is simulated using a "refluxed absorber" with no reboiler for alternative 2, where as alternative 1 is simulated using the "distillation column" module. Since a "refluxed 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 and 2, a tank is needed to accommodate liquid from the bottoms of DIB column and Purge column, respectively.

Those steady state simulation results (alternatives 1 and 2) indicate that the energy saved is 19.87% from the base case heat consumption as shown in Table 4.9.

Table 4.9:Energy integration for Butane Isomerization process (steady state simulation)



	Base case	Alternatives	
		1	2
1. Utilities usage (Btu/ hr)			
Furnace	6,223,666.57	6,227,870.62	6,227,743.37
Reboiler DIB	30,960,000	-	30,960,000
Reboiler Purge	12,190,000	12,190,000	-
Auxiliary reboiler DIB	-	25,341,590.72	-
Auxiliary reboiler Purge	-	-	6,565,625.87
Total hot utility	49,373,666.57	43,759,461.34	43,753,369.24
Total cold utility	7,118,951.11	1,510,324.23	1,499,739.09
2. Energy saving %	-	19.87	19.90

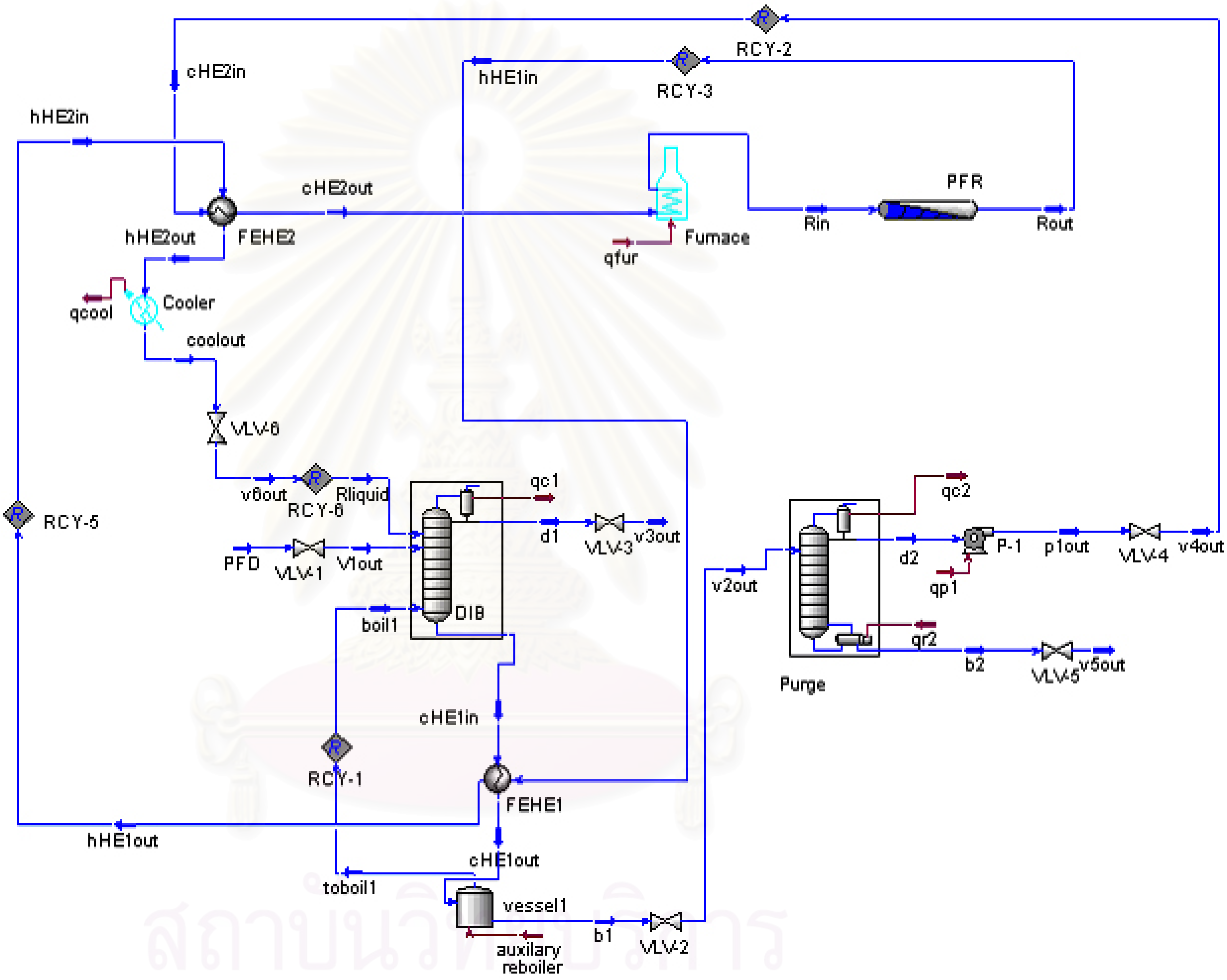


Figure 4.12: The simulated Butane isomerization process (alt.1) at steady-state by HYSYS

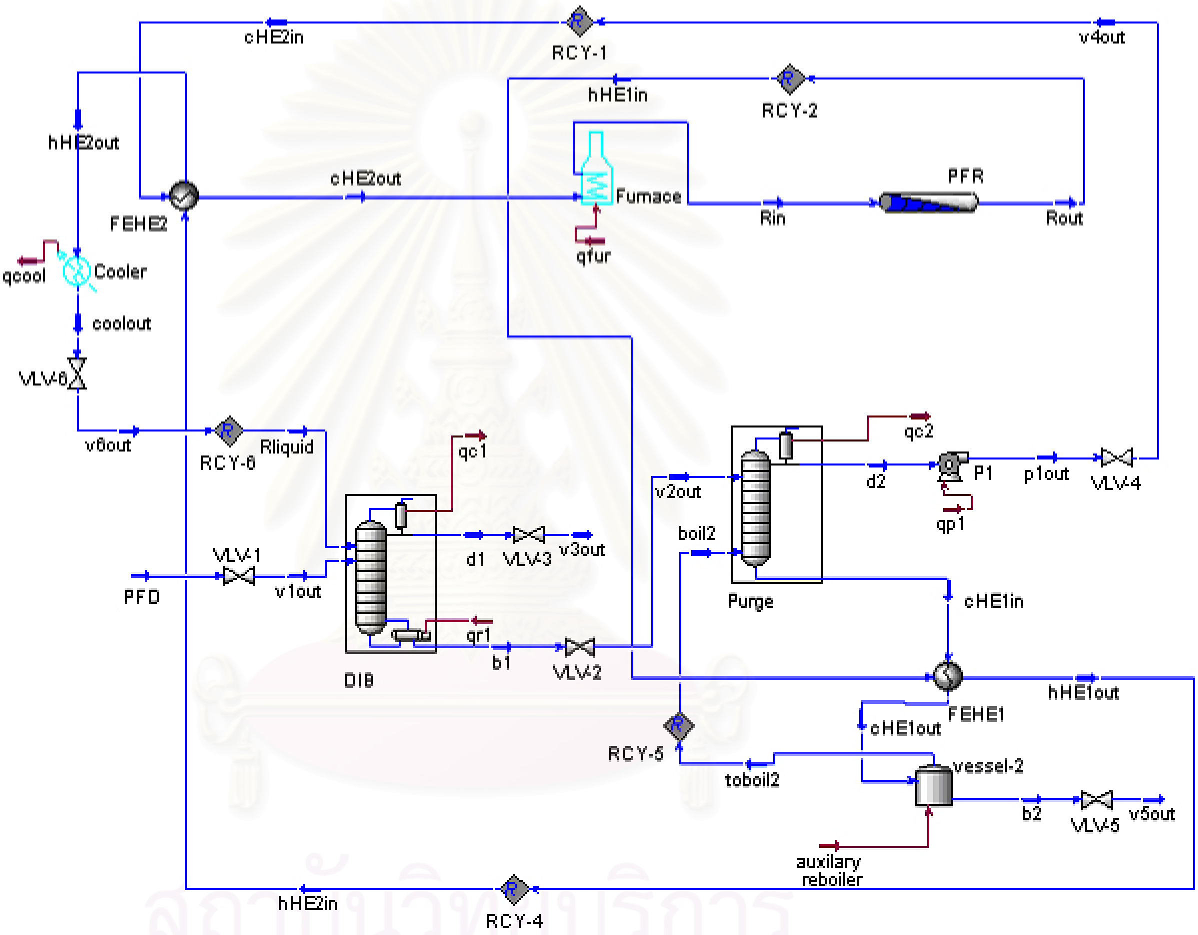


Figure 4.13: The simulated Butane isomerization process (alt.2) at steady-state by HYSYS

CHAPTER IV

CONTROL STRUCTURE DESIGE

5.1 Plantwide control design procedure

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 by 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

This process has 14 control degrees. They include fresh feed value; DIB column stream, cooling water, reflux, distillate, and bottoms valves; Purge column stream, cooling water, reflux, distillate, and bottoms valve; furnace fuel valve; flooded condenser cooling water valve; and DIB column feed valve.

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 ^{0}F 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 affluent is used to heat the reactor feed and no furnace is used. Therefore, a furnace is required to bring the reactor inlet temperature 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 the heat exchanger, the smaller the 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 ^{0}F) at the pressure in the reactor section (685 psia). As this stream is heated to the required reactor inlet temperature of 390 ^{0}F, it begins to vaporize. It is superheated vapor when fed into the reactor (390 ^{0}F at 665 psia). When a small FEHE is used, the exit temperature is 292 ^{0}F 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.

Step 4. : 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.

$$R = k_F V_R C_{nC4}$$

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. In this case the reaction rate increases by 20 percent for a 10 ^{0}F change in temperature. 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:

$$R = k_F V_R C_{nC4} - k_R V_R C_{iC4}$$

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 nC4 and iC4 dominate the rate through the relationship imposed by the equilibrium constant Keq = C_{iC4} / 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 stare. The choices for the control system made in Steps 6 and 7 must recognize this relationship between production rate and freash 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 choices 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. Because the reflux ratio is high, control of reflux drum level using level using distillate flow may be ineffective, particularly if the distillate were going directly to a downstream process. If we decide to 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 columns respond more quickly to vapor rate changes than to changes in liquid rates. Therefore, we select reboiler heat input to control nC_4 impurity in the distillate. This may seem like a poor choice 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 vale. Based 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. DIB column reflux drum level is controlled by manipulating distillate product 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.

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, however, 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; purged 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.

An obvious question at this point is ”Why don’t we just flow control the fresh feed into the process?” If we did this, we could not fix the flowrate in the recycle loop. For example, suppose we select the following control structure: fix fresh feed flowrate, control DIB column base level with DIB bottoms, control purge column base level with heat input, and control purge column reflux drum level with distillate. This structure is intuitively attractive and permits us to fix the production rate directly by setting the fresh feed flowrate. However, only level controllers set the flows around the recycle loop, so we would expect problems with snowballing. Flow disturbances can propagate around the liquid recycle loop

Step 7. : Check component balances

Four components need to be accounted for. 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 only component that is trapped inside the system and must be consumed by the reaction is the nC_4. The composition controller on the DIB distillate stream permits only a small amount (2mol%) of the nC_4 to leave in the product stream. The purge stream from the bottom of the purge column permits only a small amount of the nC_4 to escape. This purge stream can be simple flow-controlled if we don't mind losing a small amount of the nC_4 with the iC_5 purge. If the amount of the iC_5 in the fresh feed is small, this may be the simplest strategy and may have little economic penalty. Alternatively we could control the amount of the nC_4 in the purge column bottoms by manipulating bottom flowrate. Since there is a fairly large temperature change in the purge column, controlling the temperature on a suitable tray (tray 2) may be more practical since it eliminates the need for an on-line analyzer. In the simulations given later in this chapter, we adopt the simple strategy of flow-controlling the purge stream.

The amount of reactant the nC4 fed into the system must somehow be exactly balanced 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 flowrate should be increased because we are consuming more reactant than we are feeding. Table 5.1 summarizes the component balance control strategy.

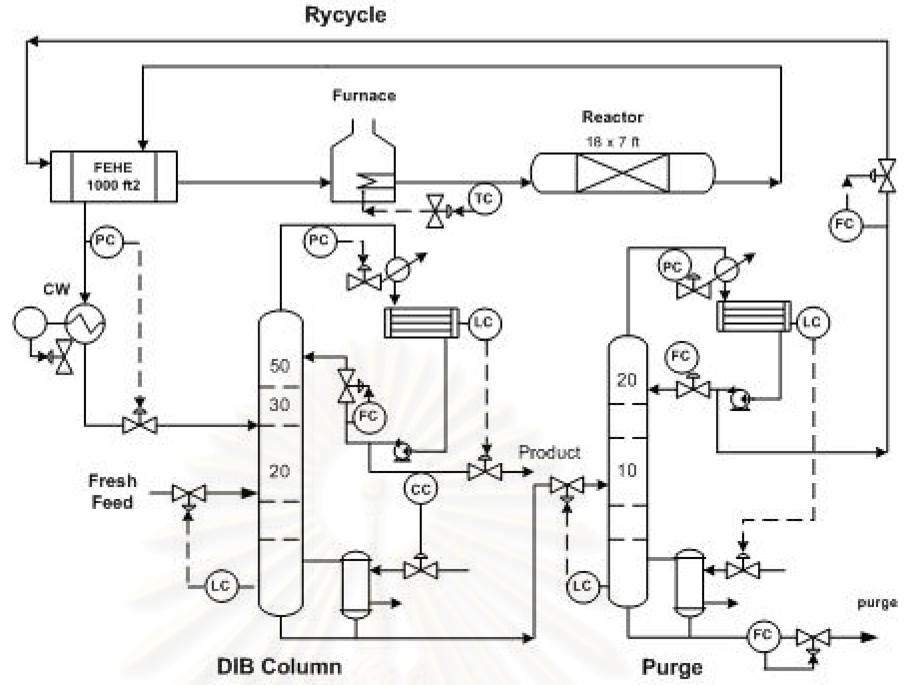


Figure 5.1: Control structure for Isomerization process (Plantwide Process Control, 1998)

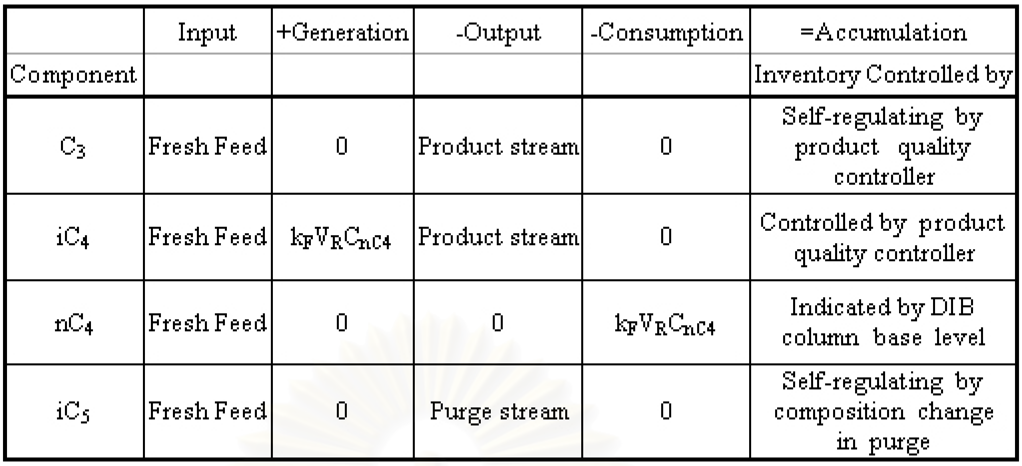
Step 8. : Control individual unit operations

The previous steps have left us at this point with two unassigned control valves, which are the reflux flows to each column. We do not need dual composition control for irreversible case because only one end of both columns is a product stream leaving the process. These two reflux flowrates are available in the step 9 to use as optimizing variables or to improve dynamic response.

Step 9. : Optimize economics or improve dynamic controllability

When we use reactor inlet temperature for production rate control (irreversible case), the only remaining degrees of freedom for optimization are the reflux flows for the two columns and the setpoint of the distillate flowrate from the purge column (recycle flow).

Table 5.1: Component Material Balance for irreversible case



	Input	+Generation	-Output	-Consumption	=Accumulation
Component					Inventory Controlled by
C_3	Fresh Feed	0	Product stream	0	Self-regulating by product quality controller
iC_4	Fresh Feed	$k_F V_R C_{nC4}$	Product stream	0	Controlled by product quality controller
nC_4	Fresh Feed	0	0	$k_F V_R C_{nC4}$	Indicated by DIB column base level
iC_5	Fresh Feed	0	Purge stream	0	Self-regulating by composition change in purge

Where V_R = reactor volume

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) and the second control structure of Luyben (1998), namely control structure 2 (CS2) to the Butane Isomerization process alternatives 1, 2 and base-case as shown in Figures 5.5 to 5.10. The new plantwide control structures CS3 and CS4 are designed for the Butane Isomerization process alternatives 1 and 2 as shown in Figures 5.11 to 5.14, respectively. In all of these control structures, the same loops are used as follows:

- Valve V1 is manipulated to control DIB column reboiler level.
- Valve V2 is manipulated to control Purge column reboiler level.
- Valve V4 is manipulated to control the flowrate in the recycle loop.
- Valve V5 is manipulated to control the bottom flowrate from the purge column.
- Valve V6 is manipulated to control the flooded condenser pressure.
- Cooler duty is manipulated to control the flooded condenser outlet temperature.
- Furnace duty is manipulated to control the reactor inlet temperature.

- DIB column condenser duty is manipulated to control the DIB column pressure.
- Purge column condenser duty is manipulated to control the Purge column pressure.
- Purge column reboiler duty is manipulated to control the level in Purge column condenser.

The main differences between CS1 to CS4 are explained below:

For Butane Isomerization process (Base Case), Poothanakul P. (2002) designed 3 control structures to reduce the effects of disturbances in order to achieved impurity of normal butane in product and desired production rate. The first control structure (S1) was modified from CS1 by controlled quality of product with fix product flow. The second control structure and the third control structure were modified from CS2. The second control structure (S2) concerned about reduction of effected of recycle by controlled temperature inside the distillation which could be controlled by adjusted reflux flow rate of column. And the last (S3) wanted to reduce effect of recycle indirectly by controlled temperature inside the distillation with outlet flow of bottom as shown in Figure Appendix D. These three control structures were compared with reference on plantwide process control book by Luyben (1998), the result shows that performances of Poothanakul's structures were better than Luyben's structures.

5.2.1 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 utility 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.

5.2.1.1 Heat Pathways

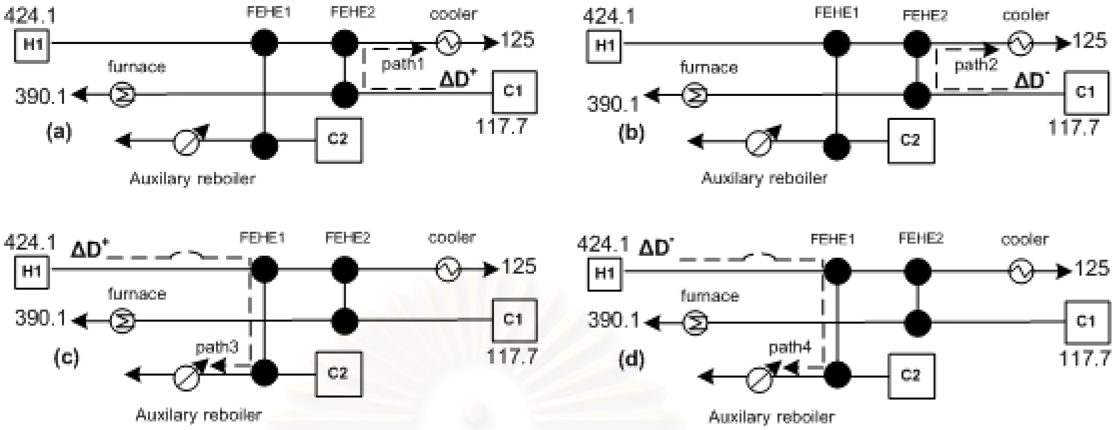


Figure 5.2: Heat Pathways through HEN in the energy-integrated Butane Isomerization Plant to achieve the highest possible dynamic MER, where:(a) path1 is used to shift the positive disturbance load of the cold stream C_1 to the cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream C_1 to the cooler, (c) path 3 is used to shift the positive disturbance load of the hot stream H_1 to the auxiliary reboiler, (d) path 4 is used to shift the negative disturbance load of the hot stream H_1 to the auxiliary reboiler

The HEN of Butane Isomerization Plant alternatives 1 and 2 as shown in Figure 5.2 is used to explain how an appropriate heat pathway should be activated to carry associated load to the utility unit (Wongsri, 1990). For instance, when the inlet temperature of a disturbed cold stream decreases, path 1 (Fig.5.2.a) should be activated by controlling the cold outlet temperature of FEHE2. This will have the effect of shifting the positive disturbance load to the cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty. Consider the case when the inlet temperature of a disturbed cold stream increases, path 2 (Fig.5.2.b) should be activated by controlling the cold outlet temperature of FEHE2 to shift its negative disturbance load to cooler. Thus, the negative disturbance load of a hot stream will result in increase of the cooler duty. On the other hand, when the inlet temperature of a disturbed hot stream increases, path 3 (Fig.5.2.c) should be activated by controlling the hot outlet temperature of FEHE1 to shift its positive disturbance load to auxiliary reboiler. As a result, the auxiliary reboiler duty of path 3 will be decreased. Consider the case when the inlet temperature of a disturbed hot stream decreases, path 4 (Fig.5.2.d) should be activated by controlling the hot inlet temperature of FEHE1 to shift its negative disturbance load to auxiliary reboiler. As a result, the auxiliary reboiler duty will be increased but, the furnace duty will be kept in the same as duty in the condition without disturbance.

5.2.1.2 Controller for Energy Management

Figure 5.3 shows control configurations for the energy-integrated Butane Isomerization plant to DMER, TC-cHE1 controller for FEHE1 and TC-cHE2 controller for FEHE2 (Fig.5.4.a and 5.4.b) are now employed in the current study to select an appropriate heat pathway to carry associated load to a utility unit.

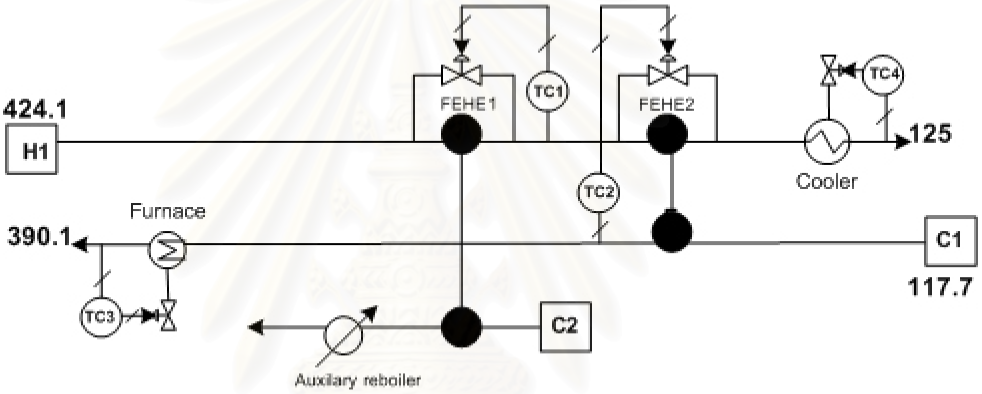
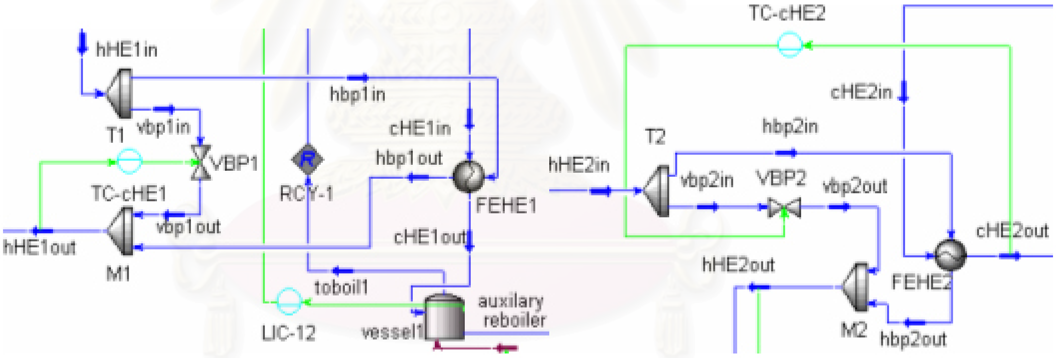


Figure 5.3: Control configurations for the energy-integrated Butane Isomerization plant to DMER

These control systems involve one manipulated variable and one controlled variables and work as follows: Figure 5.4.a shows the cold outlet temperature of FEHE1 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP1). At the same time, the hot outlet temperature of FEHE1 should not be allowed to drop below a lower limit value, which is necessary to keep the auxiliary 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 H_1, the control action to the hot temperature control (TC-hHE1out) close the valve VBP1. 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 auxiliary reboiler duty will also be increased but, the furnace duty will be kept in the same as duty in the condition without-disturbance. Whenever 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 H_1, the control action to TC-cHE1out open the valve VBP1. Consequently, the hot outlet temperature of FEHE1 will rise to its normal temperature and the cold outlet temperature of FEHE1 will be increased, so the auxiliary reboiler duty will also be decreased. Another control system is shown in Figure 5.4.b, the cold outlet temperature of FEHE2 is controlled at its nominal set point by manipulating the valve on the bypass line (VBP2). At the same time, the hot outlet temperature of FEHE2 should not be allowed to drop above an upper limit value, which is necessary to keep the cooler duty at a good level.

In order to apply control strategy in HYSYS as in Figures 5.4, a selector block can be added to the process flow diagram. On the connections page tab, all input signals are specified.



(a)TC-cHE1 controller

(b) TC-cHE2 controller

Figure 5.4: Control strategy in HYSYS

In alternative1 has two heat exchangers for preheat feed and the reboiler in the DIB column is driven by the reactor effluent stream. The DIB column is added an auxiliary reboiler, because the total heat from the reactor isn't enough to reboil the column.

In alternative2 has two heat exchangers for preheat feed and the reboiler in the Purge column is driven by the reactor effluent stream. The purge column is added an auxiliary reboiler, because the total heat from the reactor isn't enough to reboil the column.

Based on Figures 5.7 to 5.14, this loops control structures are used as follows:

- Valve VBP1 is manipulated to control the hot outlet temperature of FEHE1.
- Valve VBP2 is manipulated to control the cold outlet temperature of FEHE2.

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

5.2.2 Reference control structure I (CS1)

Based on Fig.5.5, Fig 5.7 and Fig 5.8, valveV3 is manipulated to control DIB column condenser level; DIB column reboiler duty is manipulated to control nC_4 impurity in the distillate.

5.2.3 Reference control structure II (CS2)

This control structure develops from CS1. A ratio controller is used to increase the reflux flowrate in the DIB column. The fractionating capability of the column increases as the load is increased, so the bottom does not contain less nC_4 reactant. Product rate increases.

5.2.4 Design of control structure 1 (CS3)

This control structure uses valveV3 to control impurity liquid of nC_4 in the top of DIB column (tray50), DIB column reflux flow is manipulated to control reflux drum level, and DIB column reboiler duty is manipulated to control the temperature on tray1 of DIB column. Alternatively we could control the amount of the nC_4 in the purge column bottoms by manipulating purge column reboiler duty. Since there is a fairly large temperature change in the purge column, controlling the temperature on some suitable trays (tray1 to 7) are controlled at the average temperature. We choose the level of purge column condenser is controlled by cascade to the tray temperature controller in the purge column because the tray temperature of the purge column is relative to the vapor coming overhead from the top of the column as show in Figures 5.11 and 5.12.

5.2.5 Design of control structure 2 (CS4)

This control structure develops from CS3. Due to both valveV3 which is manipulated to control impurity liquid of nC_4 in the top of DIB column (tray50) and DIB column reflux flow which is manipulated to control reflux drum level obtain poor performance. Because the distillate flowrate has large changes, this control structure switches those two variables as show in Figures 5.13 and 5.14. The other control structures are the same as CS3.

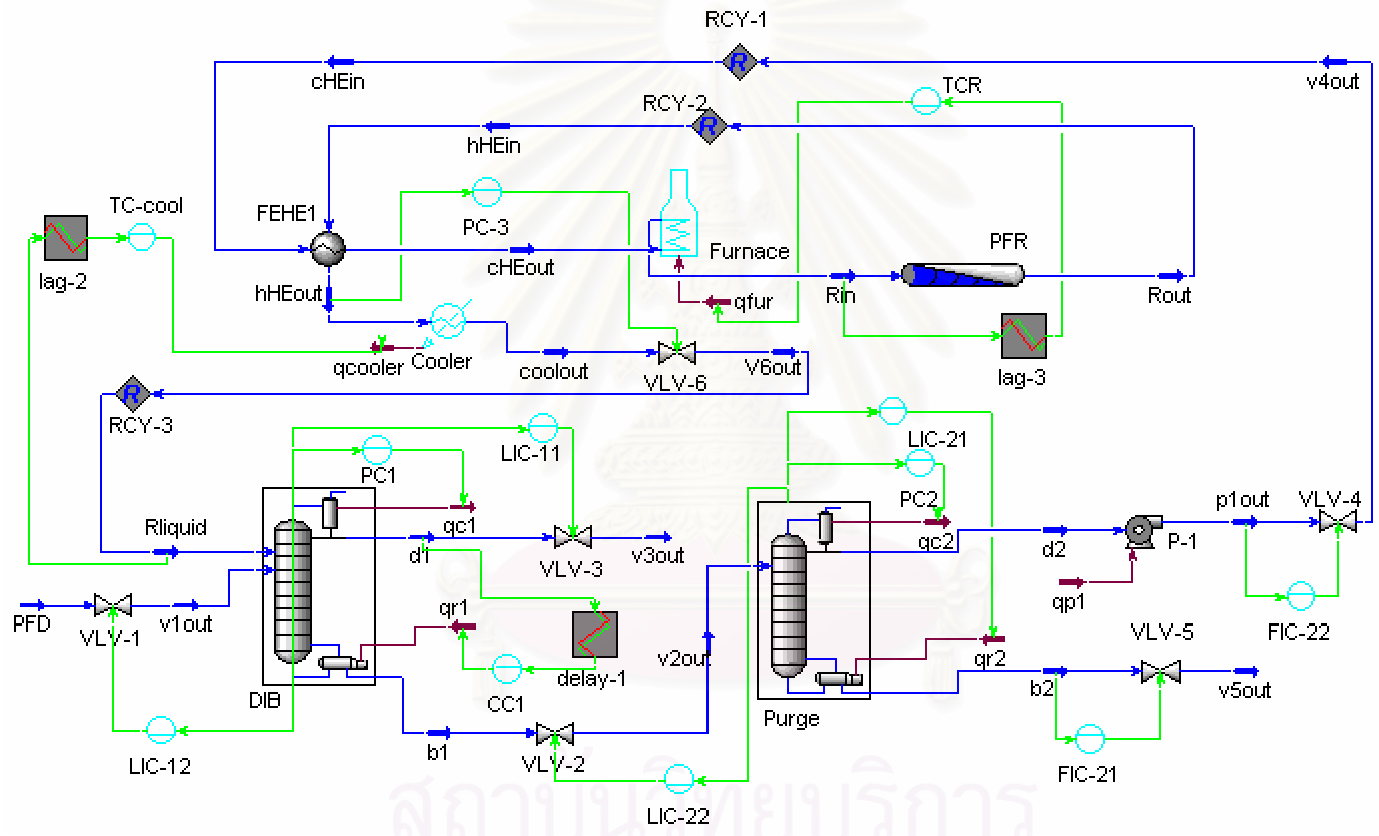


Figure 5.5: Application of reference control structure 1 (CS1) to the Butane Isomerization plant (Base Case)

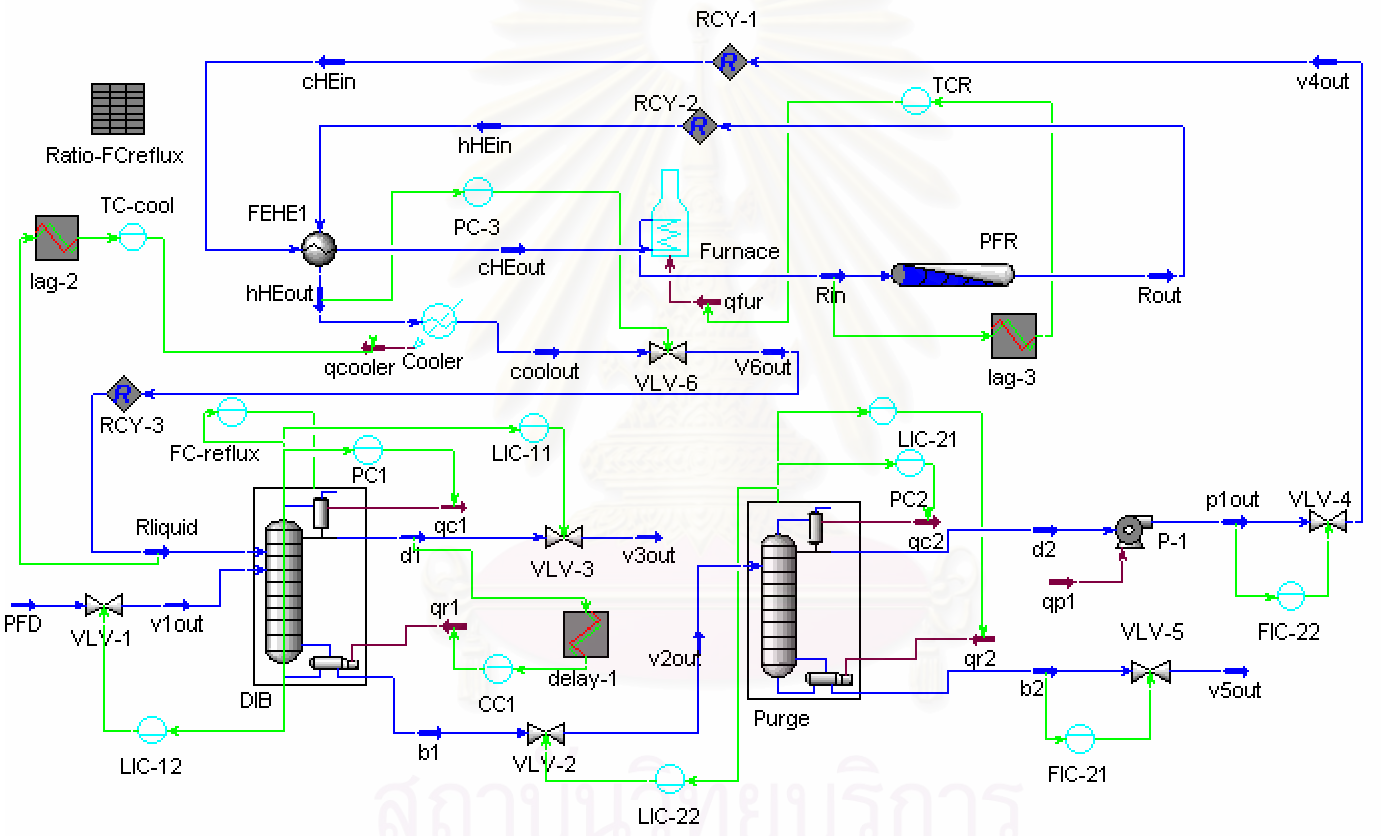


Figure 5.6: Application of reference control structure 2 (CS2) to the Butane Isomerization plant (Base Case)

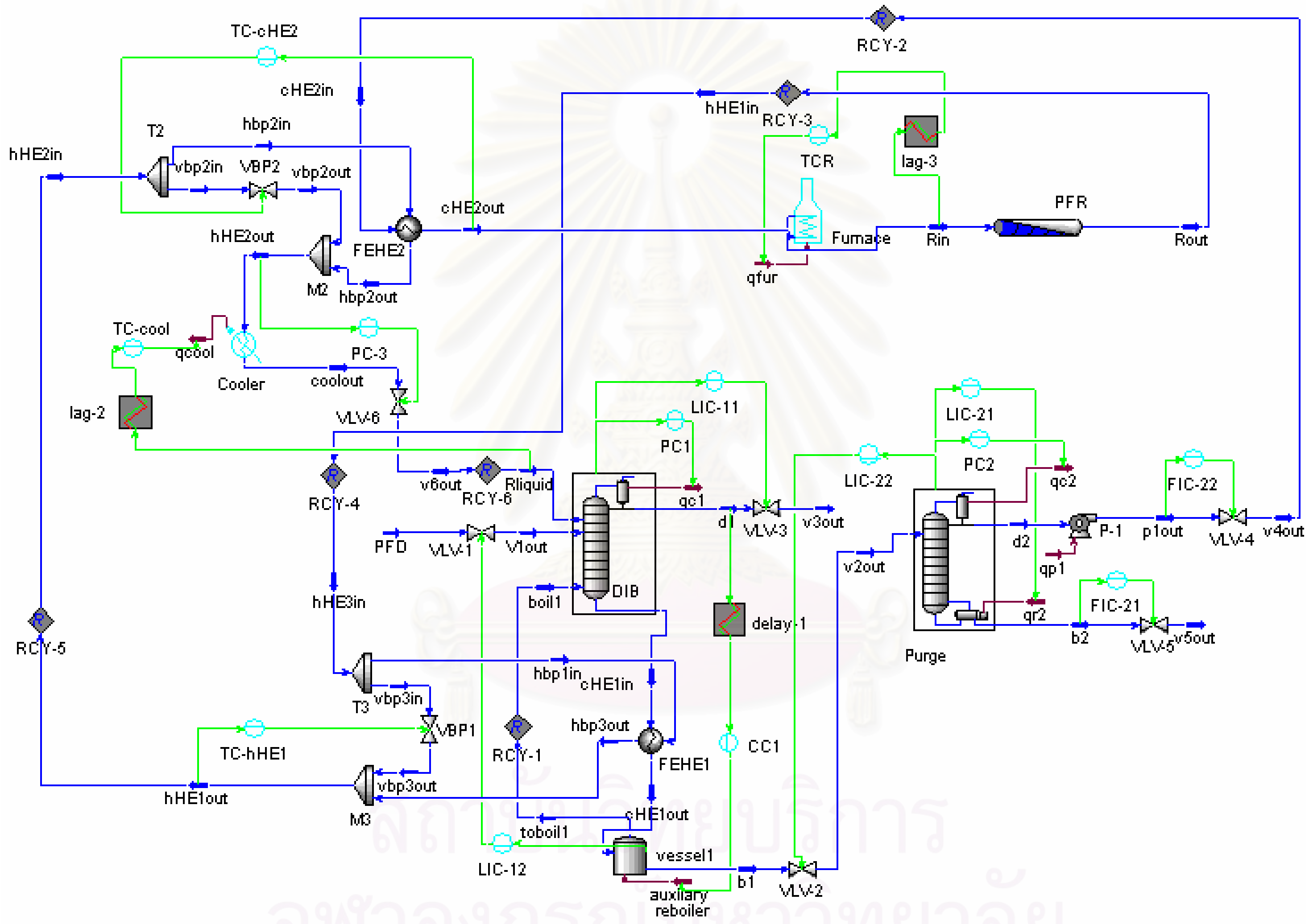


Figure 5.7: Application of reference control structure 1 (CS1) to the Butane Isomerization plant alternative 1

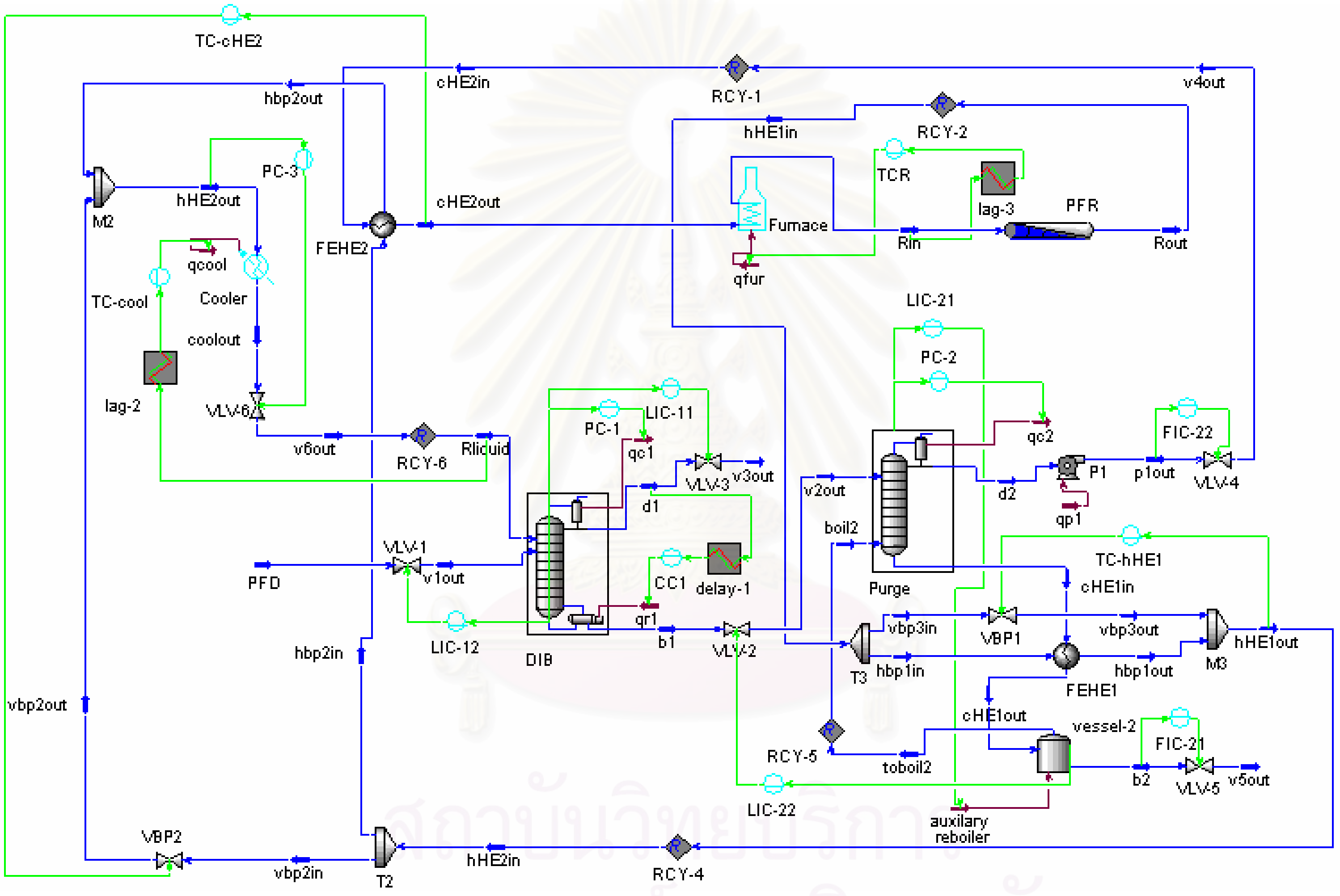


Figure 5.8: Application of reference control structure 1 (CS1) to the Butane Isomerization plant alternative 2

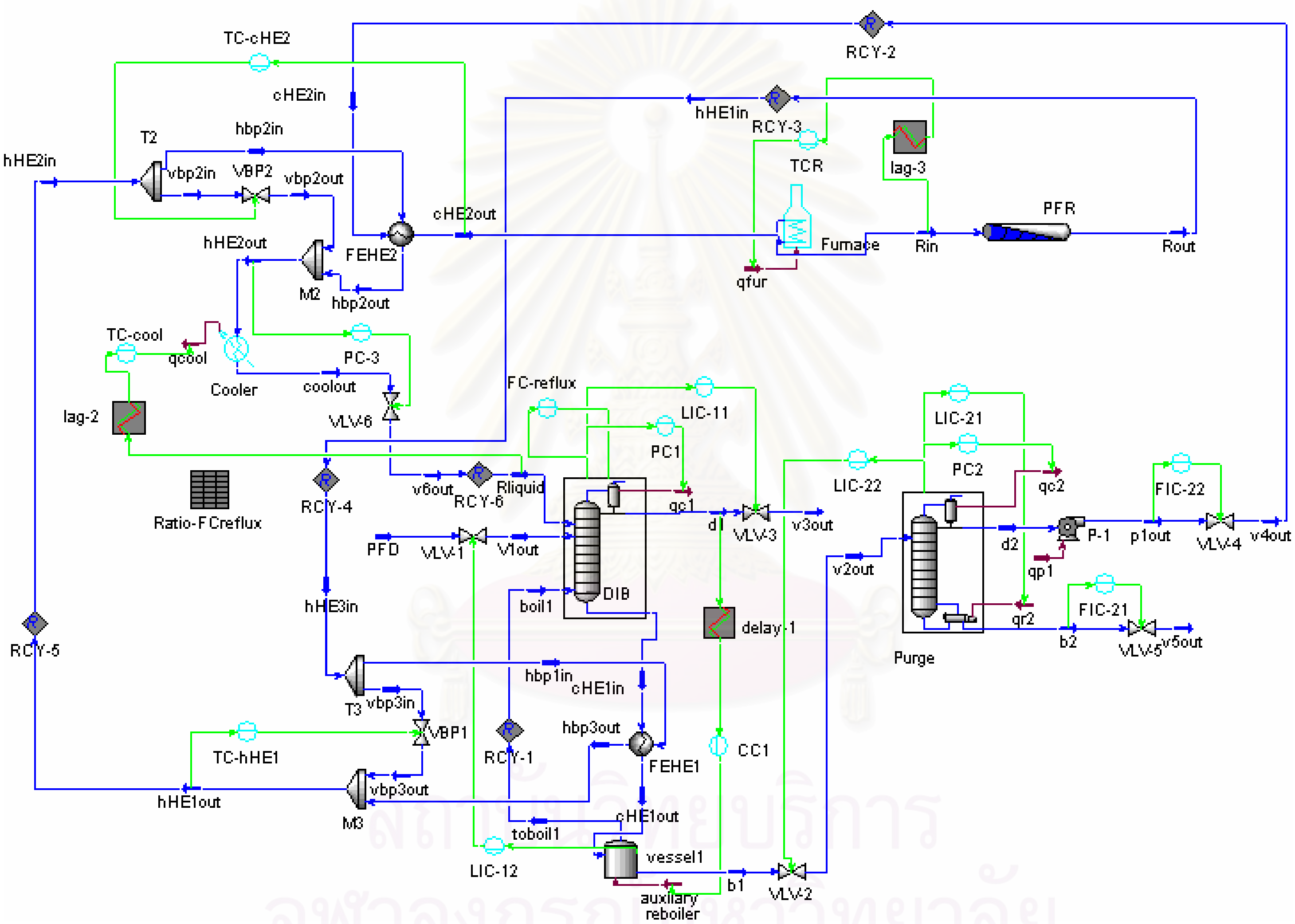


Figure 5.9: Application of reference control structure 2 (CS2) to the Butane Isomerization plant alternative1

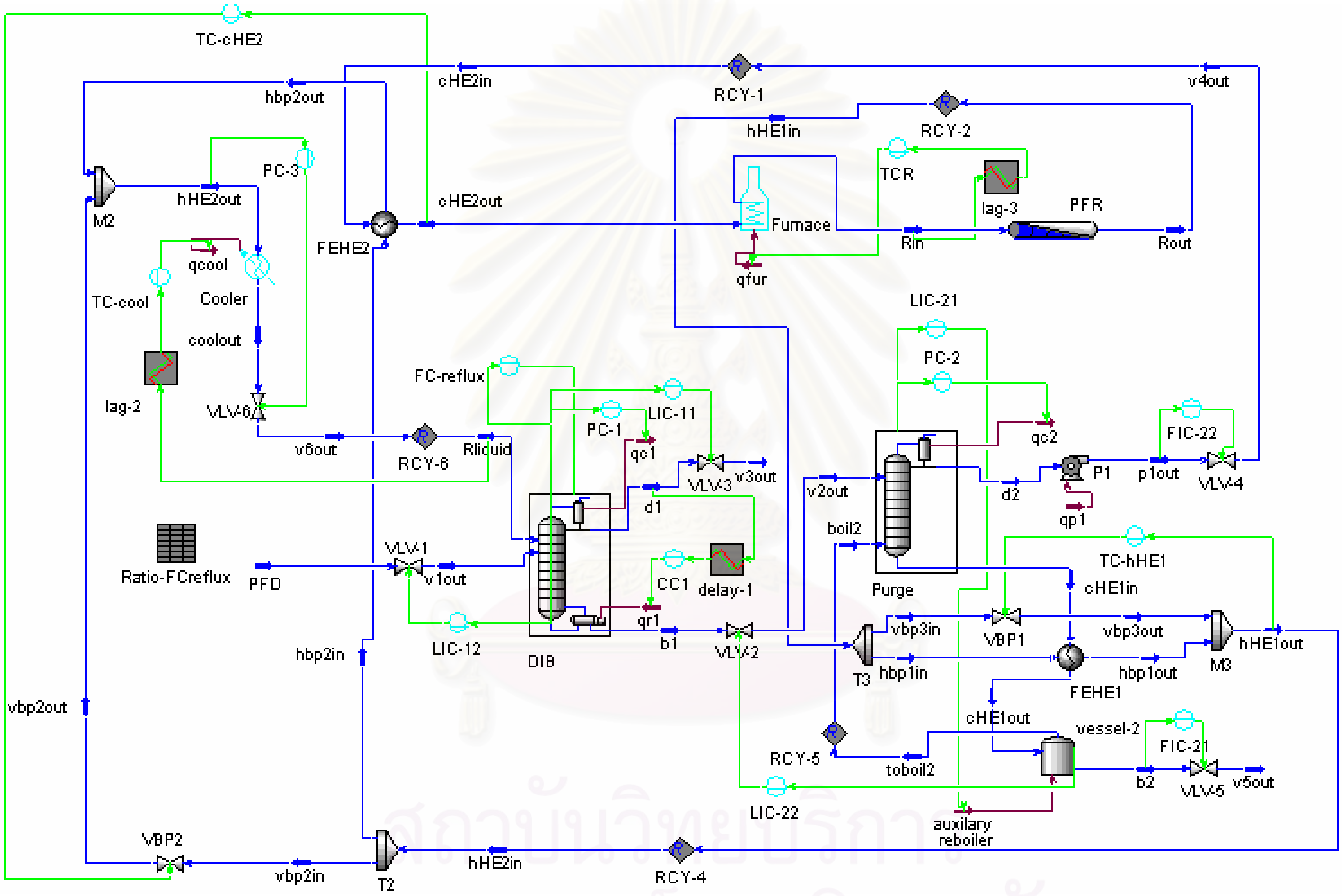


Figure 5.10: Application of reference control structure 2 (CS2) to the Butane Isomerization plant alternative 2

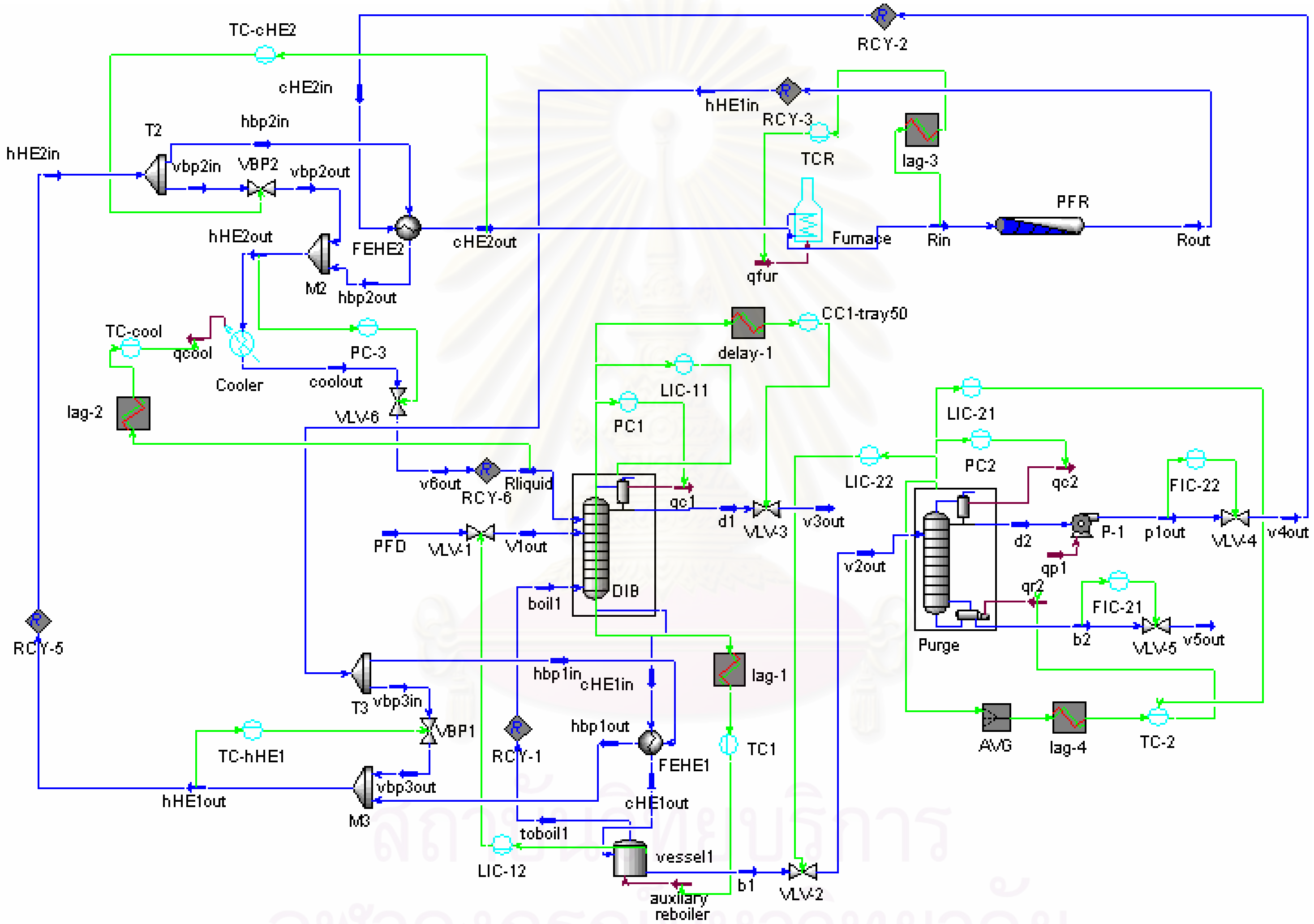


Figure 5.11: Application of control structure 3 (CS3) to the Butane Isomerization plant alternative 1

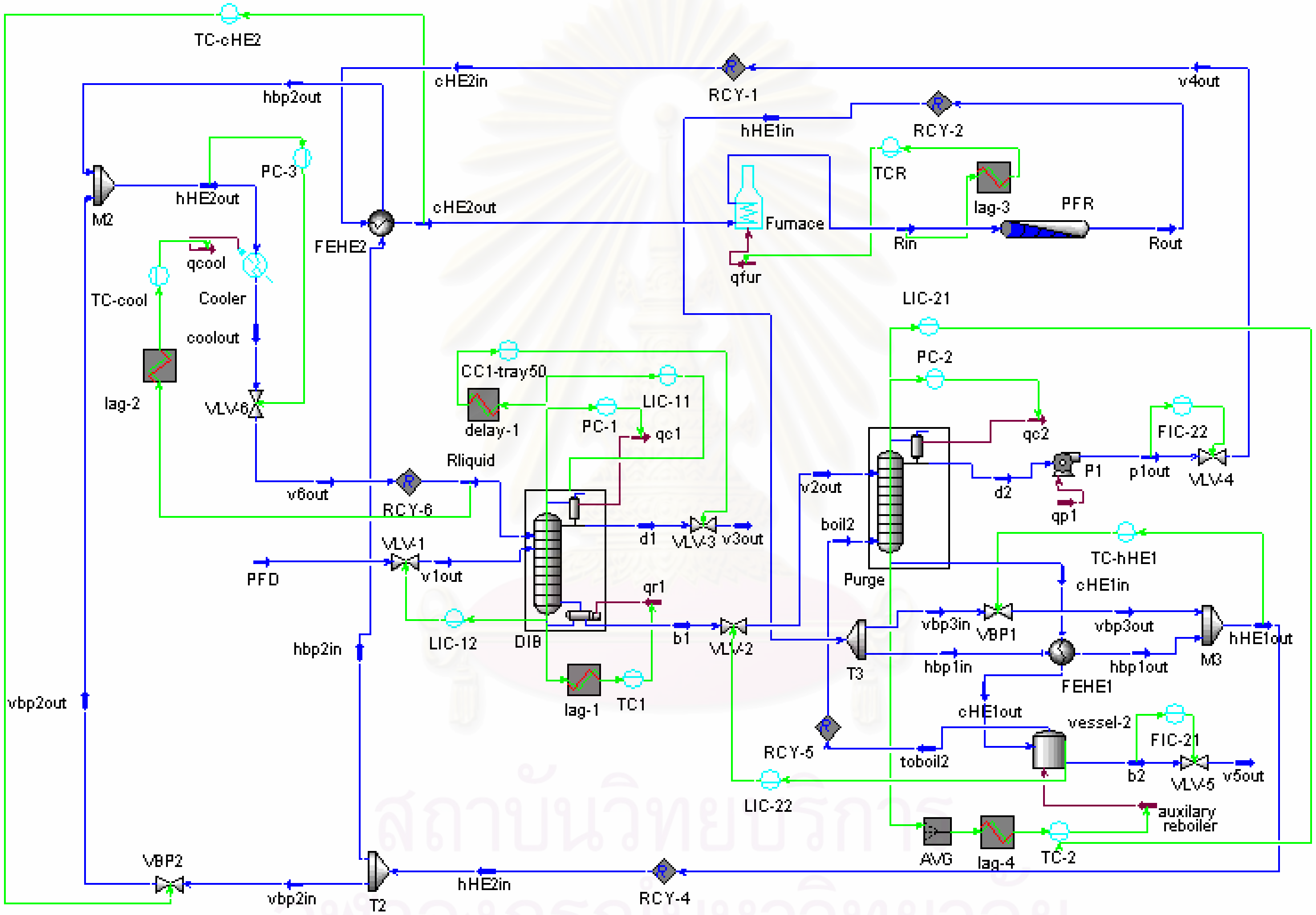


Figure 5.12: Application of control structure 3 (CS3) to the Butane Isomerization plant alternative 2

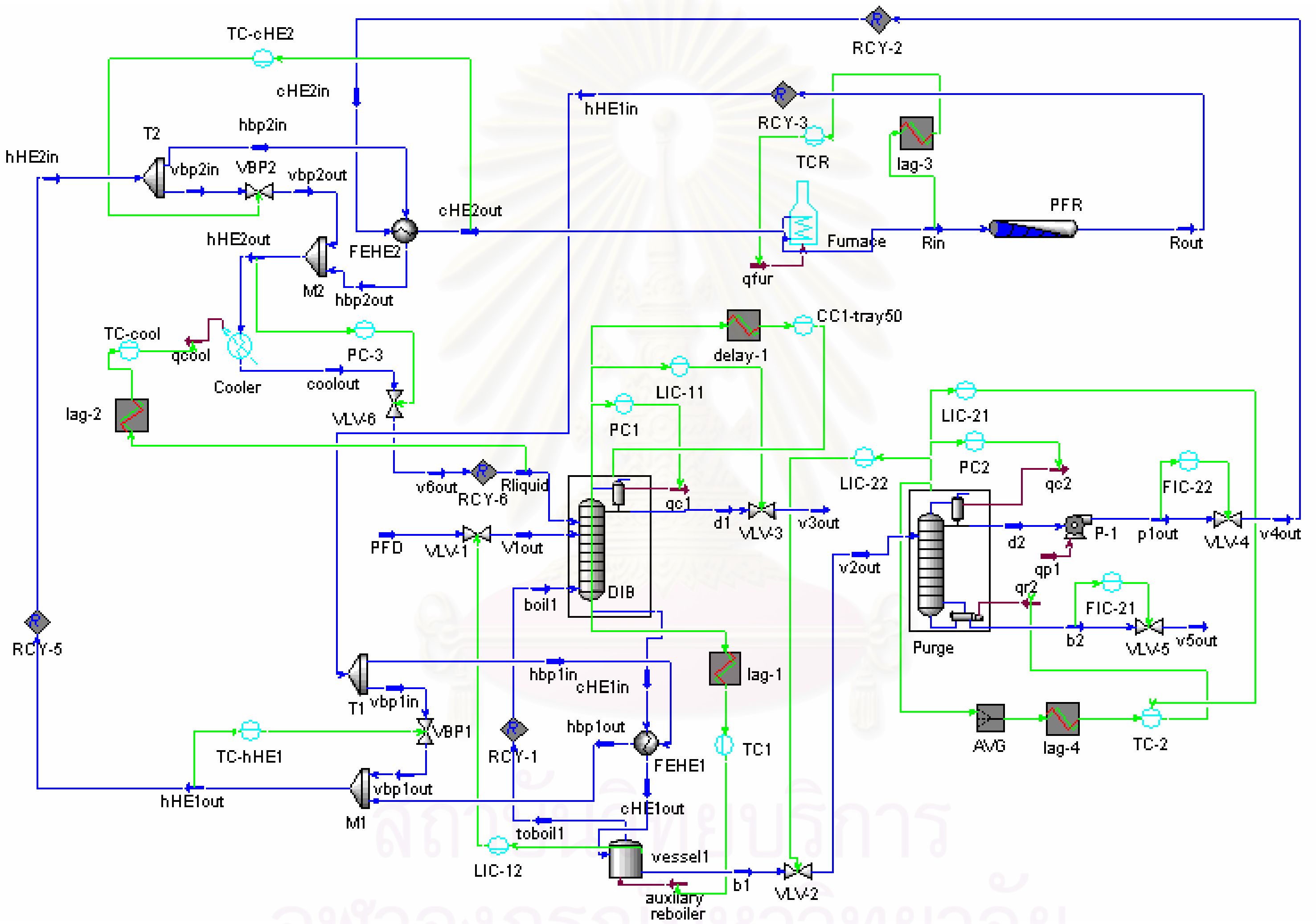


Figure 5.13: Application of control structure 4(CS4) to the Butane Isomerization plant alternative1

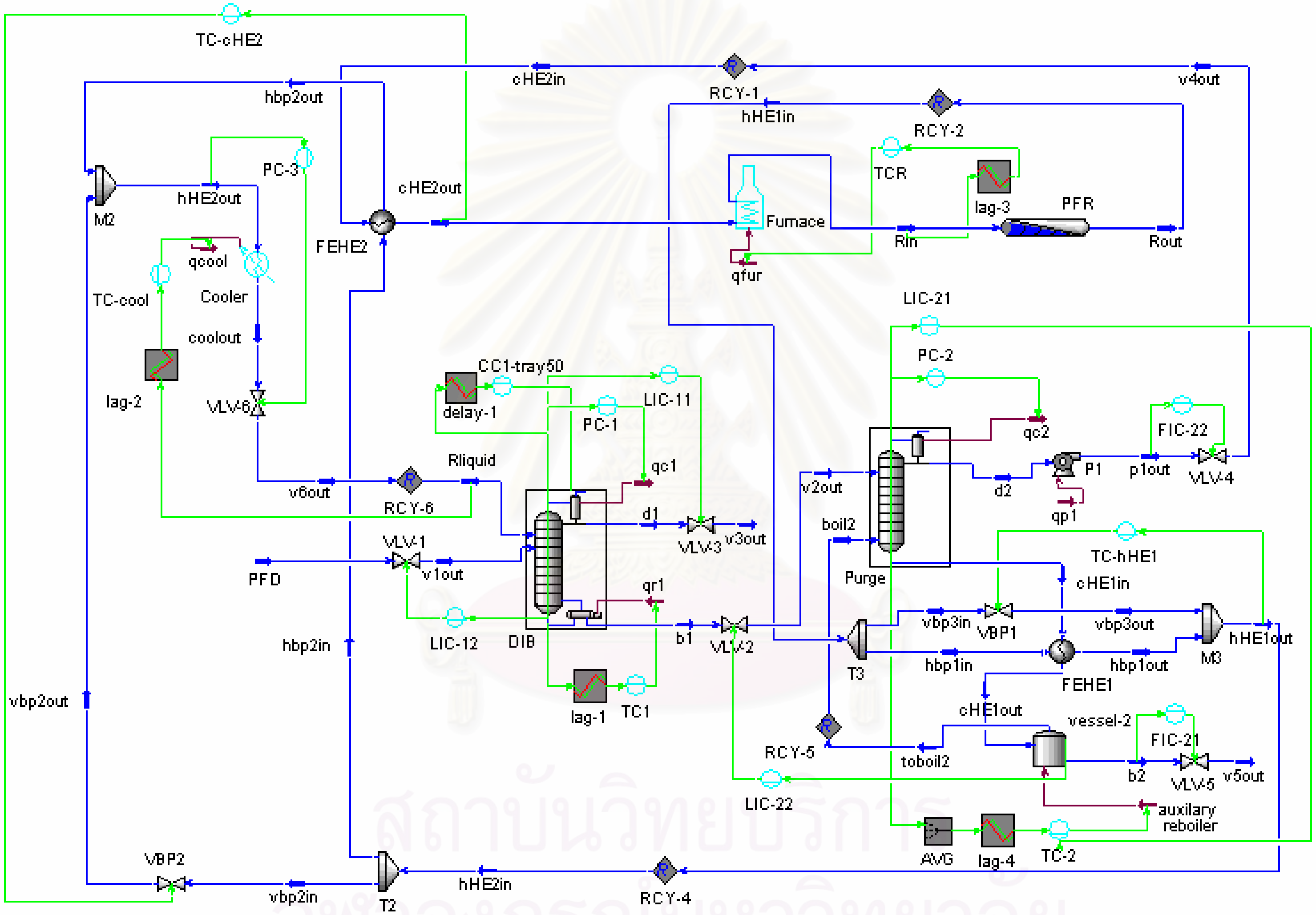


Figure 5.14: Application of control structure 4(CS4) to the Butane Isomerization plant alternative 2

5.3 Dynamic simulation result

In order to illustrate the dynamic behaviors of our control structures and the previous control structures (Luyben et al., 1999), several disturbance loads were made. The dynamic responses of CS1 and CS2 in Butane Isomerization plant alternatives 1, 2 and base-case are shown in Figures 5.15 to 5.39. Figures 5.19 to 5.27 and Figures 5.32 to 5.39 show the dynamic responses of the new control structures (CS3 and CS4) in Butane Isomerization plant alternatives 1 and 2. In general, better responses of the hot and cold utility consumptions are achieved here compared to the Luyben's control structure in the Butane Isomerization plant with no energy integration, since the duties for both hot and cold utilities could be decreased. Therefore, the proposed HPH is very useful in terms of heat load or disturbance management to achieve the highest possible dynamic MER. Results for individual disturbance load changes are as follows:

5.3.1 Change in the heat load disturbance of hot stream for CS1 and CS2 in Butane Isomerization plant (Base Case)

Figures 5.15 and 5.16 show that 10 ^{0}F step increase, occurring at time equals 10 minutes, produces an increase in product flowrate (from 550 to 623 lb.mol/hr). As more iC_4 is produced in the reactor with the increase in reaction rate at the higher temperature, the purity of the DIB distillate improves (less nC_4 in the overhead product), which causes the reboiler heat input to increase. This lowers the base level, and pulls in more fresh feed. So changing reactor inlet temperature is an effective way to set production rate when the reaction is irreversible. Figures 5.17 and 5.18 show that 10 ^{0}F step decrease, occurring at time equals 10 minutes, produces an decrease in product flowrate (from 550 to 483 lb.mol/hr).

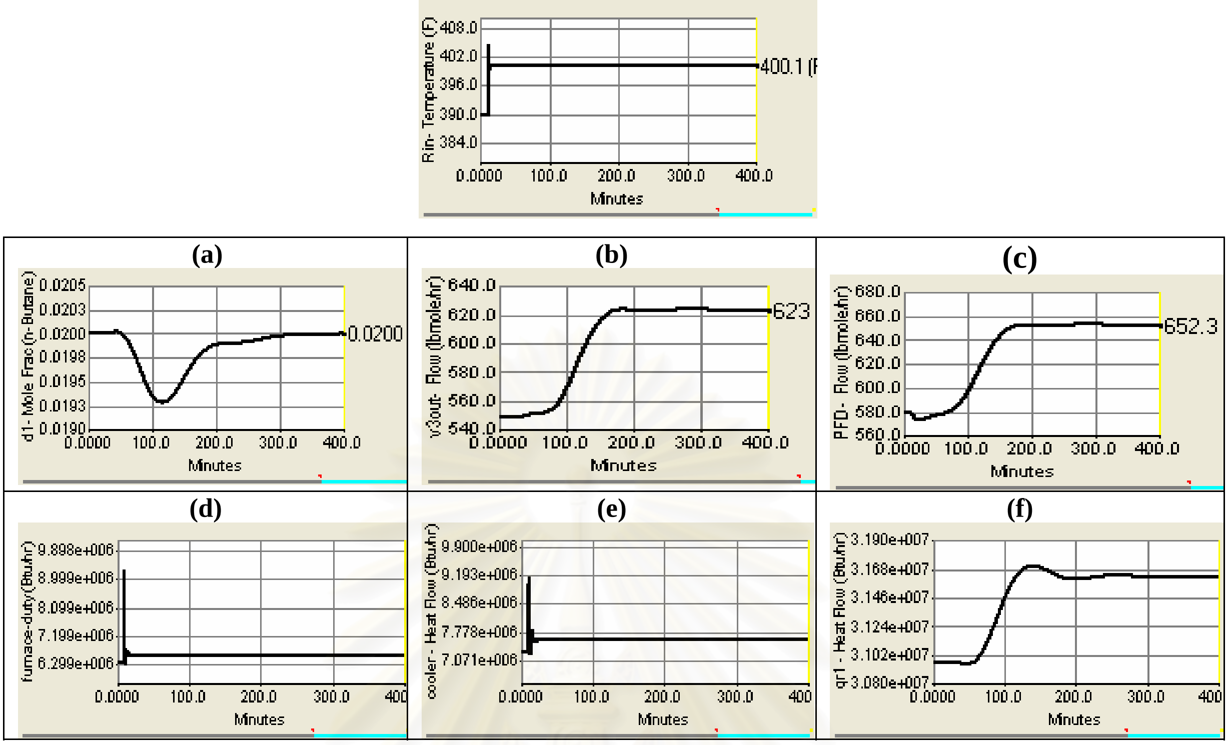


Figure 5.15: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to 10 ^oF increase in reactor inlet temperature (the heat load disturbance of hot stream), where
(a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate,(d) furnace duty, (e) cooler duty, (f) the DIB column reboiler duty.

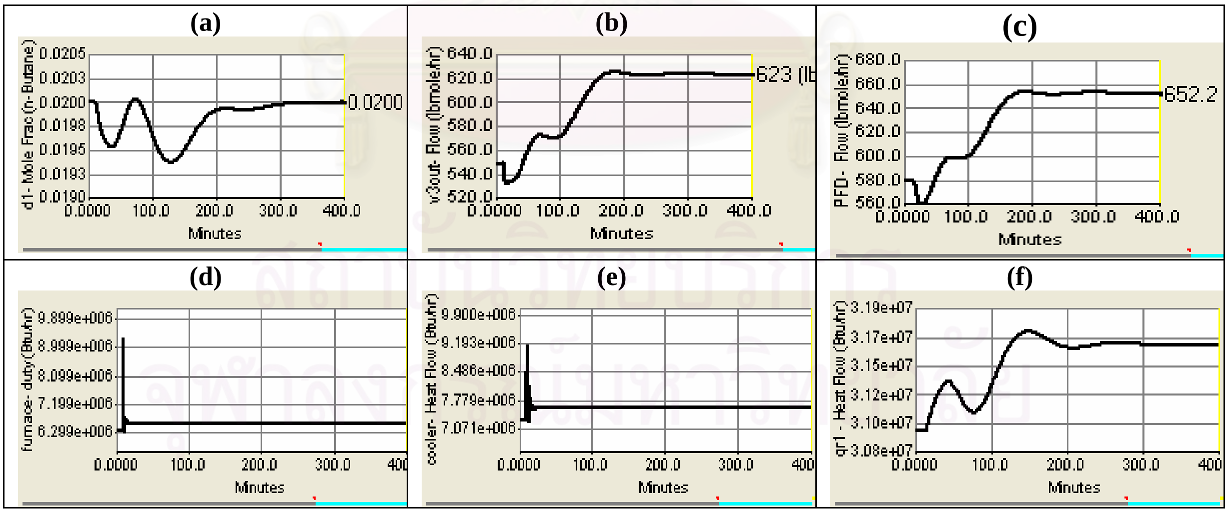
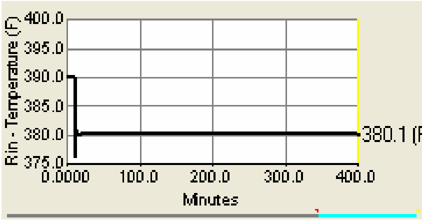


Figure 5.16: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to 10 ^oF increase in reactor inlet temperature (the heat load disturbance of hot stream), where
(a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate,(d) furnace duty, (e) cooler duty, (f) the DIB column reboiler duty.



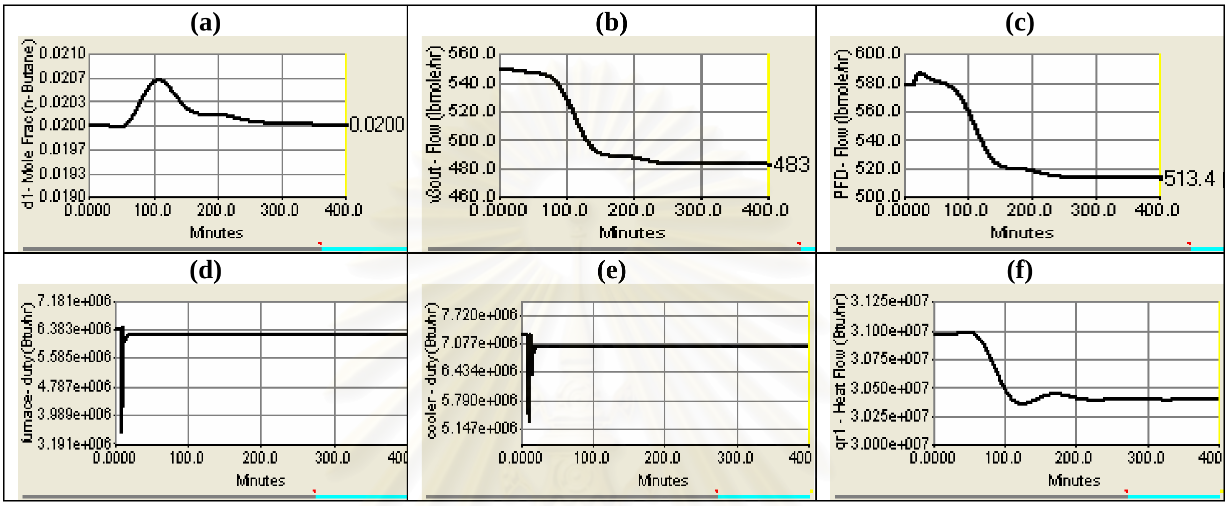


Figure 5.17: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to 10^{o}F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where
(a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate,(d) furnace duty, (e) cooler duty, (f) the DIB column reboiler duty.

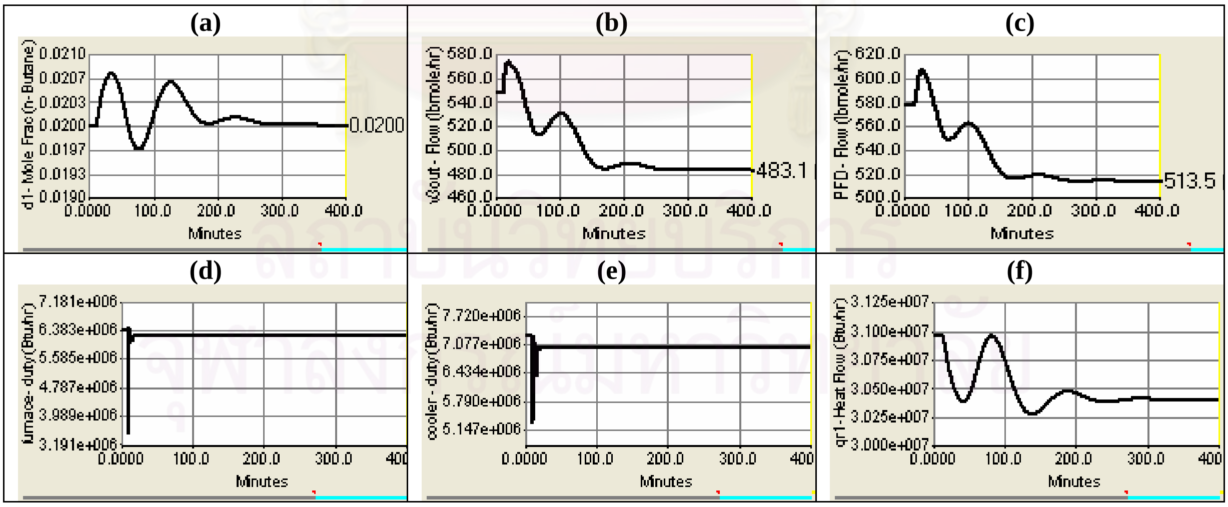


Figure 5.18: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to 10^{o}F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where
(a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate,(d) furnace duty, (e) cooler duty, (f) the DIB column reboiler duty.

5.3.2 Change in the heat load disturbance of hot stream for Butane Isomerization plant alternatives 1 and 2

Figures 5.19 to 5.27 show the dynamic responses of the Butane Isomerization plant alternatives 1 and 2 to a change in the heat load disturbance of the hot stream (the reactor inlet temperature stream). This disturbance is made as follows: The reactor inlet temperature is increased from 390.1 to 400.1 ^{0}F at time equals 10 minutes and the reactor inlet temperature is decreased from 390.1 to 380.1 ^{0}F at time equals 10 minutes (Fig.5.19).

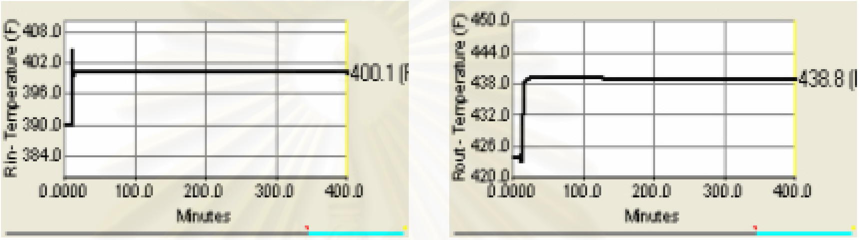
In general, the dynamic responses of the control system with the HSS for control structure 1 in Butane Isomerization plant alternatives 1 and 2 are similar with those to CS2, CS3 and CS4 in Butane Isomerization plant alternatives 1 and 2. As can be seen, the dynamic responses of the control system with the HSS in the current work are able to select proper heat pathway to carry the associated load to a utility unit.

When the hot inlet temperature of FEHE1 increases, the HSS will take an action to control the cold outlet temperature of FEHE1 (i.e. the cold outlet temperature in alternatives 1 and 2 as shown in Fig. 5.20.a and 5.21.a). The hot outlet temperature of FEHE1 quickly rises to a new steady state value (Fig. 5.20.b and 5.21.b). Fig.5.20.e and Fig.5.21e show that EHE3 duty increases due to HSS manages the positive disturbance. Therefore, the DIB column auxiliary reboiler duty in alternative 1 and Purge column auxiliary reboiler duty in alternative 2 decrease, since the hot inlet temperature of EHE3 increases.

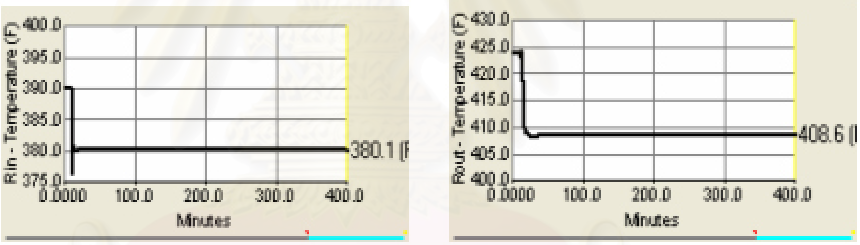
When the hot inlet temperature of FEHE1 decreases, this leads to the increase of auxiliary reboiler duty, so the HSS switches the control action from the cold outlet temperature control (TC-cHE1) to the hot outlet temperature control (TC-hHE1). Following this action, the furnace inlet temperature drops to a new steady state value (Fig. 5.22.a and 5.23.a); therefore, the furnace duty increases. The EHE3 inlet temperature rises to its set point quickly (Fig.5.22.b and 5.23.b), so the EHE3 duty also rises to its nominal value quickly. That show the EHE3 duty will be kept in the same as duty in the condition without disturbance (Fig.5.22e and 5.23.e). The hot outlet temperatures of FEHE2 and

EHE3 are well controlled.

However, the new control structures (CS3 and CS4) can handle more disturbances and are faster than the previous control structures (CS1 and CS2). Besides that the new control structures require less auxiliary reboiler utility consumptions are achieved compare to CS1 and CS2, because CS3 and CS4 are modified by manipulating auxiliary reboiler duty to control the temperature on tray1 of DIB column and Purge column.



(a) 10 °F increase



(b) 10 °F decrease

Figure 5.19: Dynamic responses to 10 ^{0}F increase and 10 ^{0}F decrease in reactor inlet temperature.

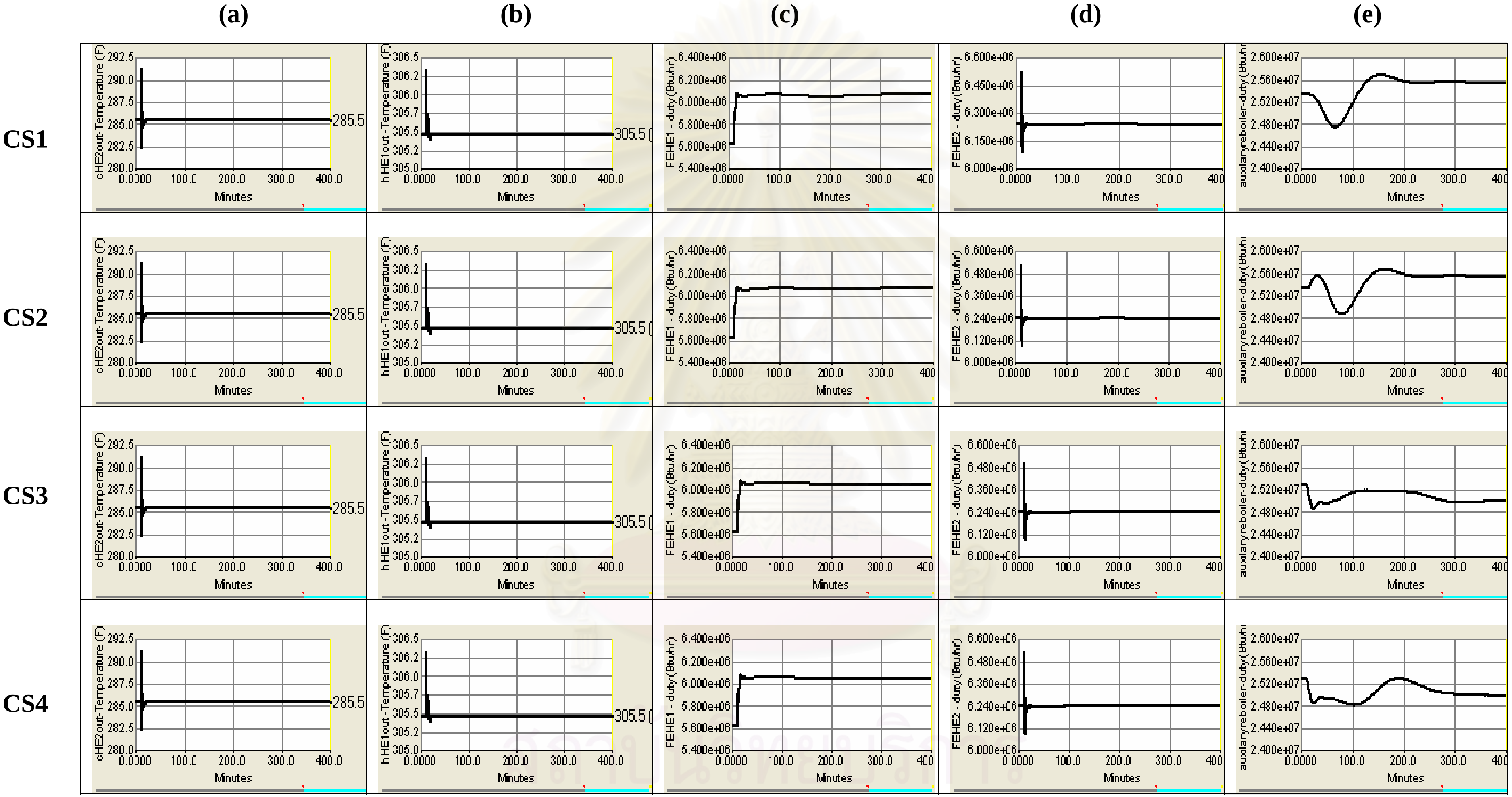


Figure 5.20: Dynamic responses of the Butane Isomerization plant alternative 1 to 10 ^{o}F increase in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the DIB column auxiliary reboiler duty; comparison between CS1, CS2, CS3 and CS4.

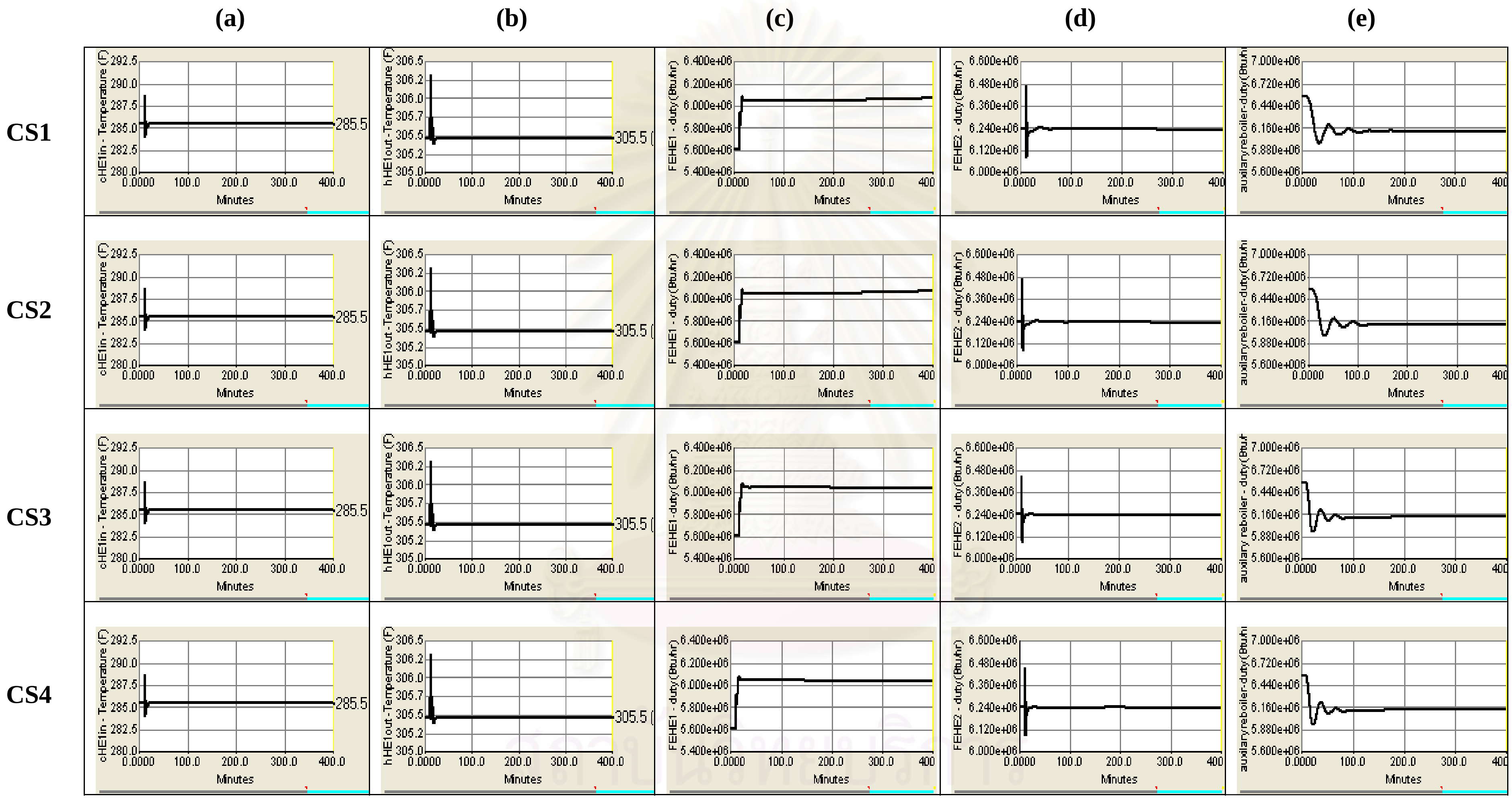


Figure 5.21: Dynamic responses of the Butane Isomerization plant alternative 2 to 10 °F increase in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the Purge column auxiliary reboiler duty; comparison between CS1, CS2, CS3 and CS4.

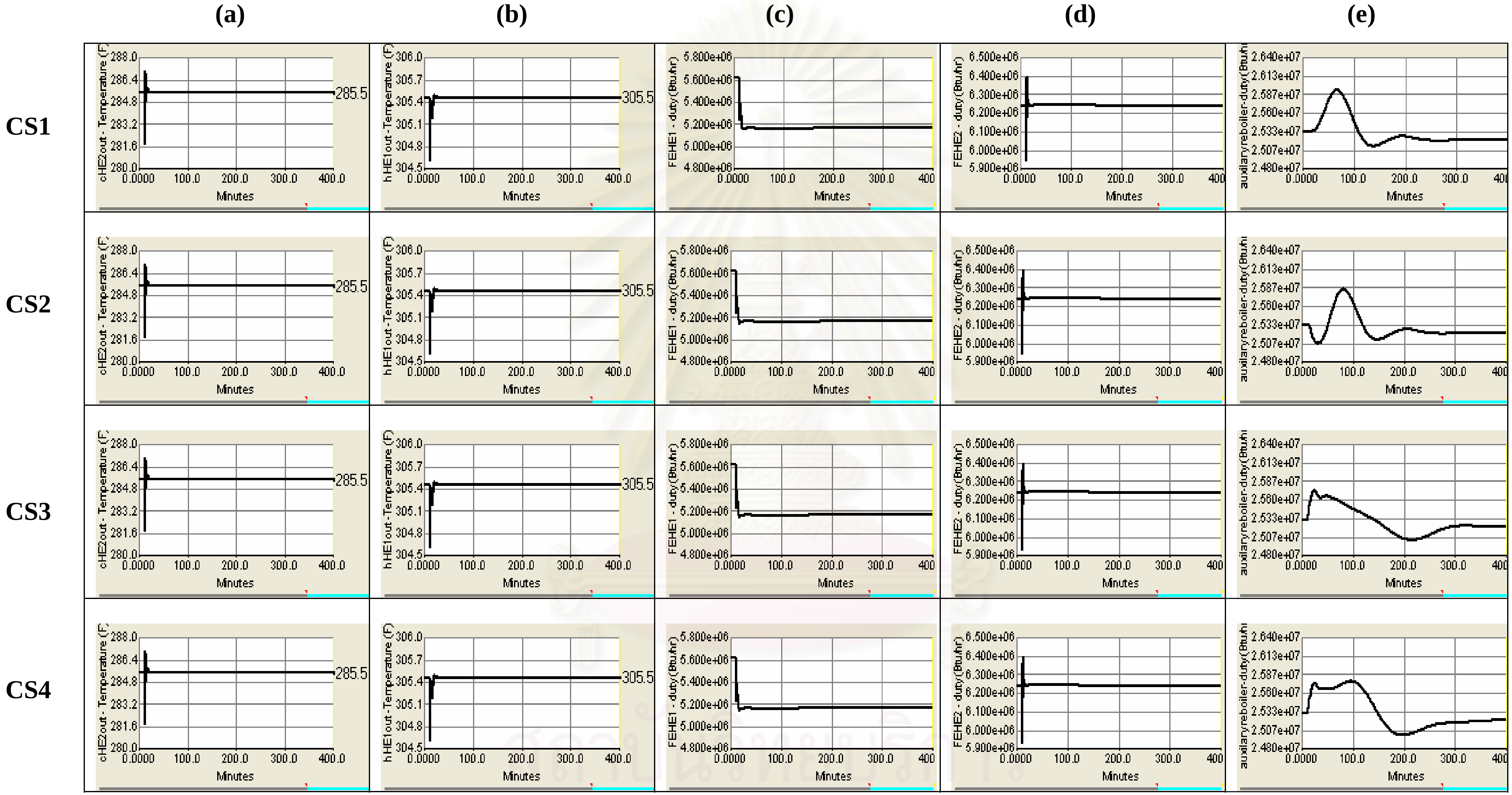


Figure 5.22: Dynamic responses of the Butane Isomerization plant alternative 1 to 10 °F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the DIB column auxiliary reboiler duty; comparison between CS1, CS2, CS3 and CS4.

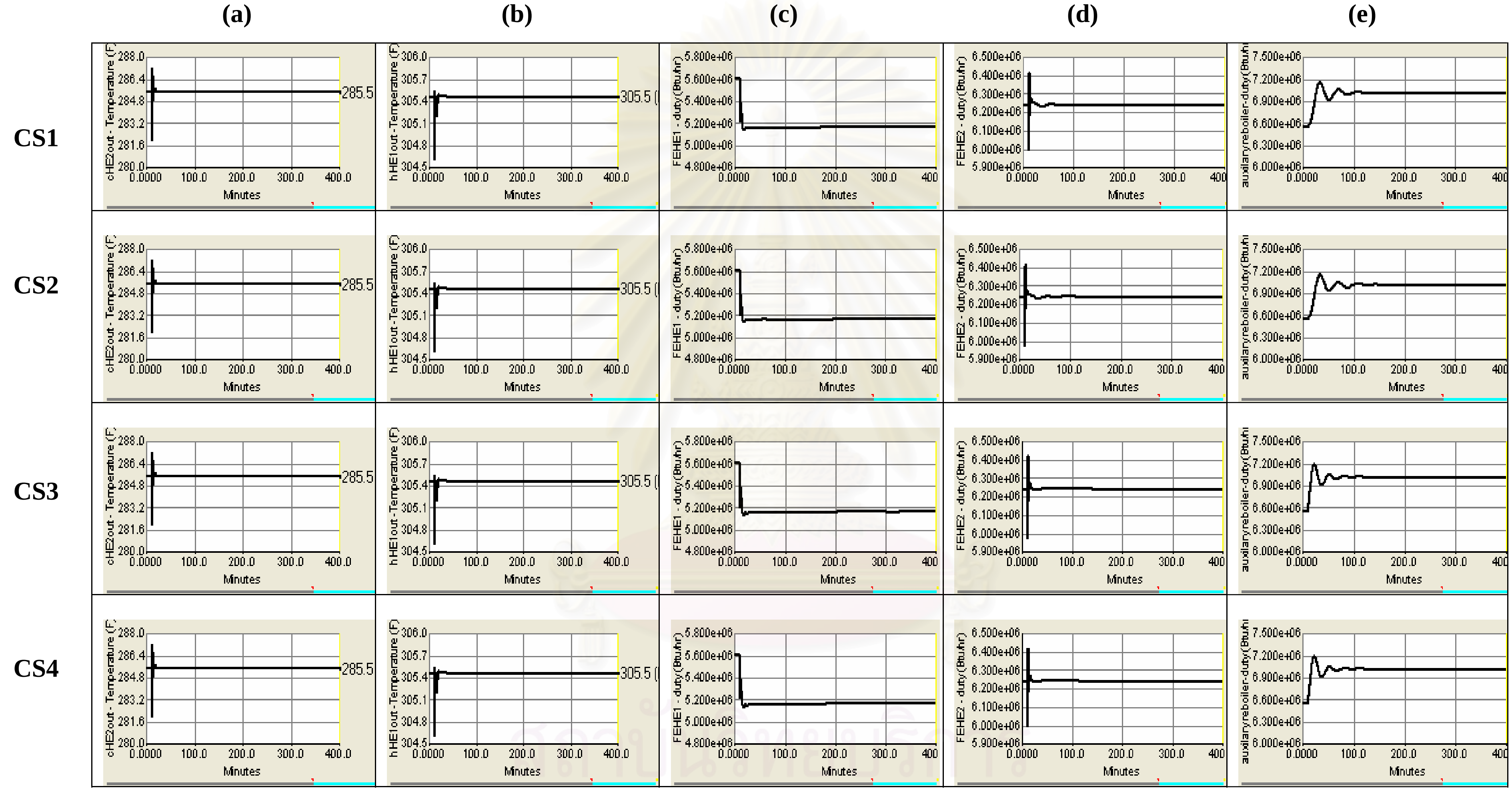


Figure 5.23: Dynamic responses of the Butane Isomerization plant alternative 2 to 10 °F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the Purge column auxiliary reboiler duty; comparison between CS1, CS2, CS3 and CS4.

5.3.2.1 The dynamic responses of CS1 control structure

Figures 5.24 and 5.25 give the simulation results for increasing the reactor inlet temperature. The temperature response is oscillatory and it comes to new setpoint within 30 minutes. Effect from the temperature increase, the rate of reaction of Butane Isomerization process increase because of increasing temperature can raise the reaction rate. Figures 5.24.a,b,c and 5.25.a,b,c show the impurity of nC_4 in the product, the iC_4 product flow and the fresh feed flow. The fresh feed flow and the iC_4 product flow are slowly increased about 200 minute to new steady-state due to reaction rate increasing. But nC_4 impurity in product is slowly decreased and it takes over 300 minutes to return to its set point.

Figures 5.26 and 5.27 show that, the simulation results for decreasing the reactor inlet temperature. Effect from the temperature decrease, the fresh feed flow and the iC4 product flow are decreased. But nC_4 impurity in product is slowly increased and it takes long time to achieve setpoint.

As can be seen, the dynamic responses of CS1 in Butane Isomerization process alternative 1 are slower than those in Butane Isomerization process (Base Case).

Again, the dynamic responses of CS1 in Butane Isomerization alternative 2 are slower than those in alternative 1. Most of control loops in alternative 2 are more oscillatory than those in alternative 1. The reactor inlet temperature and the cooler outlet temperature are slightly well controlled (Fig 5.24.f to 5.27.f). But, the dynamic response of the nC_4 impurity in product is less oscillatory than those in alternative 1.

For a complex energy-integrated plant, it is important to control the temperature on bottom tray of column such as the dynamic responses of CS1 and CS2 in Butane Isomerization plant alternatives 1 and 2 don't control the temperature on tray1 of DIB column, so when more iC_4 is produced in the reactor with the increase in reaction rate at the higher temperature, the purity of DIB distillate improves (less nC_4 in the overhead product),which causes the DIB column auxiliary reboiler duty in alternative 1 and DIB column reboiler duty in alternative 2 to increase (Fig 5.24.i and 5.25.i).

In contrast, when less iC_4 is produced in the reactor with the decrease in reaction rate at the lower temperature, the purity of DIB distillate improves (more nC4 in the overhead product),which causes the DIB column auxiliary reboiler duty in alternative 1 and DIB column reboiler duty in alternative 2 to decrease (Fig 5.26.i and 5.27.i).

5.3.2.2 The dynamic responses of CS2 control structure

Figures 5.24 to 5.27 show the dynamic responses of the process for 10 ^{0}F increase and 10 ^{0}F decrease in the reactor inlet temperature. This control structure has the same dynamic responses as CS1, but CS1 can handle more disturbances and is faster than CS2.

As can be seen, the dynamic responses of CS2 in Butane Isomerization process alternative 1 are slower than those in Butane Isomerization process (Base Case).

Again, the dynamic responses of CS2 in Butane Isomerization alternative 2 are slower than those in alternative 1. Most of control loops in alternative 2 are more oscillatory than those in alternative 1. The reactor inlet temperature and the cooler outlet temperature are slightly well controlled (Fig 5.24.f to 5.27.f). But, the dynamic response of the nC_4 impurity in product is less oscillatory than those in alternative 1 (Fig 5.24.a to 5.27.a).

5.3.2.3 The dynamic responses of CS3 control structure

Figures 5.24 to 5.27 show the dynamic responses of the process for 10 ^{0}F increase and 10 ^{0}F decrease in the reactor inlet temperature. The dynamic responses of this control structure are faster than others because the reflux flow can control the reflux drum level more effective than the distillate flow. But we control distillate composite manipulating the distillate flowrate, so the iC_4 product flow has large changes. However, in this case we assume that the distillate is going to a storage tank or cavern.

Figures 5.24.g to 5.27.g and Figures 5.24.h to 5.27.h show the temperature control in 2 distillation columns. The temperature response of DIB column does not see the changing. But the temperature response of Purge column will change to follow the level of Purge column condenser (cascade from level control of Purge column condenser).

As can be seen, the dynamic responses of CS3 in Butane Isomerization process alternative 1 are similar with those in alternative 2. Some control loops (such as the tray temperature of Purge column, the reactor inlet temperature, the cooler outlet temperature and the pressure of Purge column condenser) in Butane Isomerization process alternative 2 are more oscillatory than those in alternative 1. But, the dynamic response of the nC_4 impurity of product in alternative 3 is less oscillatory than those in alternative 1.

5.3.2.4 The dynamic responses of CS4 control structure

Figures 5.24 to 5.27 show the dynamic responses of the process for 10 ^{0}F increase and 10 ^{0}F decrease in reactor inlet temperature. The dynamic responses of this control structure are similar to CS3 except composition control in DIB column. The dynamic response of this control loop is faster than others because the reflux flow can control the nC_4 impurity in product more effective than the distillate flow.

Figures 5.24.g to 5.27.g and Figures 5.24.h to 5.27.h show the temperature control in 2 distillation columns. The temperature response of DIB column does not see the changing. But the temperature response of Purge column will change to follow the level of Purge column condenser (cascade from level control of Purge column condenser).

As can be seen, the dynamic responses of CS4 in Butane Isomerization process alternative 1 are similar with those in alternative 2. Some control loops (such as the tray temperature of Purge column, the reactor inlet temperature, the cooler outlet temperature and the pressure of Purge column condenser) in Butane Isomerization process alternative 2 are more oscillatory than those in alternative 1. But, the dynamic response of the nC_4 impurity of product in alternative 2 is less oscillatory than those in alternative 1.

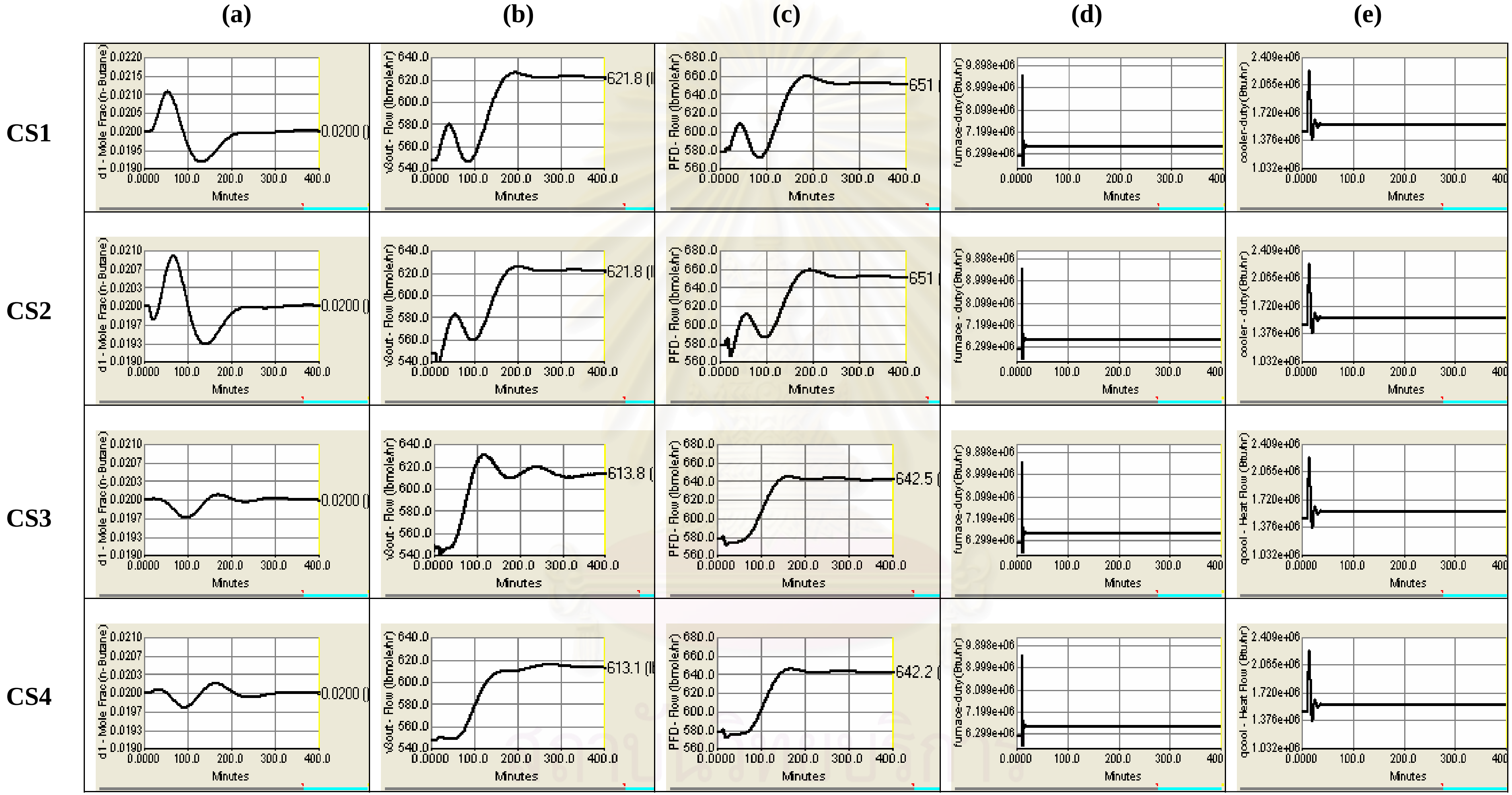


Figure 5.24: Dynamic responses of the Butane Isomerization plant alternative 1 to 10 °F increase in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1,CS2,CS3 and CS4.

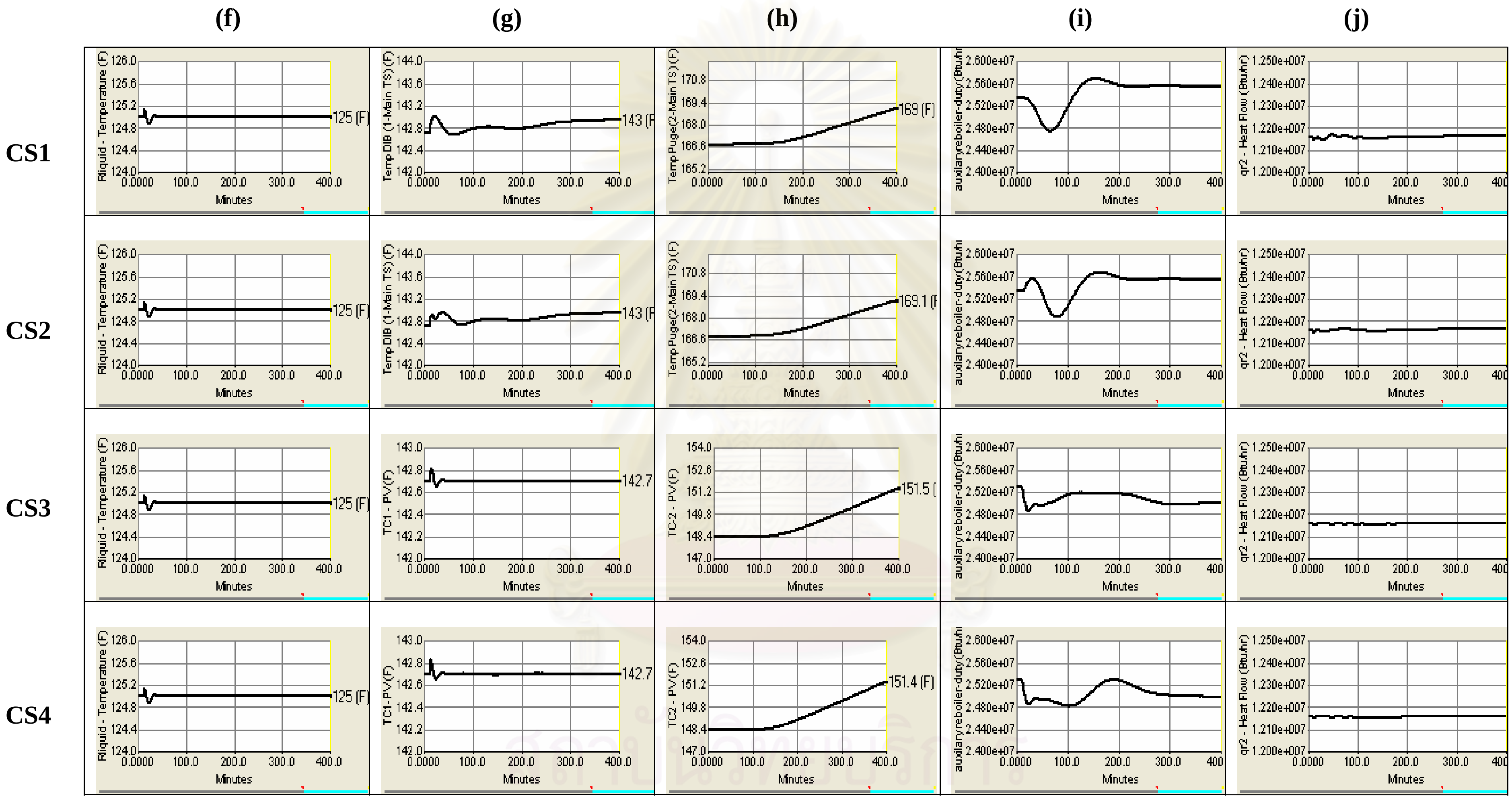


Figure 5.24: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

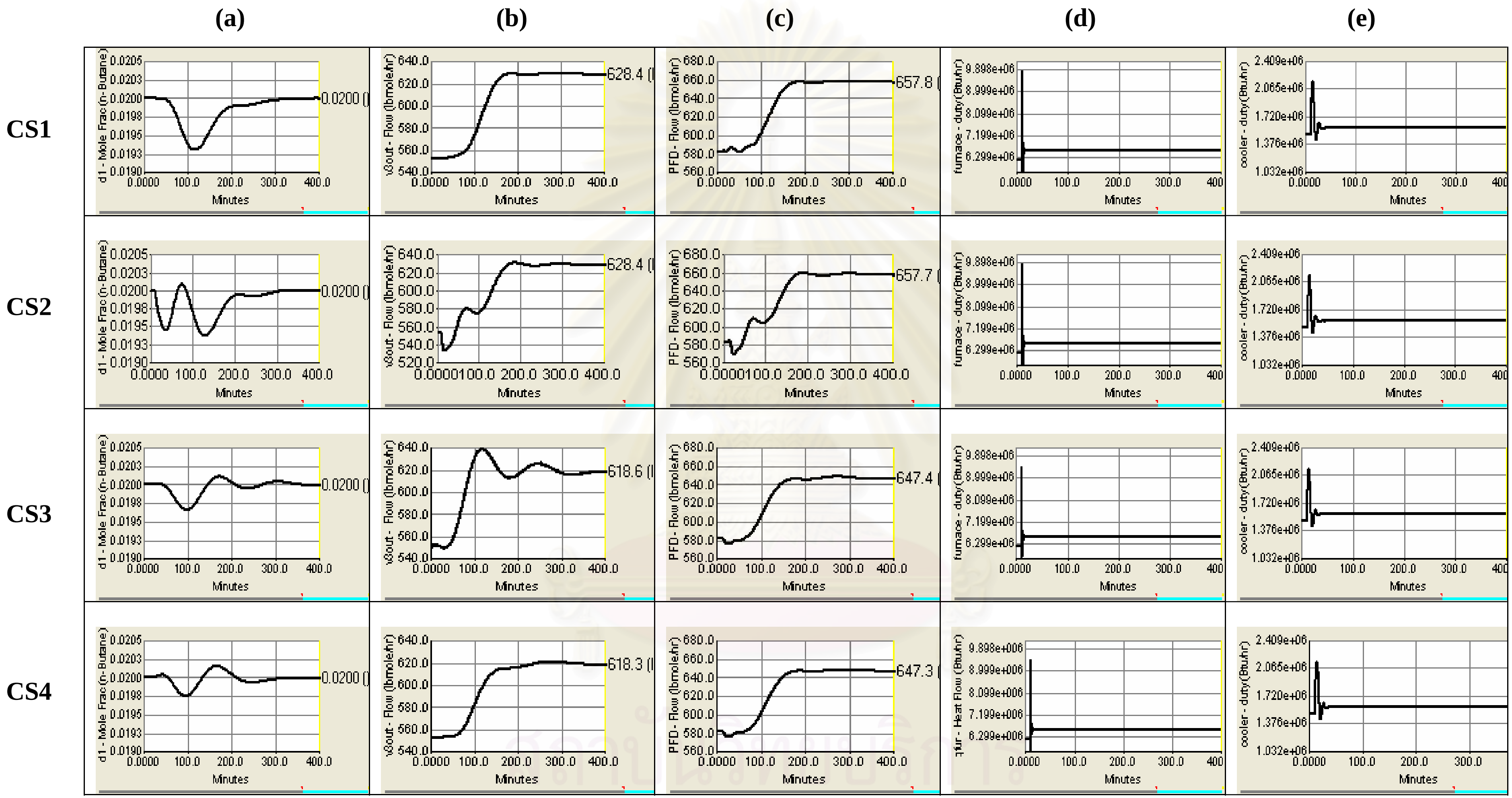


Figure 5.25: Dynamic responses of the Butane Isomerization plant alternative 2 to 10 ^{o}F increase in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the impurity of nC$_4$ in the product, (b) the iC$_4$ product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

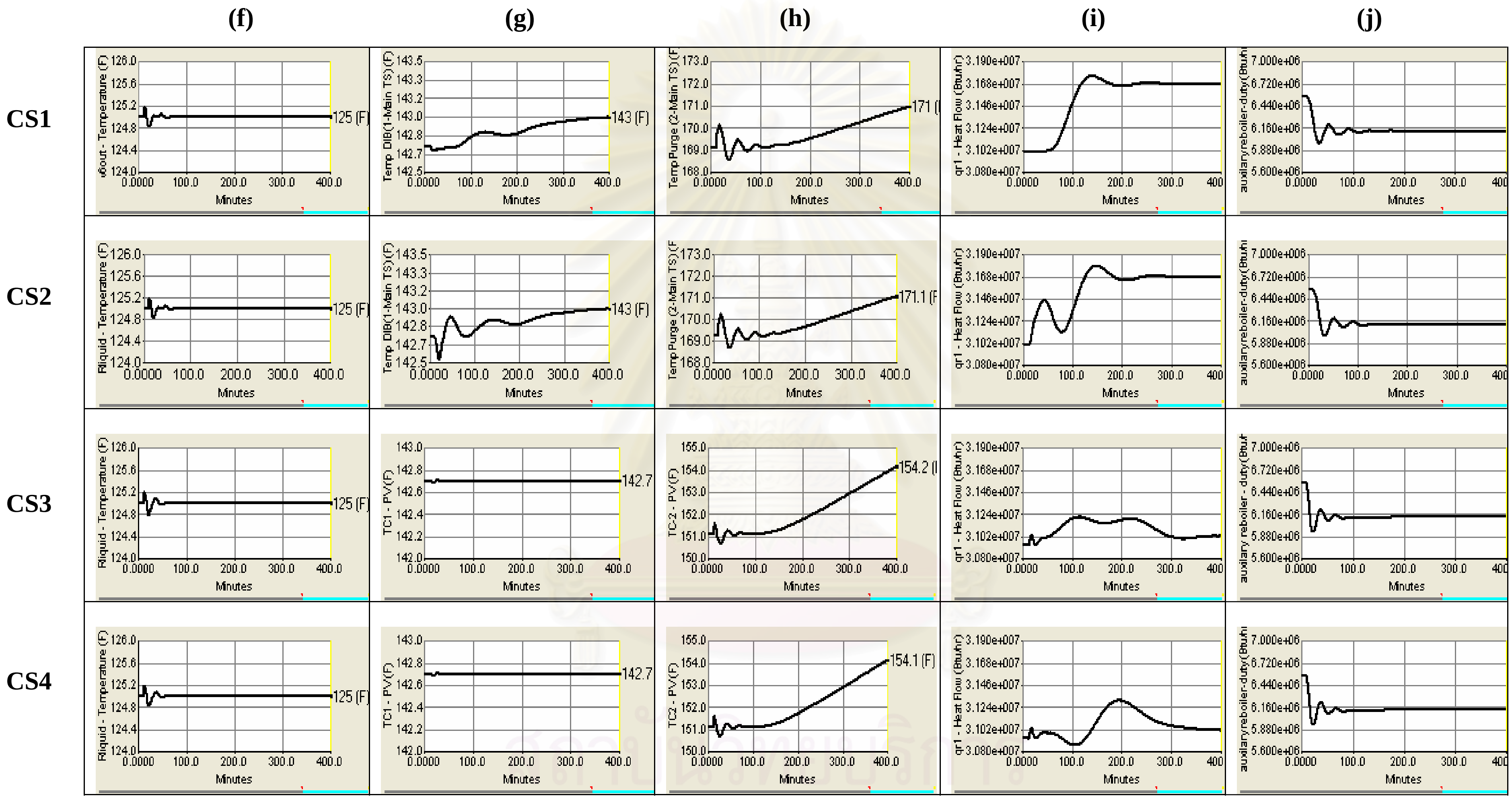


Figure 5.25: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

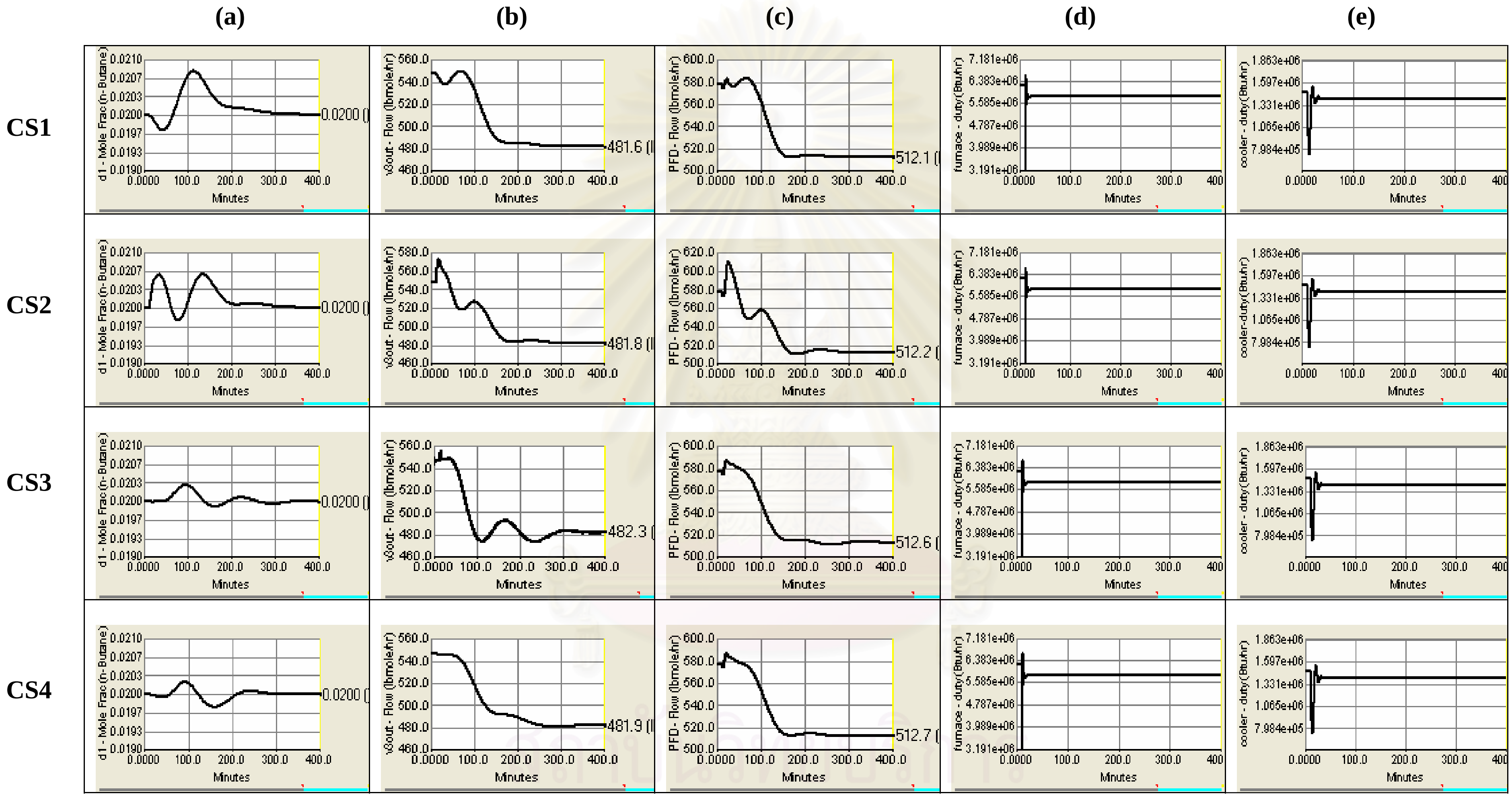


Figure 5.26 Dynamic responses of the Butane Isomerization plant alternative1 to 10 °F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

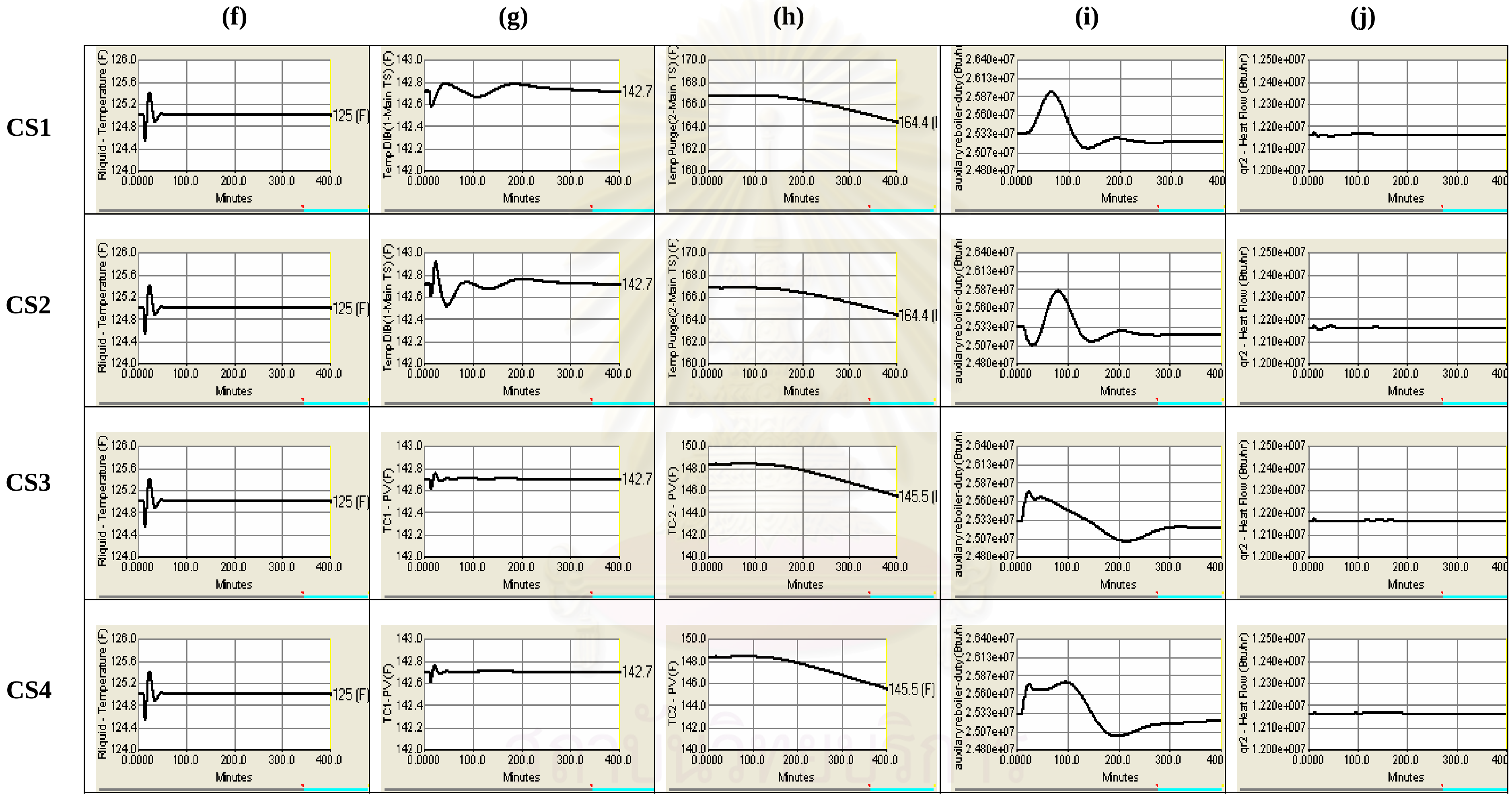


Figure 5.26: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

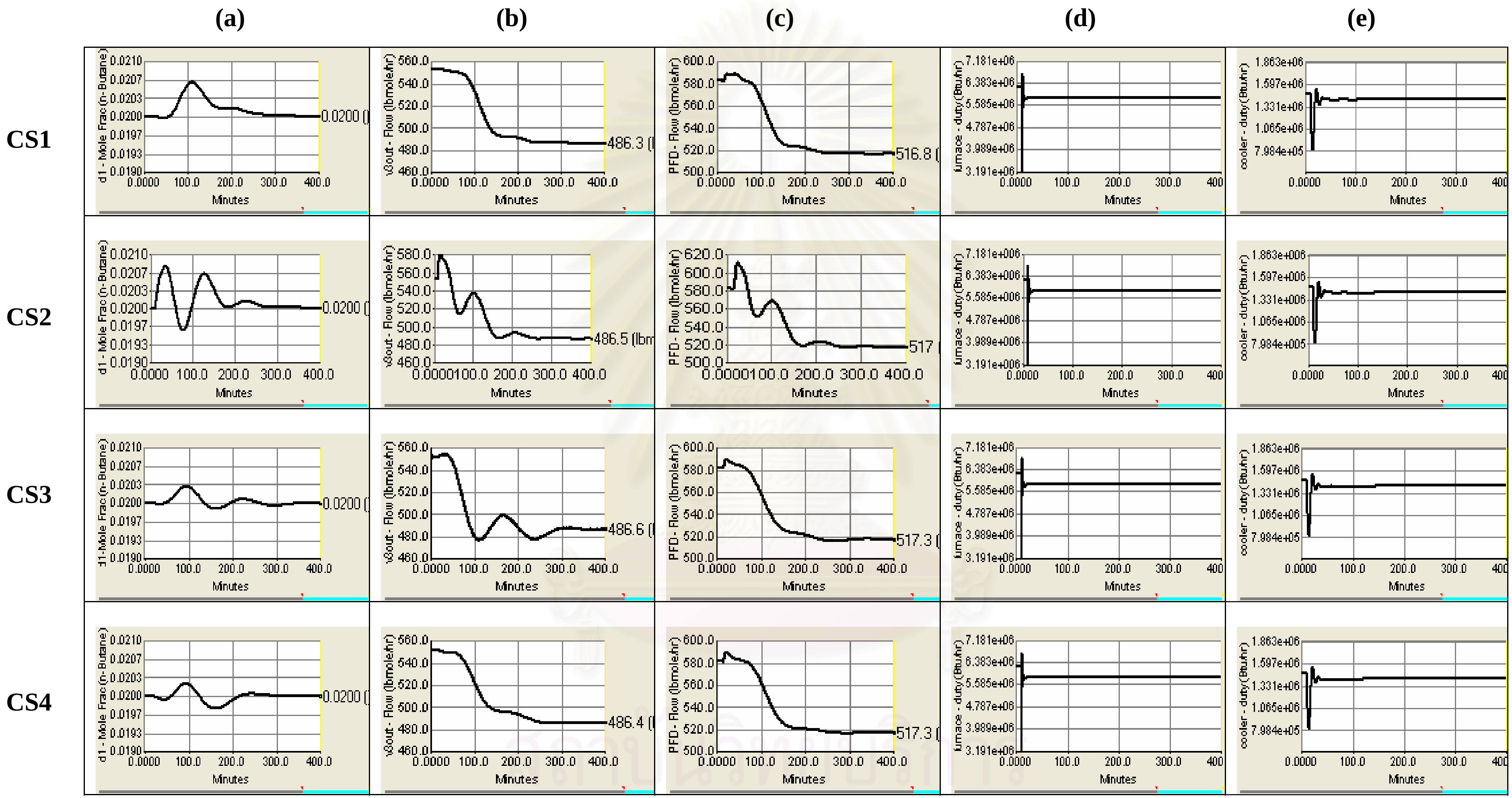


Figure 5.27: Dynamic responses of the Butane Isomerization plant alternative 2 to 10 ^{o}F decrease in reactor inlet temperature (the heat load disturbance of hot stream), where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

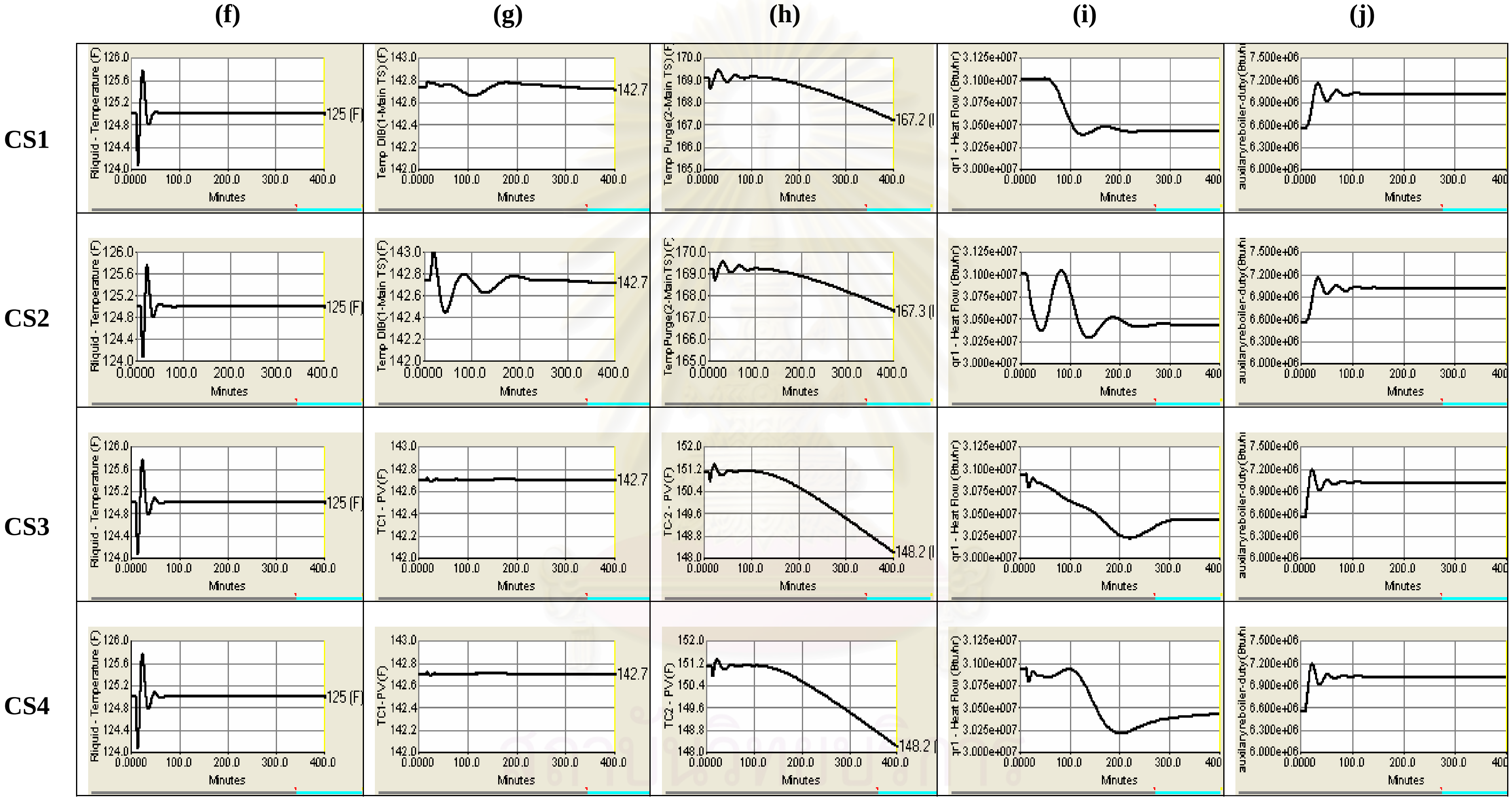


Figure 5.27: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

5.3.3 Change in the recycle flowrates for CS1 and CS2 in Butane Isomerization plant (Base Case)

Figure 5.28 shows the dynamic responses of CS1 in Butane Isomerization plant (Base Case) for increasing the recycle flowrate from 870 to 940.1lb.mol/h. If no other change is made, the effect is a slight decrease in production rate! This is certainly not what we would intuitively expect. This unusual behavior can be explained by considering what happens in the DIB column. More recycle means a higher feed rate to this column, which increases the column load. Since we are holding the purity of the distillate, the variability is all reflected in the bottoms stream. Thus there is an increase in the iC_4 impurity in the bottoms. This changes the reactor inlet composition to have a lower reactant (nC4) concentration. The result is a slight drop in the overall reaction rate.

Figure 5.29 gives results of CS1 in Butane Isomerization plant alternative1 for a step change in the setpoint of the recycle flowrate controller from 870.1 to 800.1lb.mol/h. The nC_4 impurity in the distillate (xD) slowly drops, and distillate flowrate is increased by the composition controller. It takes over four hours for distillate composition to return close to its setpoint (Figure 5.29d).

However, the fresh feed increases to match the distillate flow rate. These two streams must be identical at steady state. The increase in fresh feed is from 580 to about 600 lb-mol/hr (Figure 5.29f).

You might find it counter-intuitive that a decrease in the recycle results in an increase in production rate. This interesting effect occurs in adiabatic irreversible reactors with constant inlet temperature. It results because the lower flowrate through the adiabatic reactor means a higher exit temperature. The higher the temperature, the larger the reaction rate. Note in Figure 5.29b the increase in the reactor exit temperature Tout from its initial value of 424 ^{0}F up to 428 ^{0}F. So production increase when recycle flowrate decrease for irreversible reactions.

Figure 5.30 shows the dynamic responses of CS2 in Butane Isomerization plant alternative1 for increasing the recycle flowrate from 870 to 940.1 lb.mol/h and Figure 5.31 shows the effect of decreasing in the recycle flowrate from 870.1

to 800.1lb.mol/h. Fig 5.30 shows what happens if a ratio controller is used to increase the reflux flowrate in the DIB column as the recycle flowrate is increased. Now the fractionating capability of the column increase as the load is increased, so the bottom does not contain less nC_4 reactant. Product rate increases from 550 to 560.5lb.mol/h (Figure 5.30e).

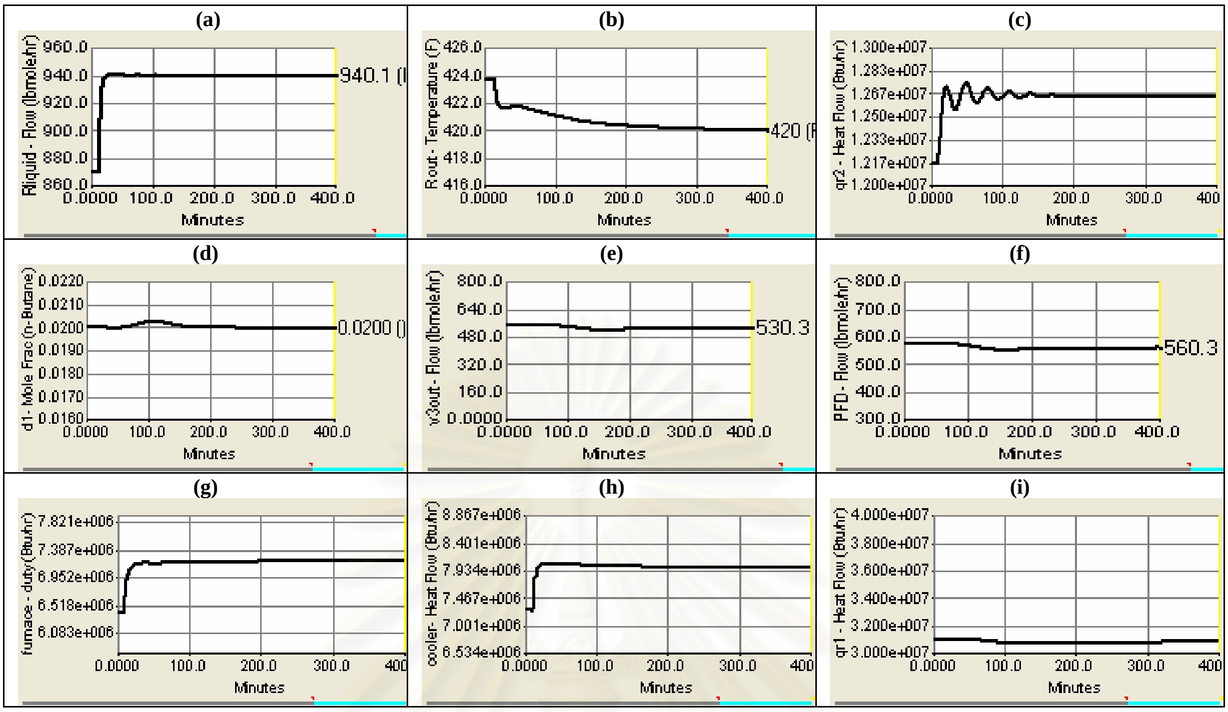


Figure 5.28: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1 lb.mol/h, where (a) the recycle flowrate, (b) the reactor outlet temperature, (c) the Purge column reboiler duty, (d) the impurity of nC_4 in the product, (e) the iC_4 product flowrate, (f) the fresh feed flowrate, (g) furnace duty, (h) cooler duty, (i) the DIB column reboiler duty.

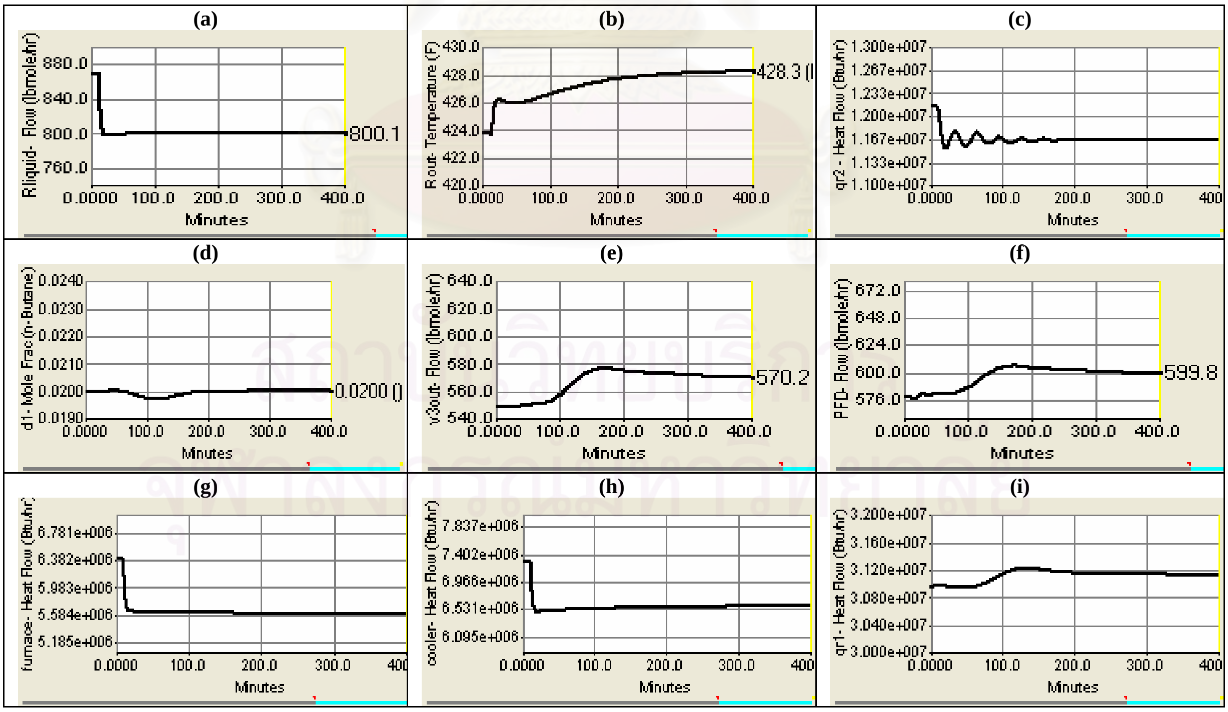


Figure 5.29: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to decrease in recycle flow from 870 to 800.1 lb.mol/h, where (a) the recycle flowrate, (b) the reactor outlet temperature, (c) the Purge column reboiler duty, (d) the impurity of nC_4 in the product, (e) the iC_4 product flowrate, (f) the fresh feed flowrate, (g) furnace duty, (h) cooler duty, (i) the DIB column reboiler duty.

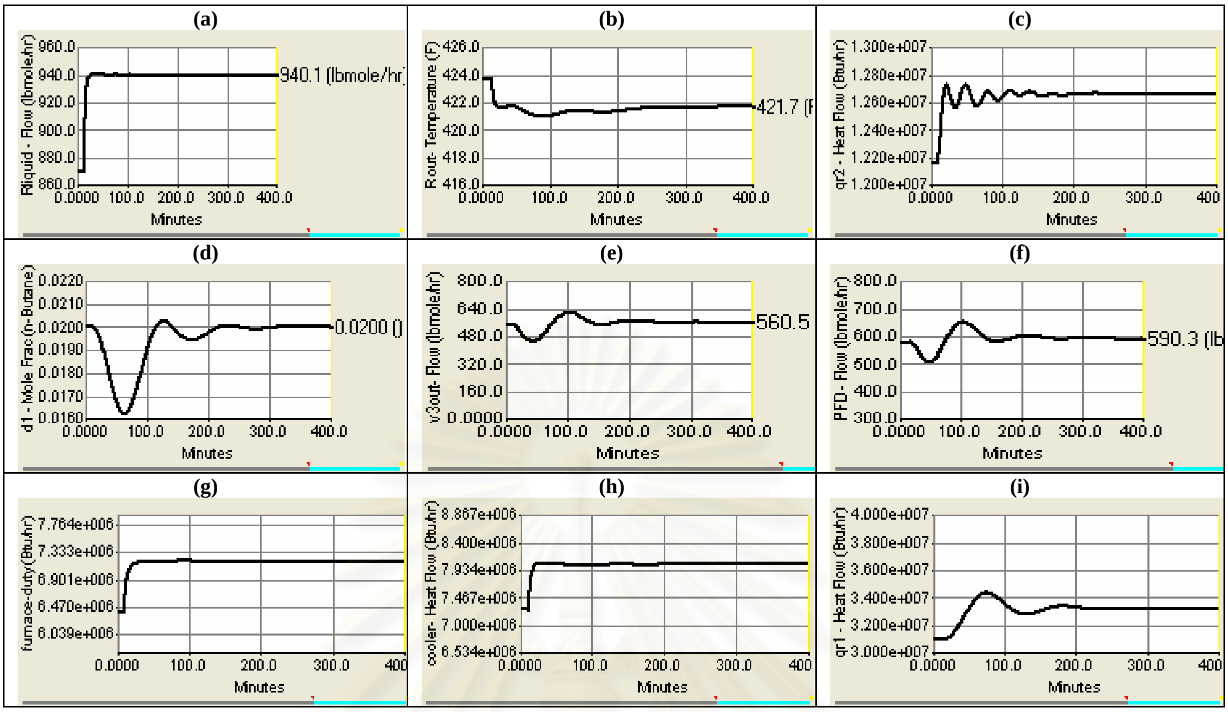


Figure 5.30: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1 lb.mol/h, where (a) the recycle flowrate, (b) the reactor outlet temperature, (c) the Purge column reboiler duty, (d) the impurity of nC_4 in the product, (e) the iC_4 product flowrate, (f) the fresh feed flowrate, (g) furnace duty, (h) cooler duty, (i) the DIB column reboiler duty.

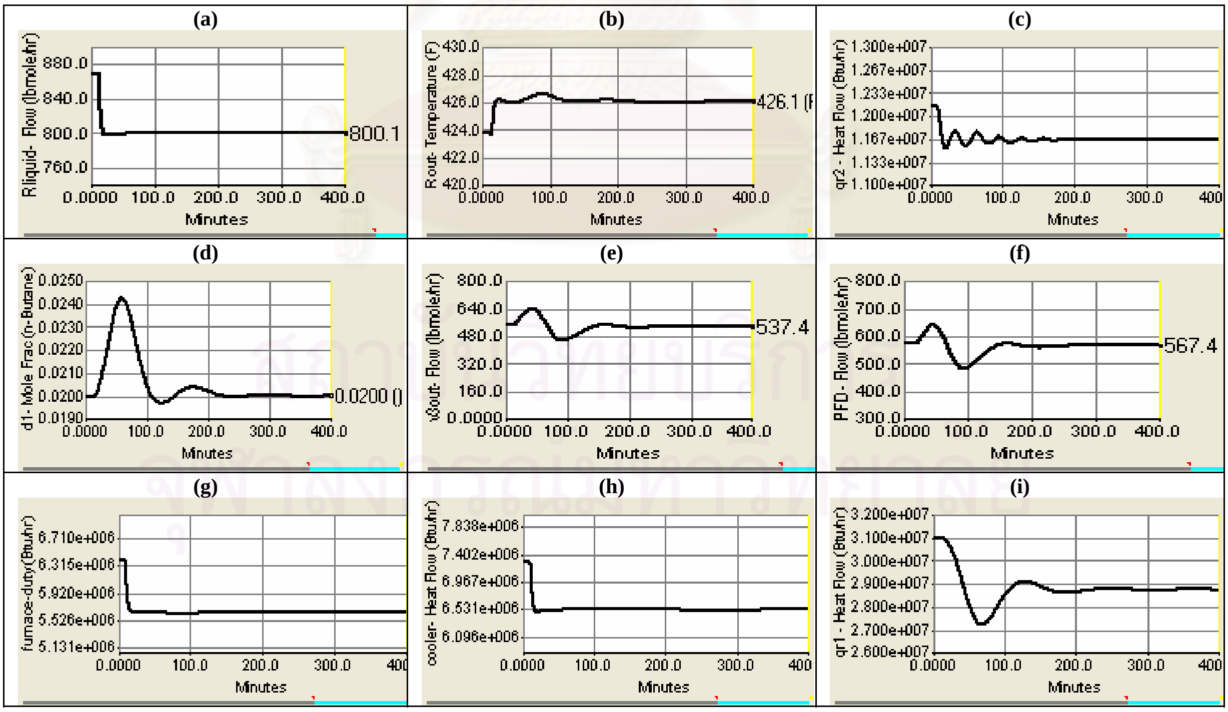


Figure 5.31: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to decrease in recycle flow from 870 to 800.1 lb.mol/h, where (a) the recycle flowrate, (b) the reactor outlet temperature,(c) the Purge column reboiler duty, (d) the impurity of nC_4 in the product, (e) the iC_4 product flowrate, (f) the fresh feed flowrate, (g) furnace duty, (h) cooler duty,(i) the DIB column reboiler duty.

5.3.4 Change in the recycle flowrates for Butane Isomerization plant alternatives 1 and 2

On the other case, a disturbance in the production rate is also made for this study. Figures 5.32 to 5.39 show the dynamic responses of the Butane Isomerization plant alternatives 1 and 2 to a change in the recycle flowrates (the disturbance loads of cold steam). This disturbance is made as follows: The recycle flowrates is increased from 870.1 to 940.1lb.mol/h at time equals 10 minutes, and the recycle flowrates is decreased from 870.1 to 800.1lb.mol/h at time equals 10 minutes. Again, the recycle flowrates response is very rapid; the new steady state is reached very quickly.

In general, the dynamic responses of the control system with the LSS for control structure 1 in Butane Isomerization plant alternatives 1 and 2 are similar with those to CS2, CS3 and CS4 in Butane Isomerization plant alternatives 1 and 2. As can be seen, the dynamic responses of the control system with the LSS in the current work are able to select proper heat pathway to carry the associated load to a utility unit.

When the cold inlet temperature of FEHE2 (Fig.5.32.e and 5.33.e) decreases due to the rise in recycle flowrates, the LSS will take an action to control the cold outlet temperature of FEHE2 (i.e. FEHE1 inlet temperature as shown in Fig.5.32.b and 5.33.b). The hot outlet temperature of FEHE2 quickly drops to a new steady state value (Fig.5.32.a and 5.33.a). Therefore, the cooler duty decreases (Fig.5.32c and 5.33.c), since the cooler inlet temperature (or the hot outlet temperature of FEHE2) decreases.

When the cold inlet temperature of FEHE2 (Fig.5.34.e and 5.35.e) increases due to the drop in recycle flowrates, the LSS switches the control action from TC-cHE2 to TC-hHE2. As a result, the hot outlet temperature of FEHE2 drops to its nominal value (Fig.5.34.a and 5.35.a). Therefore it is understandable that why the furnace duty decreases significantly (Fig. 5.34c and 5.35.c), since the cold outlet temperature of FEHE2 increases (Fig.5.34.b and 5.35.b). Thus, the negative disturbance load of cold stream will result in decrease of the furnace duty. The cooler duty is slightly maintained at its good level. The hot outlet temperatures of FEHE1 and EHE3 are well controlled.

However, the new control structures (CS3 and CS4) can handle more disturbances and are faster than the previous control structures (CS1 and CS2). Besides that the new control structures require less auxiliary reboiler utility consumptions are achieved compare to CS1 and CS2, because CS3 and CS4 control structures are modified by manipulating auxiliary reboiler duty to control the temperature on tray1 of DIB column and Purge column.

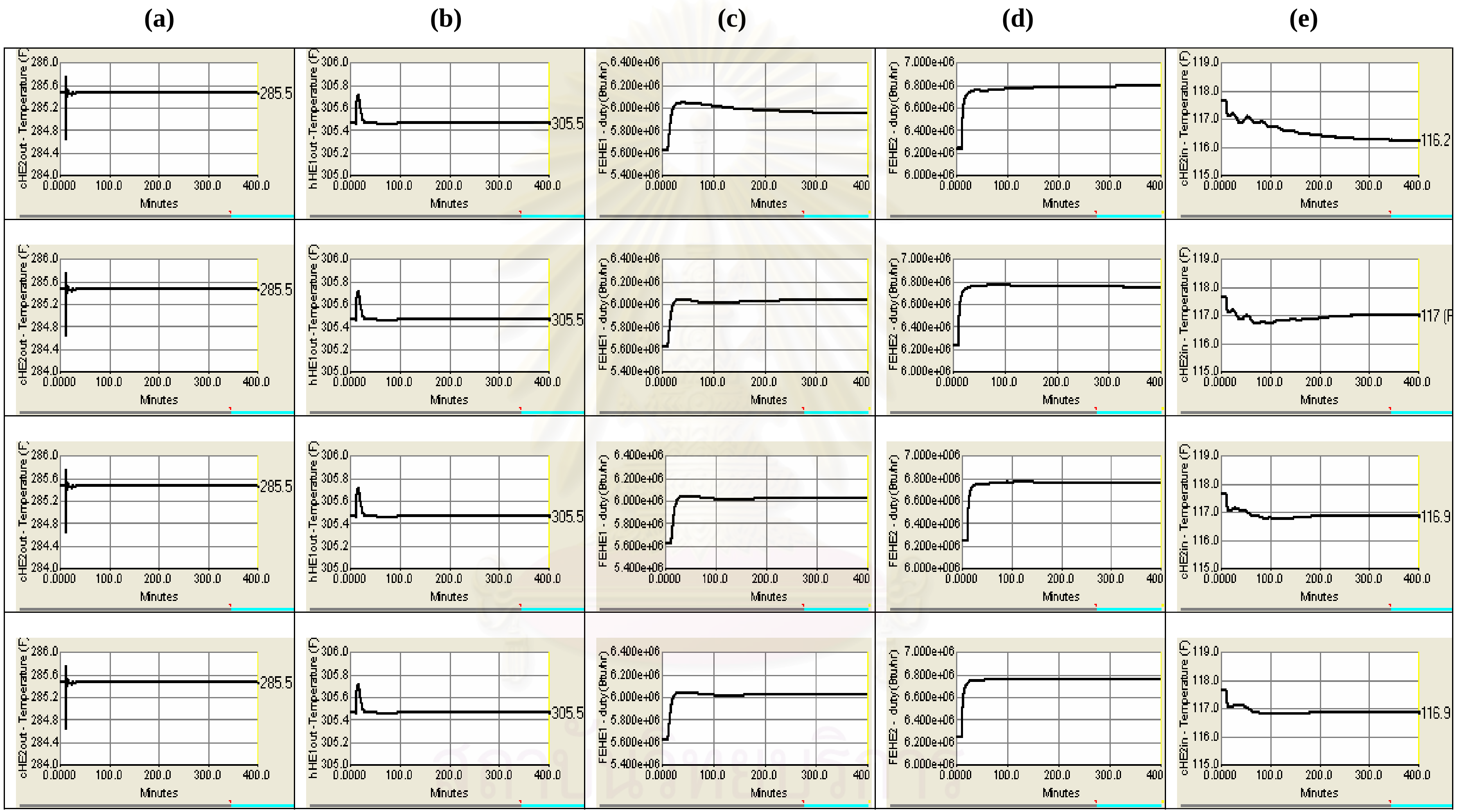


Figure 5.32: Dynamic responses of the Butane Isomerization plant alternative 1 to increase in recycle flow from 870 to 940.1lb.mol/h ,where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the cold inlet temperature of FEHE2; comparison between CS1,CS2,CS3 and CS4.

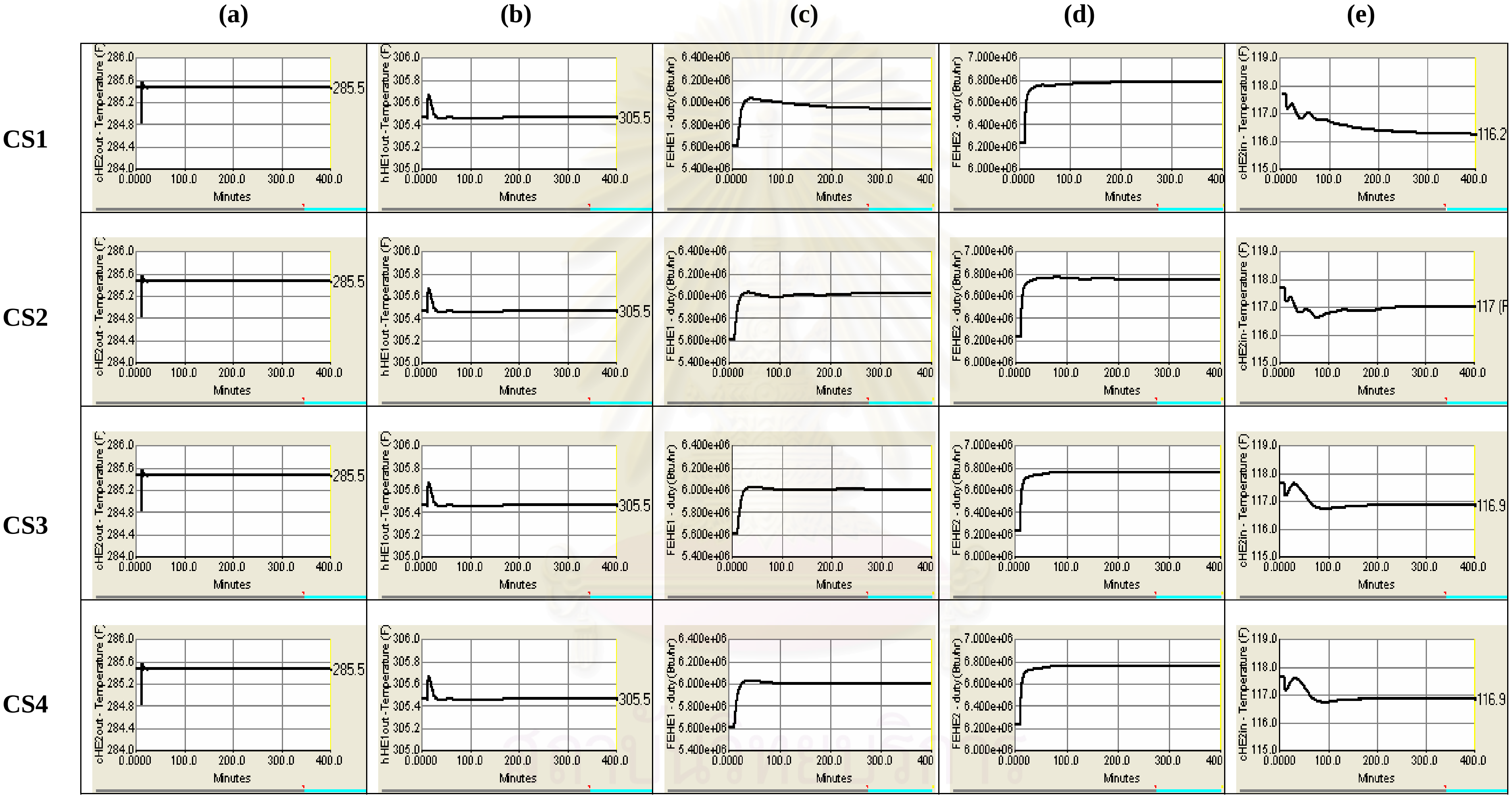


Figure 5.33: Dynamic responses of the Butane Isomerization plant alternative 2 to increase in recycle flow from 870 to 940.1lb.mol/h ,where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the cold inlet temperature of FEHE2; comparison between CS1,CS2,CS3 and CS4.

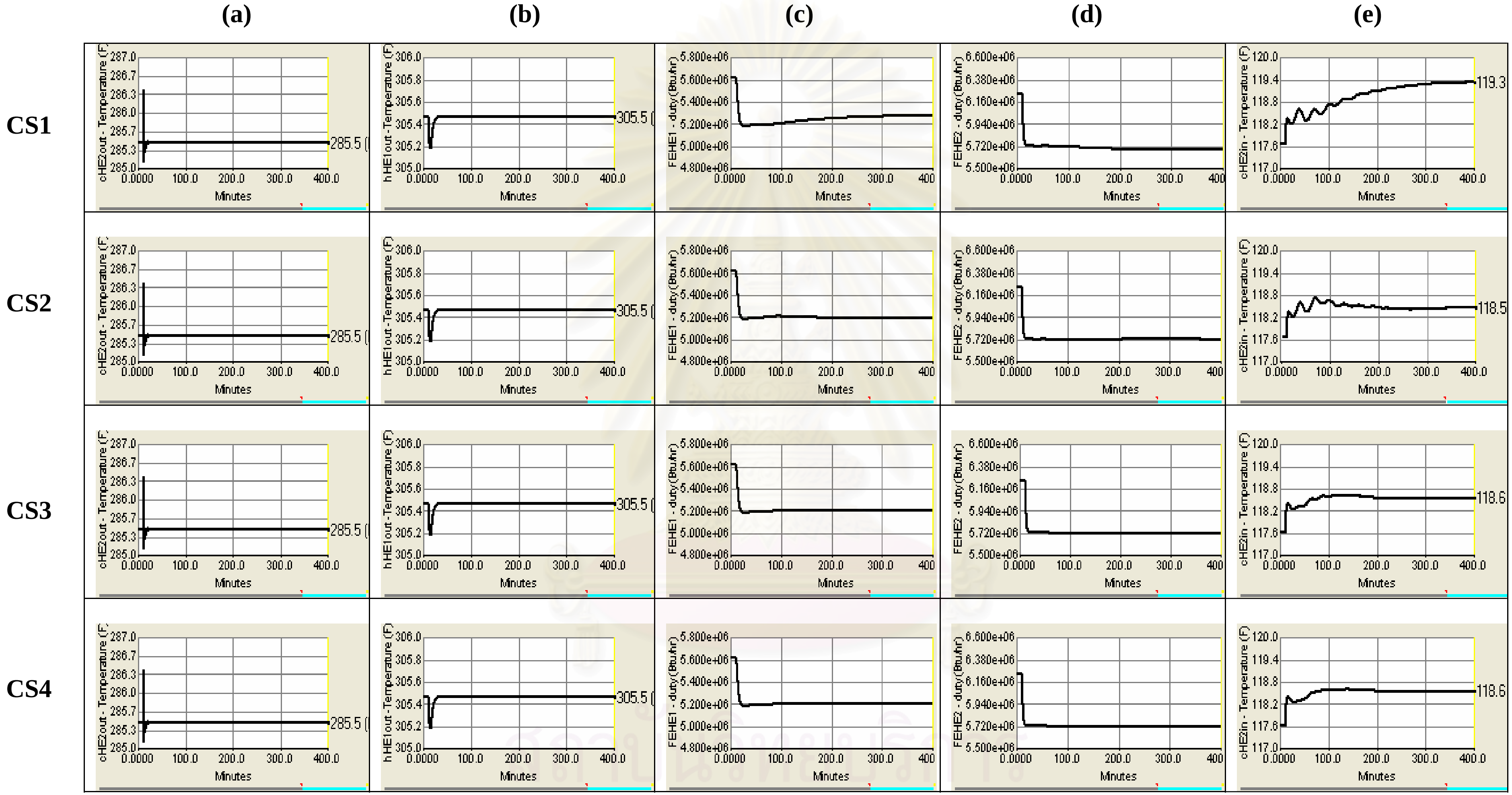


Figure 5.34: Dynamic responses of the Butane Isomerization plant alternative 1 to decrease in recycle flow from 870 to 800.1lb.mol/h. ,where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the cold inlet temperature of FEHE2; comparison between CS1,CS2,CS3 and CS4.

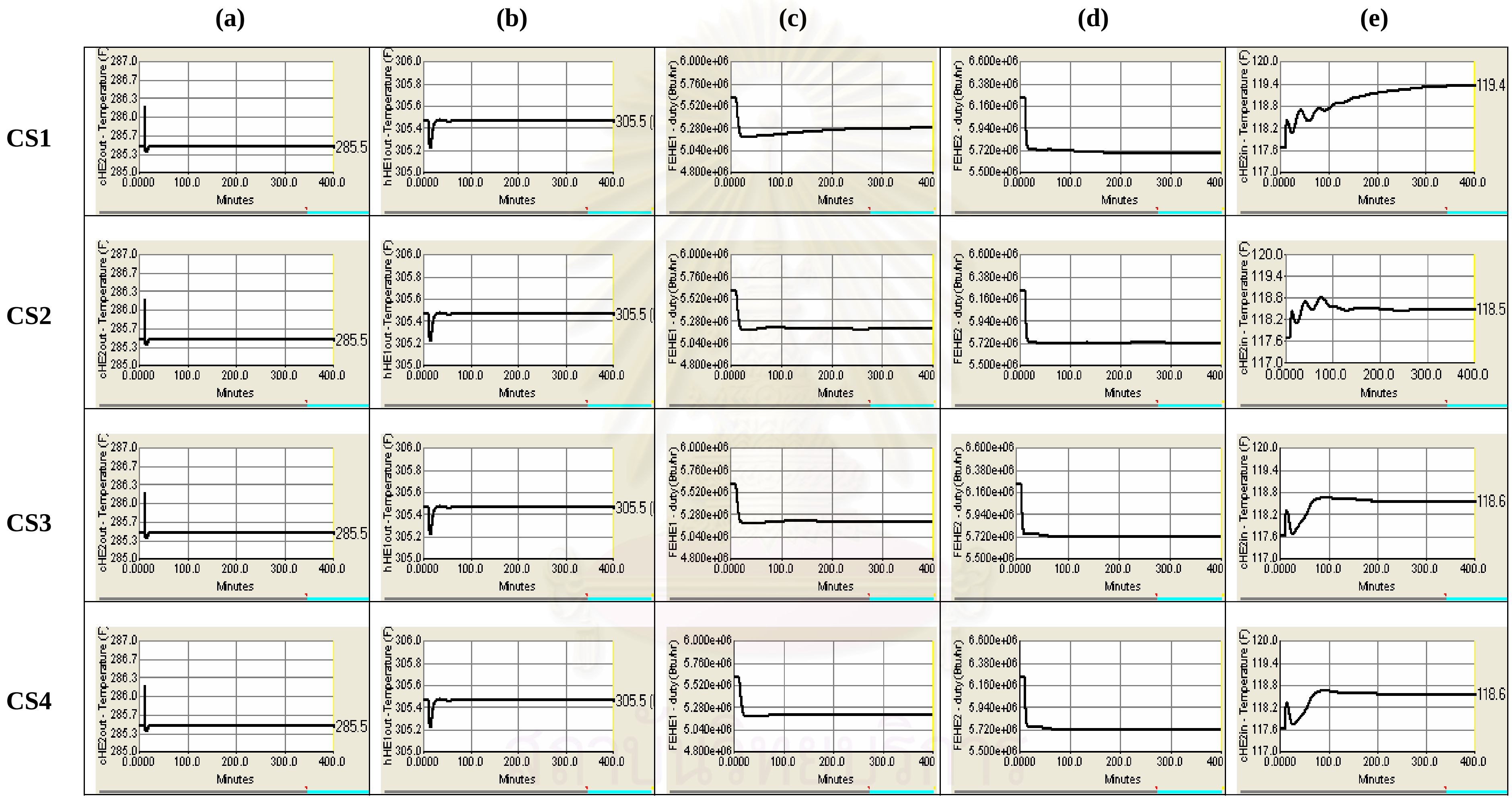


Figure 5.35: Dynamic responses of the Butane Isomerization plant alternative 2 to decrease in recycle flow from 870 to 800.1lb.mol/h. ,where (a) the cold outlet temperature of FEHE2, (b) the hot outlet temperature of FEHE1, (c) FEHE1 duty, (d) FEHE2 duty, (e) the cold inlet temperature of FEHE2; comparison between CS1,CS2,CS3 and CS4.

5.3.4.1 The dynamic responses of CS1 control structure

Figures 5.36 and 5.37 give the simulation results for increasing the recycle flowrate from 870 to 940.1lb.mol/h. If no other change is made, the effect 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.

Figures 5.36.a,b,c and 5.37.a,b,c show the impurity of nC_4 in the product, the iC_4 product flow and the fresh feed flow. The fresh feed flow and the iC_4 product flow are slowly decreased about 200 minute to new steady-state due to reaction rate decreasing. But the impurity of nC_4 in product does not see the changing.

Figures 5.38 and 5.39 give results for a step change in the setpoint of the recycle flowrate controller from 870.1 to 800.1lb.mol/h. The nC_4 impurity in the distillate (xD) slowly drops, and distillate flowrate is increased by the composition controller. It takes over four hours for distillate composition to return close to its setpoint. Fresh feed initially decreases because the decrease in the bottom flow raises base level. However, eventually the fresh feed increases to match the distillate flow rate. These two streams must be identical at steady state. The increase in fresh feed is from 580 to about 600 lb-mol/hr (Fig 5.38c and Fig5.39c).

As can be seen, the dynamic responses of CS1 in Butane Isomerization process alternative 1 are slower than those in Butane Isomerization process (Base Case).

Again, the dynamic responses of CS1 in Butane Isomerization alternative 2 are slower than those in alternative 1. Most of control loops in alternative 2 are more oscillatory than those in alternative 1. The reactor inlet temperature and the cooler outlet temperature (Fig 5.36.f to 5.39.f) are slightly well controlled. But, the dynamic response of the nC_4 impurity in product is less oscillatory than those in alternative 1.

For a complex energy-integrated plant, it is important to control the temperature on bottom tray of column such as the dynamic responses of CS1 and CS2 in Butane Isomerization plant alternatives 1 and 2 don't control the temperature on tray1 of DIB column, so when less iC_4 is produced in the reactor with increasing the recycle flowrate at constant reactor inlet temperature, the purity of DIB distillate improves (more nC_4 in the overhead product), which causes the DIB column auxiliary reboiler duty in alternative 1 and DIB column reboiler duty in alternative 2 to decrease (Fig 5.36.i and 5.37.i).

In contrast, when more iC_4 is produced in the reactor with decreasing the recycle flowrate at constant reactor inlet temperature, the purity of DIB distillate improves (less nC_4 in the overhead product), which causes the DIB column auxiliary reboiler duty in alternative 1 and DIB column reboiler duty in alternative 2 to increase.(Fig 5.38.i and 5.39.i).

5.3.4.2 The dynamic responses of CS2 control structure

Figures 5.36 and 5.37 show the dynamic responses of the process for increasing the recycle flowrate from 870 to 940.1lb.mol/h. The dynamic responses of CS2 are slower than CS1, but the CS2 control structure can increase the product flowrate in the DIB column. It results because a ratio controller is used to increase the reflux flowrate in the DIB column as the recycle flowrate is increased.

Figures 5.36a and 5.37a show the nC_4 impurity in the distillate (xD) slowly drops. It takes over four hours for distillate composition to return close to its setpoint.

Figures 5.38 and 5.39 give results for a step change in the setpoint of the recycle flowrate controller from 870.1 to 800.1lb.mol/h. The nC_4 impurity in the distillate (xD) slowly raises (Fig 5.38.a and 5.39.a), and distillate flowrate is decreased. It takes over four hours for distillate composition to return close to its setpoint.

As can be seen, the dynamic responses of CS2 in Butane Isomerization process alternative 1 are slower than those in Butane Isomerization process (Base Case).

Again, the dynamic responses of CS2 in Butane Isomerization alternative 2 are slower than those in alternative 1. Most of control loops in alternative 2 are more oscillatory than those in alternative 1. The reactor inlet temperature and the cooler outlet temperature (Fig 5.36.f to 5.39.f) are slightly well controlled. But, the dynamic response of the nC_4 impurity in product is less oscillatory than those in alternative 1.

5.3.4.3 The dynamic responses of CS3 control structure

Figures 5.36 to 5.39 show the dynamic responses of the process for increasing the recycle flowrate and decreasing the recycle flowrate. The dynamic responses of this control structure are faster than CS1 and CS2 because the reflux flow can control the reflux drum level more effective than the distillate flow. But we control distillate composite manipulating the distillate flowrate, so the iC_4 product flow has large changes. However, in this case we assume that the distillate is going to a storage tank or cavern.

Figures 5.36a to 5.39a show the nC_4 impurity in the distillate (xD) is less oscillatory than other control structures and this control structure can increase the iC4 product flowrate.

Figures 5.36.g to 5.39.g and Figures 5.36.h to 5.39.h show the temperature control in 2 distillation columns. The temperature response of DIB column does not see the changing. But the temperature response of Purge column will change to follow the level of Purge column condenser (cascade from level control of Purge column condenser).

As can be seen, the dynamic responses of CS3 in Butane Isomerization process alternative 1 are similar with those in alternative 2. Some control loops (such as the tray temperature of Purge column, the reactor inlet temperature, the cooler outlet temperature and the pressure of Purge column condenser) in Butane Isomerization process alternative 2 are more oscillatory than those in alternative 1. But, the dynamic response of the nC_4 impurity of product in alternative is less oscillatory than those in alternative 1.

5.3.4.4 The dynamic responses of CS4 control structure

Figures 5.36 to 5.39 show the dynamic responses of the process for increasing the recycle flowrate and decreasing the recycle flowrate. The dynamic responses of this control structure are the fastest compare with the other control structures because the reflux flow can control the nC4 impurity in product more effective than the distillate flow.

Figures 5.36a to 5.39a show the nC_4 impurity in the distillate (xD) is slight change from the setpoint and this control structure can increase the iC_4 product flowrate.

Figures 5.36.g to 5.39.g and Figures 5.36.h to 5.39.h show the temperature control in 2 distillation columns. The temperature response of DIB column does not see the changing. But the temperature response of Purge column will change to follow the level of Purge column condenser (cascade from level control of Purge column condenser).

As can be seen, the dynamic responses of CS4 in Butane Isomerization process alternative 1 are similar with those in alternative 2. Some control loops (such as the tray temperature of Purge column, the reactor inlet temperature, the cooler outlet temperature and the pressure of Purge column condenser) in Butane Isomerization process alternative 2 are more oscillatory than those in alternative 1. But, the dynamic response of the nC_4 impurity of product in alternative is less oscillatory than those in alternative 1.

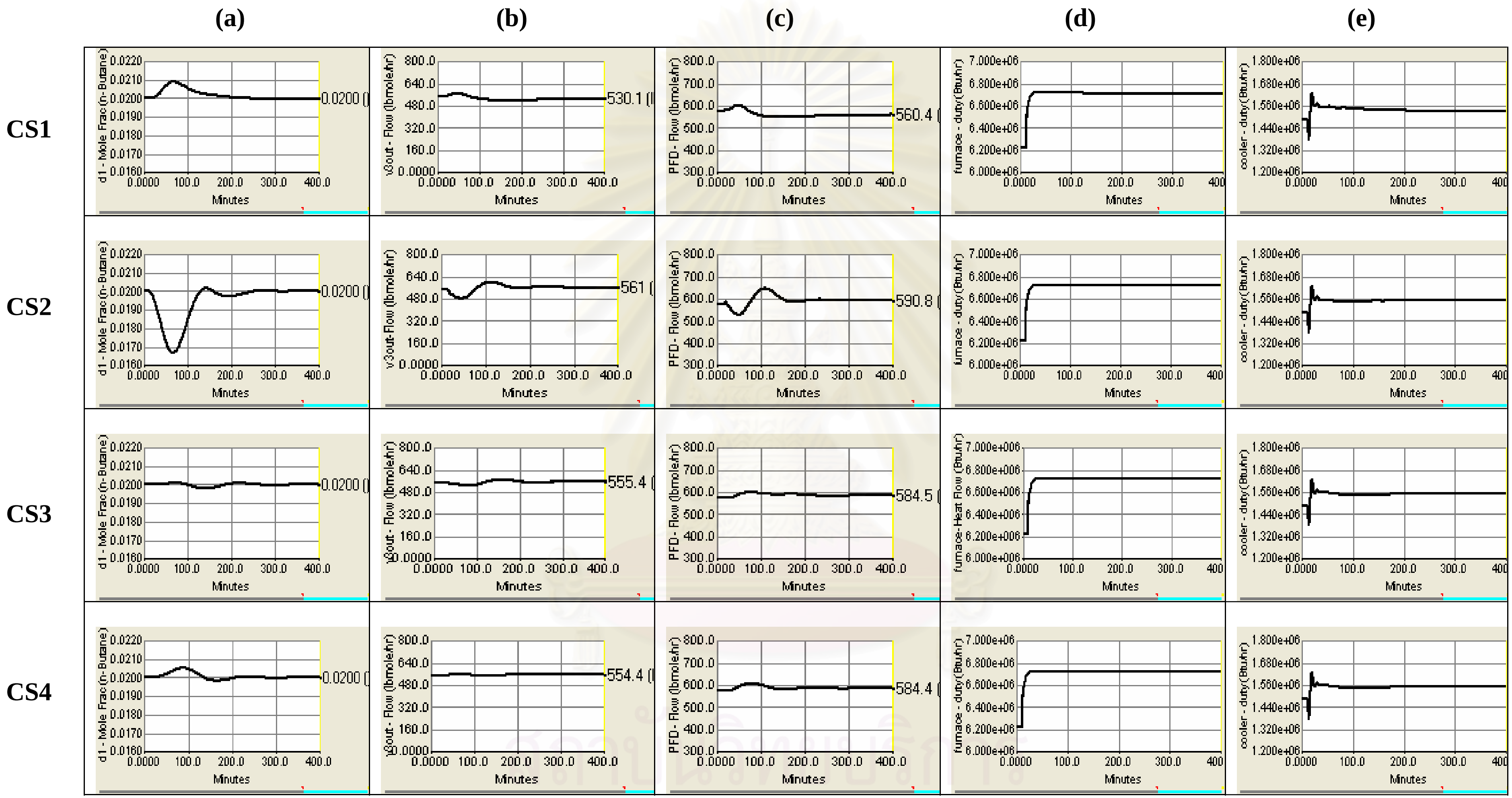


Figure 5.36: Dynamic responses of the Butane Isomerization plant alternative 1 to increase in recycle flow from 870 to 940.1lb.mol/h , where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

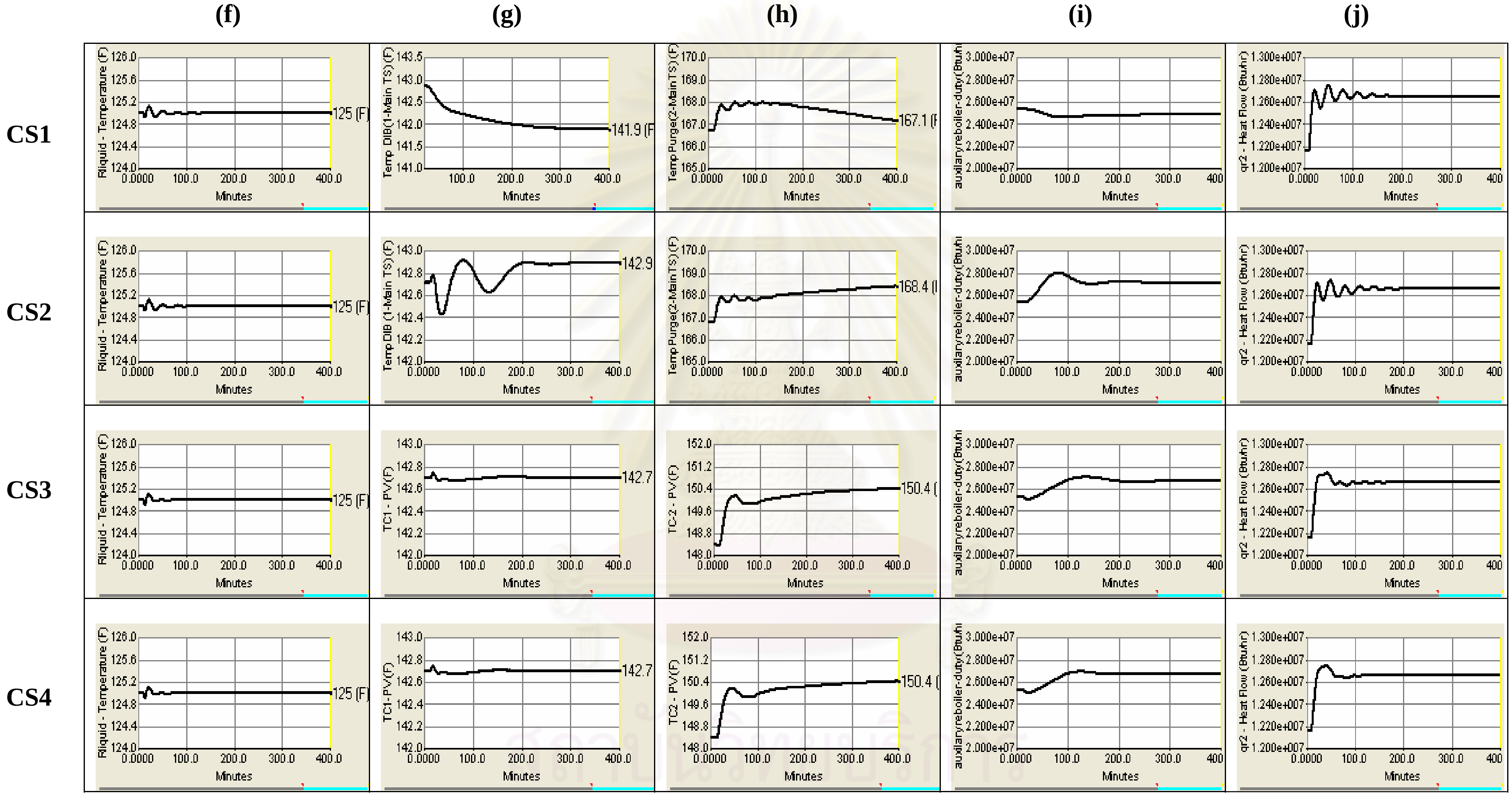


Figure 5.36: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

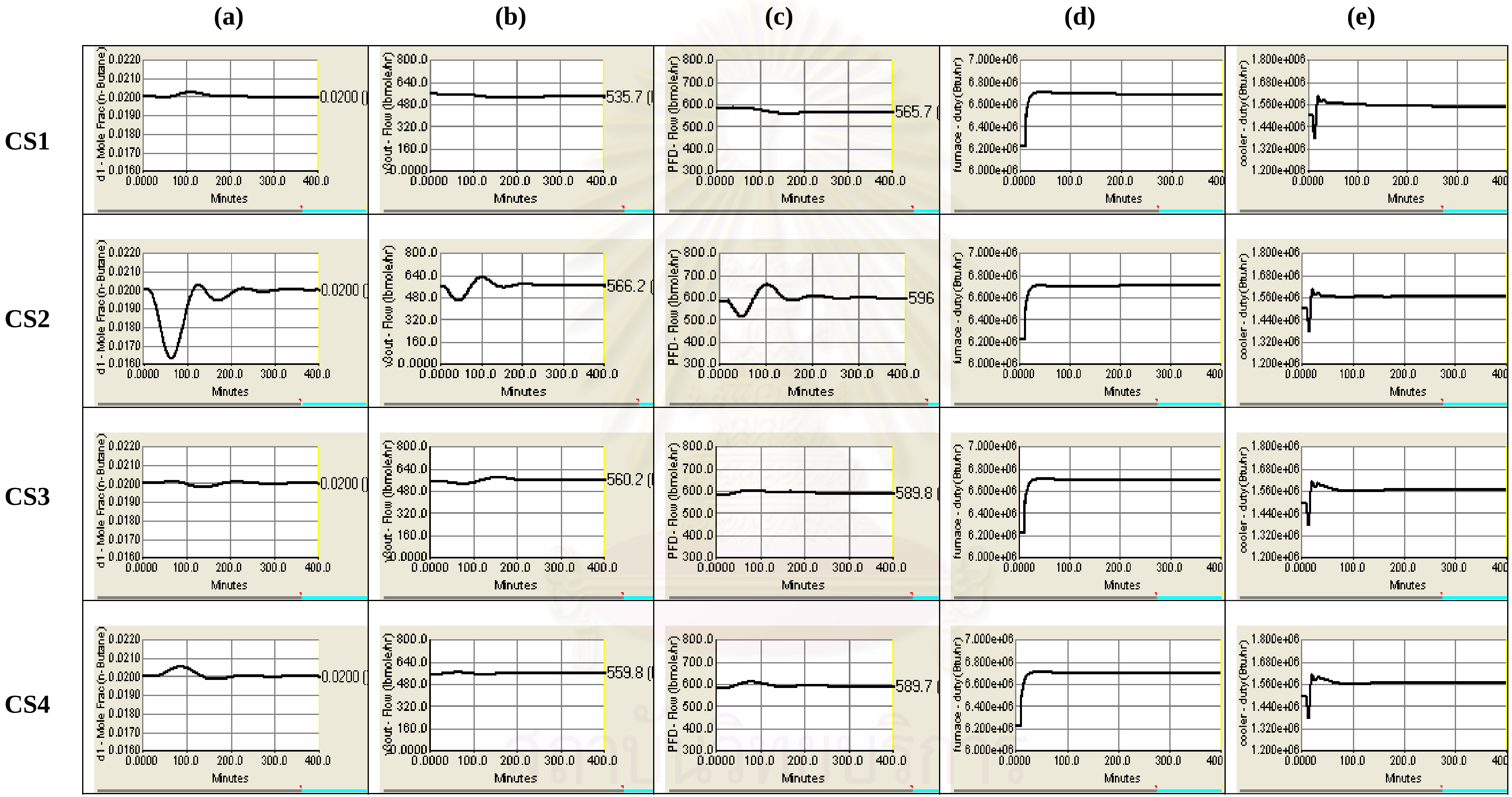


Figure 5.37: Dynamic responses of the Butane Isomerization plant alternative 2 to increase in recycle flow from 870 to 940.1lb.mol/h , where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

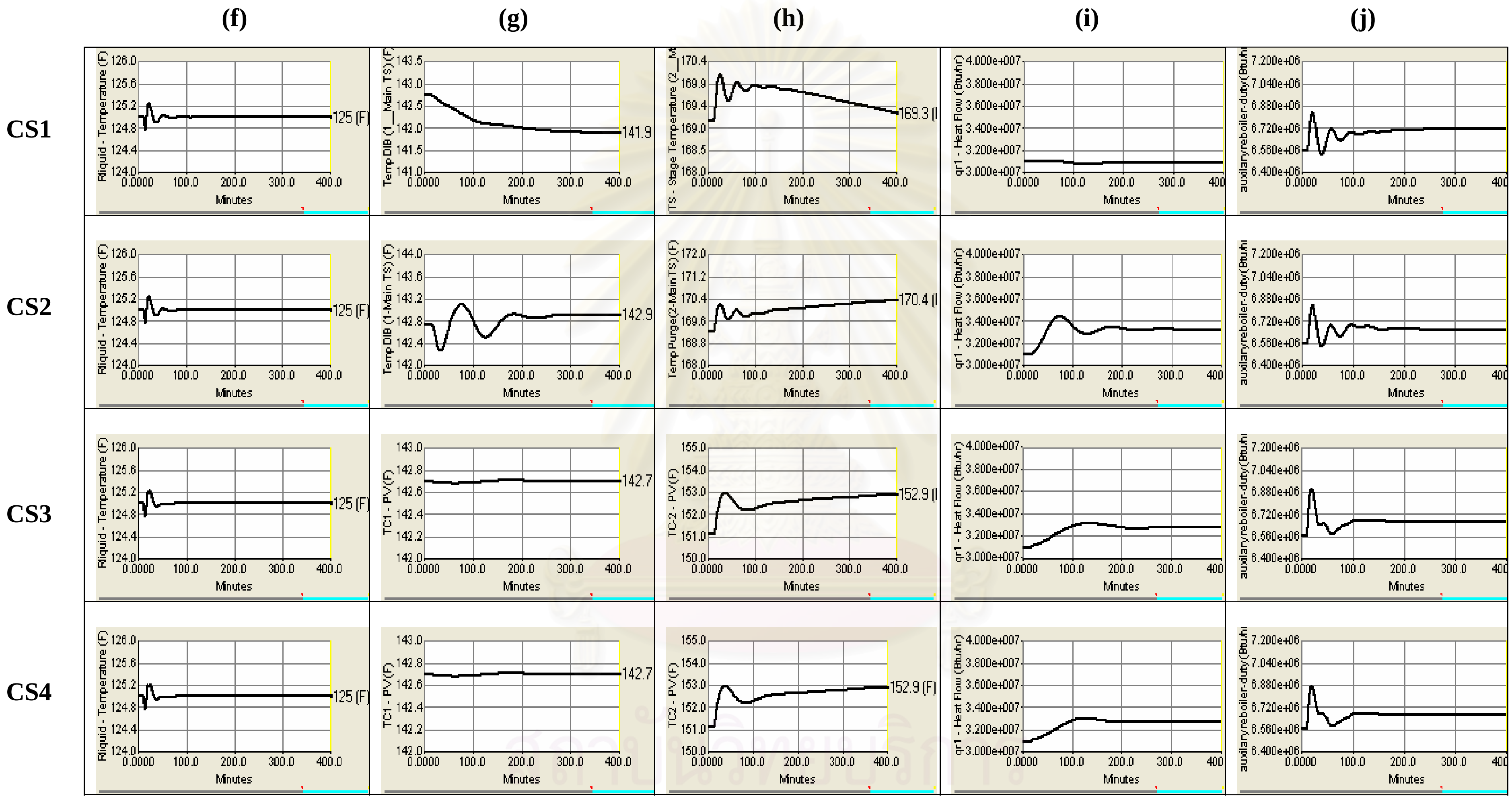


Figure 5.37: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

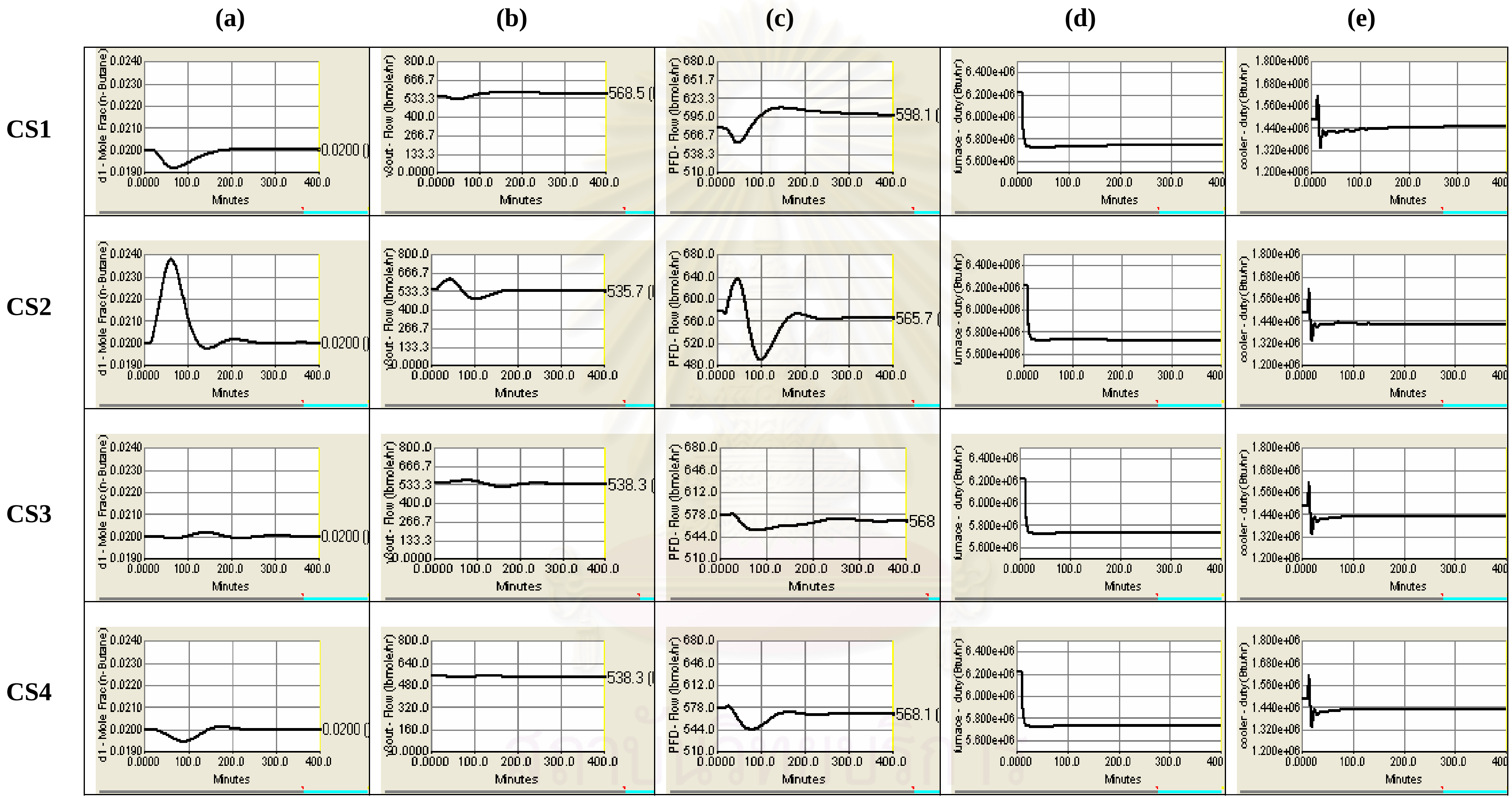


Figure 5.38: Dynamic responses of the Butane Isomerization plant alternative 1 to decrease in recycle flow from 870 to 800.1lb.mol/h. , where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

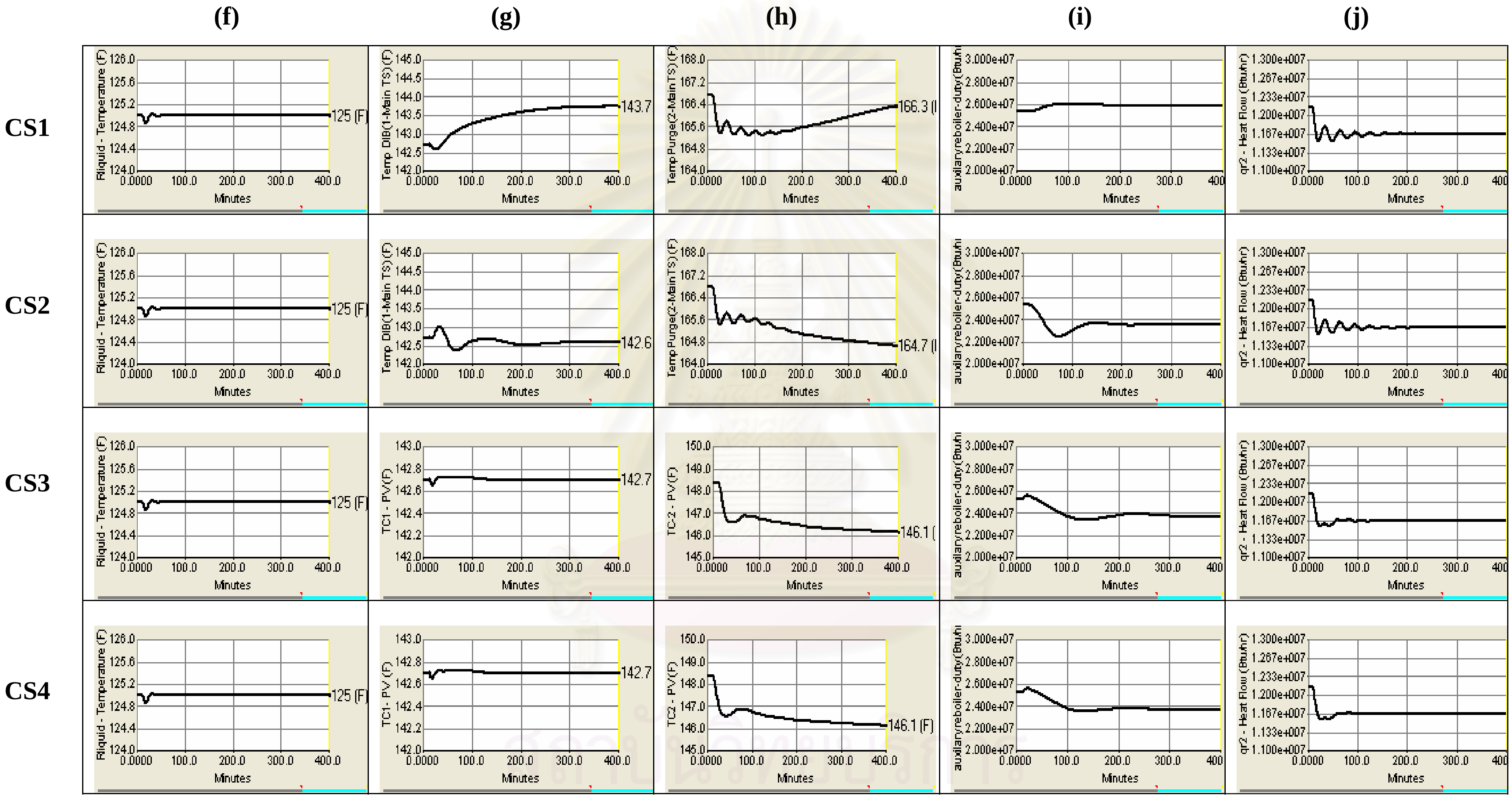


Figure 5.38: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

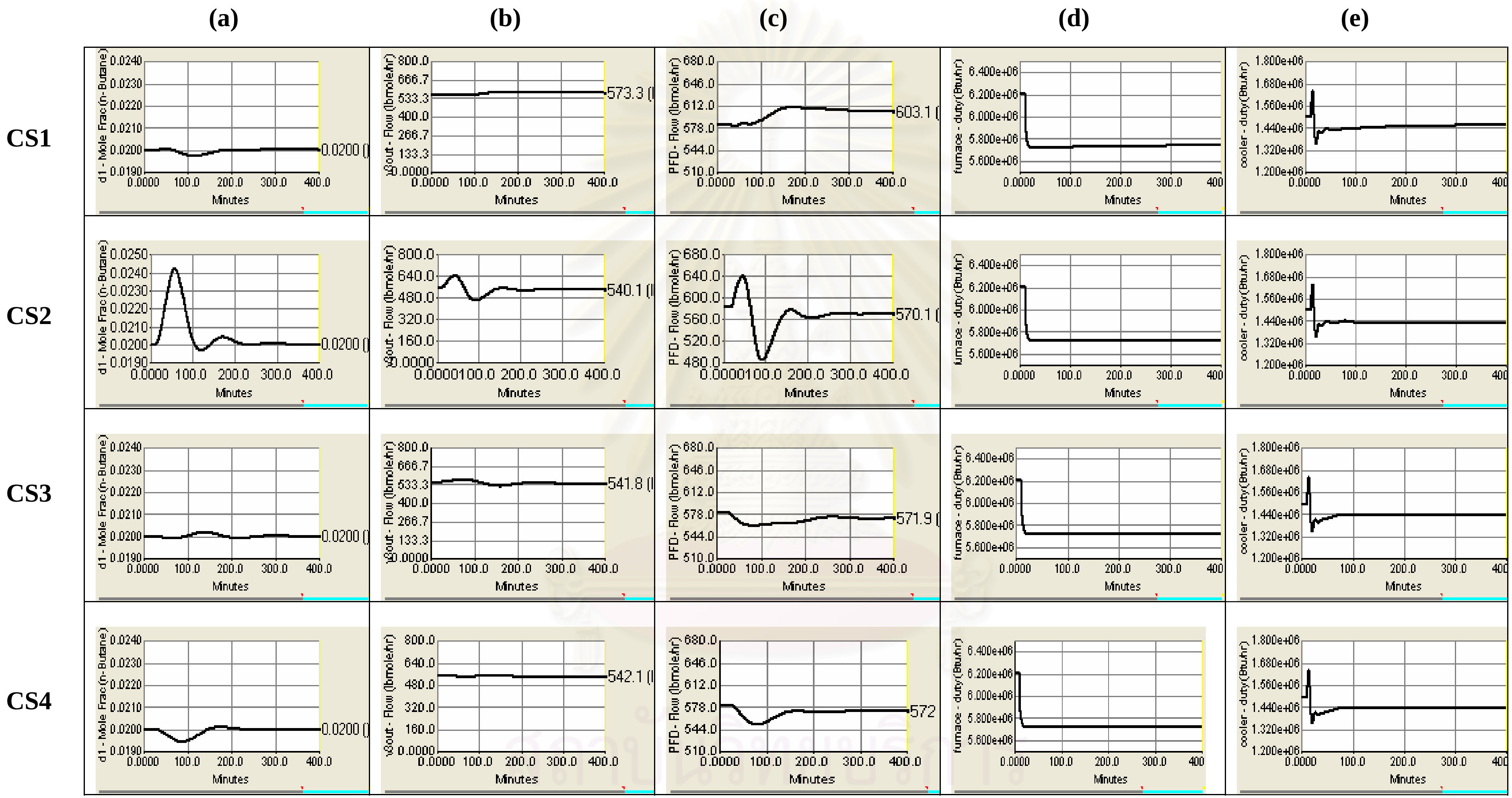


Figure 5.39: Dynamic responses of the Butane Isomerization plant alternative 2 to decrease in recycle flow from 870 to 800.1lb.mol/h. , where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1, CS2, CS3 and CS4.

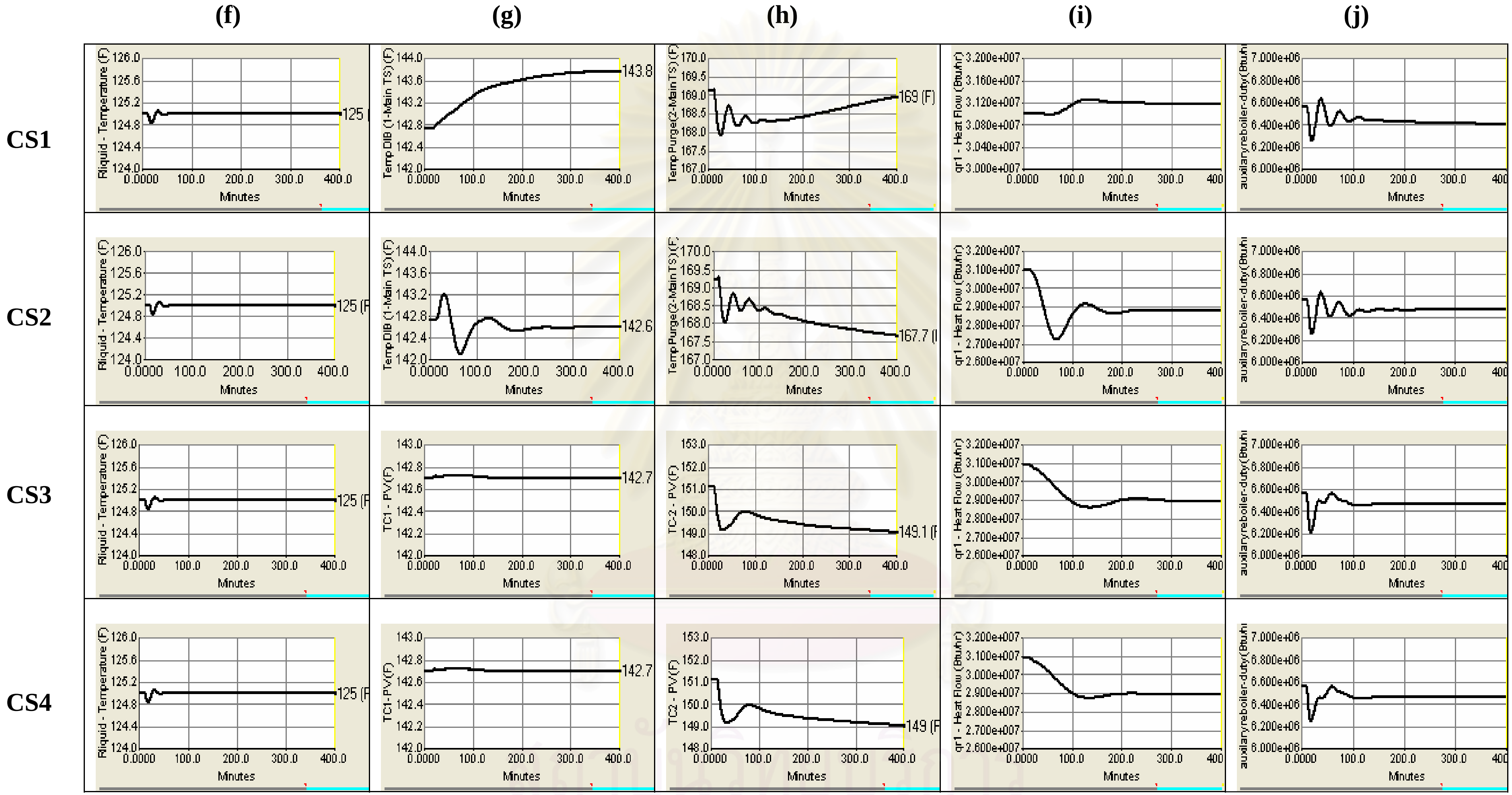


Figure 5.39: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

5.4 Evaluation of the dynamic performance

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

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

Note that $|\epsilon(t)|$ = y_{sp}(t)-y(t) is the deviation (error) of the response form the desired set point.

In this study, IAE method is used to evaluate the dynamic performance of the designed control system. Tables 5.2 and 5.3 show the IAE of some temperature controllers in the butane isomerization process with different energy integration schemes (alternatives 1, 2 and base-case) for CS1 control structure to CS4 control structure. The IAE results for the change in the setpoint of the reactor inlet temperature (the disturbance loads of hot steam) are listed in Tables 5.2. Whereas, Table 5.3 shows the IAE results for the change in the recycle flowrates (the disturbance loads of cold steam).

5.4.1 Evaluation of the dynamic performance for CS1 control structure

In general, the control system for CS1 in the butane isomerization process (Base Case) is the most effective one compared with the other two alternatives, i.e. the value of IAE in the butane isomerization process (Base Case) is smaller than those in alternatives 1 and 2, but the value of IAE in the butane isomerization process alternative 1 is smaller than that in alternative 2.

As can be seen that the IAE results for CS1 control structure are smaller than CS2 control structure, but the IAE results for CS1 control structure are larger than CS3 and CS4.

5.4.2 Evaluation of the dynamic performance for CS2 control structure

In general, the control system for CS2 in the butane isomerization process (Base Case) is the most effective one compared with the other two alternatives, i.e. the value of IAE in the butane isomerization process (Base Case) is smaller than those in alternatives 1 and 2, but the value of IAE in the butane isomerization process alternative 1 is smaller than that in alternative 2.

As can be seen, the IAE results for CS2 control structure are the worst one compared with those in CS1, CS3 and CS4.

5.4.3 Evaluation of the dynamic performance for CS3 control structure

In general, the control system for CS3 in the butane isomerization process alternative 1 is better than that in alternative 2, i.e. the value of IAE in the butane isomerization process alternative 1 is smaller than that in the alternative

As can be seen that the IAE results for the change in the setpoint of the reactor inlet temperature in the butane isomerization process of CS3 control structure are the smallest one compared with those in CS1, CS2 and CS4, but IAE results for the change in the recycle flowrates in the butane isomerization process of CS3 control structure are larger than CS4 control structure.

5.4.4 Evaluation of the dynamic performance for CS4 control structure

In general, the control system for CS4 in the butane isomerization process alternative 1 is better than that in alternative 2, i.e.the value of IAE in the butane isomerization process alternative 1 is smaller than that in the alternative 2.

As can be seen that the IAE results for CS3 control structure look just the same as CS4 control structure results, but IAE results for the change in the recycle flowrates in the butane isomerization process of CS3 control structure are larger than CS4 control structure. The performance of these control structures can be arranged from the best to lowest performance (error of controllability point of view) as the following sequences: CS4, CS3, CS1, and CS2.

Table 5.2: The IAE results of the control systems to change in the setpoint of the reactor inlet temperature

Decrease Reactor Inlet Temperature 10^oF										
A	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.057695	0.07109	0.085311	0.056981	0.081458	0.067016	0.034656	0.03552	0.039015	0.036485
TCR	8.228	8.228667	8.9551	9.2048	8.9553	9.9532	9.6792	10.091	9.679	9.0308
TC-cool	3.641833	3.6425	9.9974	11.324	10.032	11.33	9.9947	11.305	9.9943	11.29
PC1	7.346167	19.33333	14.994	7.5843	16.992	18.035	3.7125	3.3717	7.9194	7.8105
PC2	0.2011	0.3914	0.34949	10.57	0.25894	10.318	0.49767	5.2841	0.53325	5.4601
Total A	19.4748*	31.66699	34.38130	38.74008	36.31970	49.70322	23.91873	30.08732	28.16497	33.62789
B	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1			2.3813	2.3514	2.499	2.399	2.3273	2.249	2.3383	2.3504
TC-cHE2			6.3007	5.7529	6.3114	5.9726	6.4615	5.9568	6.4613	5.7624
Total B			8.682	8.1043	8.8104	8.3716	8.7888	8.2058	8.7996	8.1128
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B			43.06330	46.84438	45.13010	58.07482	32.7075*	38.29312	36.96457	41.74069
C	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1							1.2784	0.90308	1.4748	1.0107
TC2							0.21633	6.0746	0.19975	5.9508
ToltalA+B+C							34.2022*	45.27080	38.63912	48.70219

Increase Reactor Inlet Temperature 10^oF										
A	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.065815	0.065783	0.094986	0.065609	0.084309	0.067632	0.037046	0.039031	0.03753	0.034758
TCR	7.933833	7.933833	9.3817	9.7136	9.381	9.7141	9.3439	8.4347	9.5051	8.4358
TC-cool	3.073833	3.073833	10.626	11.157	10.672	11.148	10.65	11.032	10.627	11.031
PC1	10.09167	15.169	18.234	10.507	18.933	17.327	2.2277	2.3727	8.3989	8.1949
PC2	0.146825	0.282617	0.33564	10.86	0.26331	10.55	0.50928	5.32	0.54737	5.4932
Total A	21.31197*	26.52507	38.67233	42.30321	39.33362	48.80673	22.76793	27.19843	29.11590	33.18966
B	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1			2.3548	2.2987	2.4273	2.2776	2.1438	2.2273	2.2102	2.2043
TC-cHE2			5.8256	5.2169	5.8425	5.2228	5.7079	5.0336	5.8682	5.0342
Total B			8.1804	7.5156	8.2698	7.5004	7.8517	7.2609	8.0784	7.2385
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B			46.85273	49.81881	47.60342	56.30713	30.6196*	34.45933	37.19430	40.42816
C	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1							0.96817	0.63342	1.3289	0.84675
TC2							0.22833	6.1027	0.218	6.0147
ToltalA+B+C							31.8161*	41.19545	38.74120	47.28961

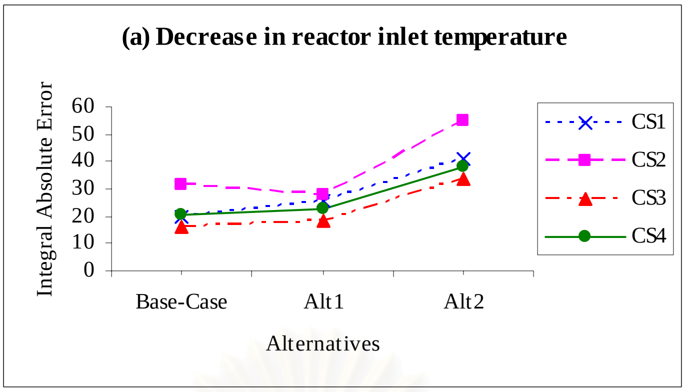
Note * = Minimum IAE value

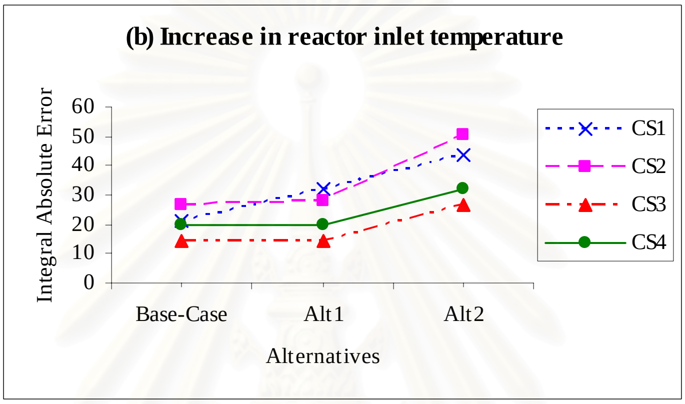
Table 5.3: The IAE results of the control systems to change in recycle flowrates

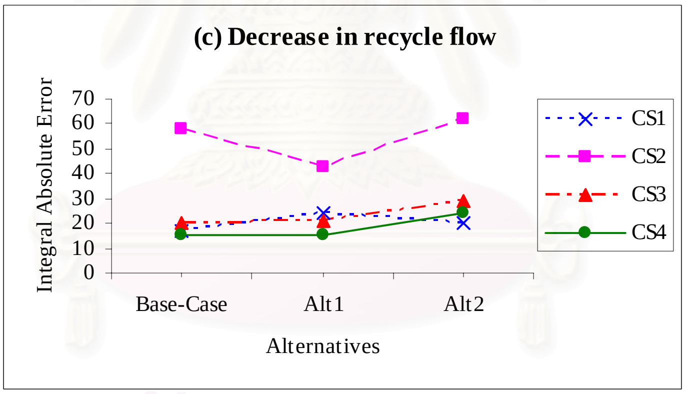
Increase recycle flow from 870.1 to 940.1lb.mol/h.										
A	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.020062	0.2358	0.071032	0.017826	0.22501	0.23226	0.026925	0.027007	0.057011	0.054587
TCR	1.577333	1.577583	0.82075	0.7395	0.82092	0.746	0.82075	0.73783	0.82108	0.73833
TC-cool	0.645667	0.650417	2.6171	2.905	2.6162	2.9318	2.4943	2.9668	2.4918	2.9655
PC1	3.837333	46.01	9.9174	3.6714	30.089	47.422	12.537	12.506	6.7598	7.1435
PC2	7.926	7.793667	7.7947	9.0804	7.6293	8.8699	5.3243	23.136	5.135	23.785
Total A	14.006*	56.26747	21.22098	16.41413	41.38043	60.20196	21.20328	39.37364	15.26469	34.68692
B	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1			2.9003	2.3594	2.6648	2.5271	2.5231	2.3454	2.4913	2.3323
TC-cHE2			1.0482	0.892	1.0758	0.91675	1.0297	0.90508	1.0337	0.902
Total B			3.9485	3.2514	3.7406	3.44385	3.5528	3.25048	3.525	3.2343
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B			25.16948	19.66553	45.12103	63.64581	24.75608	42.62412	18.7897*	37.92122
C	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1							2.6009	2.2357	2.2803	1.792
TC2							4.7699	4.5769	4.1638	4.1738
ToltalA+B+C							32.12688	49.43672	25.2338*	43.88702

Decrease recycle flow from 870.1 to 800.1lb.mol/h.										
A	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.021682	0.236083	0.074623	0.019996	0.23089	0.23098	0.026034	0.0261	0.056591	0.054226
TCR	1.538167	1.533333	0.81825	0.73592	0.81883	0.73617	0.81825	0.73517	0.81817	0.73575
TC-cool	0.658167	0.666167	3.0472	3.7158	3.0333	3.6762	2.873	3.6794	2.8718	3.6552
PC1	4.213167	44.735	10.614	4.1326	29.474	45.674	12.847	12.641	7.2028	7.6006
PC2	10.74817	10.6035	10.545	11.716	10.359	11.716	5.7449	23.335	5.2777	23.905
Total A	17.17935	57.77408	25.09907	20.32032	43.91602	62.03335	22.30918	40.41667	16.2271*	35.95078
B	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1			2.7919	2.4614	2.2445	2.1825	2.1588	2.019	2.1455	1.9854
TC-cHE2			1.3537	1.3478	1.3062	1.3143	1.2947	1.337	1.2995	1.3168
Total B			4.1456	3.8092	3.5507	3.4968	3.4535	3.356	3.445	3.3022
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B			29.24467	24.12952	47.46672	65.53015	25.76268	43.77267	19.6721*	39.25298
C	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1							2.9172	2.4011	2.4298	1.8408
TC2							5.4264	4.8257	4.4128	4.3511
ToltalA+B+C							34.10628	50.99947	26.5147*	45.44488

Note * = Minimum IAE value







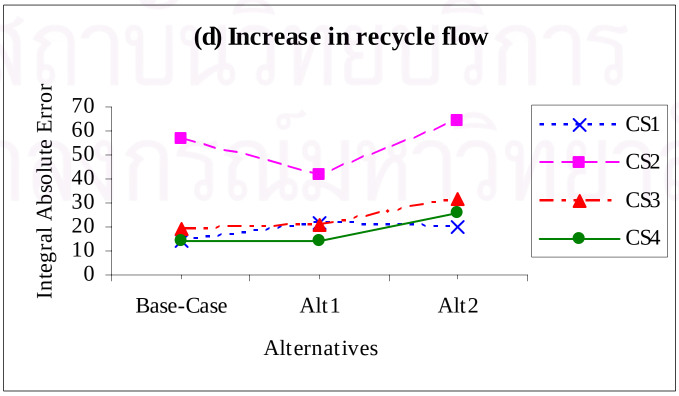
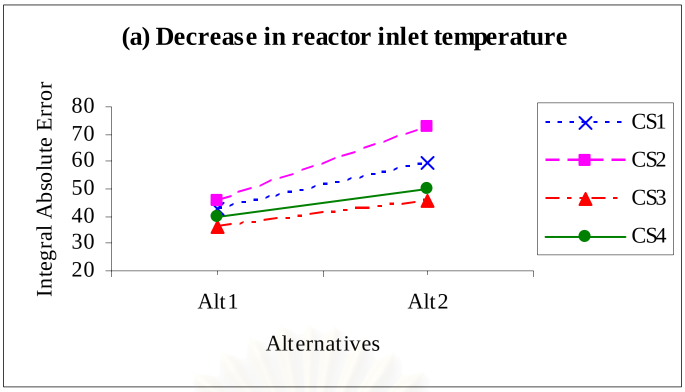
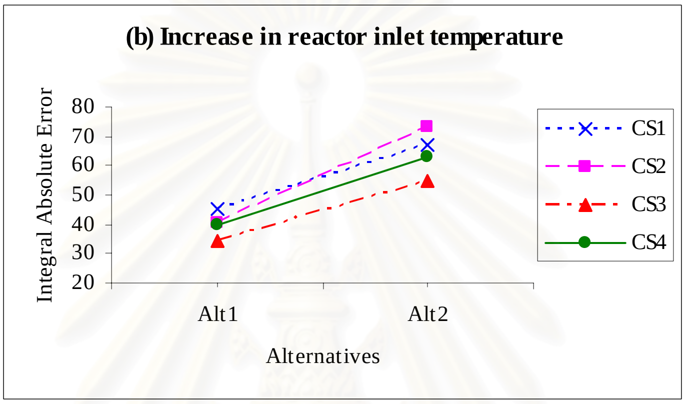
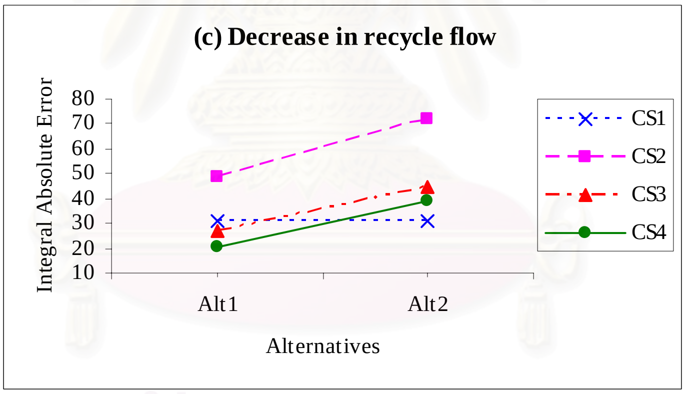


Figure 5.40: The IAE results of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1, 2 and base-case) from disturbance load changes, where (a) decrease in reactor inlet temperature, (b) increase in reactor inlet temperature, (c) decrease in recycle flow, (d) increase in recycle flow.







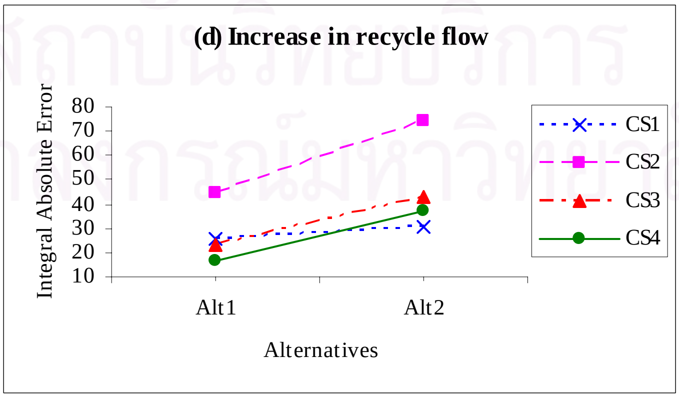


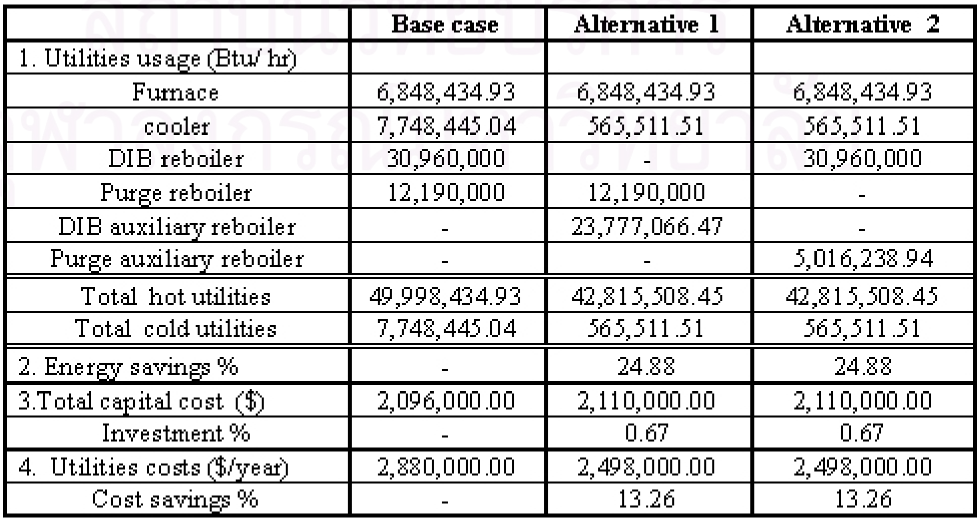
Figure 5.41: The IAE results of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1 and 2) from disturbance load changes, where (a) decrease in reactor inlet temperature, (b) increase in reactor inlet temperature, (c) decrease in recycle flow, (d) increase in recycle flow.

5.5 Economic analysis for the butane isomerization process

In this work, the capital equipment-costing program CAPCOST is chosen for cost estimation of the butane isomerization process with energy integration. This program is based on the module factor approach to costing that was originally introduced by Guthrie and modified by Ulrich. In addition, we must update the value for the Chemical Engineering Plant Cost Index (CEPCI) before using this program.

From steady state point view, on the evaluation of the economics of a butane isomerization process, the term economics refers to the evaluation of capital costs and operating costs associated with the construction and operation of a butane isomerization process. The methods by which the one-time costs associated with the construction of the plant and the continuing costs associated with the daily operation of the process are combined into meaningful economic criteria are provided. The benefit obtained from energy integration with the alternatives1 to the others is given in Table 5.4. From Table 5.4, we see that when we install the various heat-exchanger network alternatives on the base-case design for the Butane Isomerization processes, the energy saved is 24.88% from the design without heat integration. The utilities cost per year saved is 13.26 %, but the capital cost raised is 0.67 %.

Table 5.4: Results of energy integration and cost estimation for Butane Isomerization process with different energy integration schemes



	Base case	**Alternative 1**	**Alternative 2**
1. Utilities usage (Btu/ hr)			
Furnace	6,848,434.93	6,848,434.93	6,848,434.93
cooler	7,748,445.04	565,511.51	565,511.51
DIB reboiler	30,960,000	-	30,960,000
Purge reboiler	12,190,000	12,190,000	-
DIB auxiliary reboiler	-	23,777,066.47	-
Purge auxiliary reboiler	-	-	5,016,238.94
Total hot utilities	49,998,434.93	42,815,508.45	42,815,508.45
Total cold utilities	7,748,445.04	565,511.51	565,511.51
2. Energy savings %	-	24.88	24.88
3.Total capital cost ($)	2,096,000.00	2,110,000.00	2,110,000.00
Investment %	-	0.67	0.67
4. Utilities costs ($/year)	2,880,000.00	2,498,000.00	2,498,000.00
Cost savings %	-	13.26	13.26

The energy consumption before disturbance loads testing of the four control structures for Butane Isomerization process with different energy integration schemes are summarized in Table 5.5 and Figure 5.42. The result shows the utility consumption of the fourth control structure is less than those of the other control structures.

Table 5.5: The energy consumption of the four control structures

	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Utilities usage (Btu/ hr)										
Furnace	6.397E+06	6.397E+06	5.449E+06	4.383E+06	5.449E+06	4.383E+06	5.450E+06	4.386E+06	5.450E+06	4.386E+06
cooler	7.278E+06	7.278E+06	3.957E+05	3.955E+05	3.957E+05	3.955E+05	3.956E+05	3.946E+05	3.956E+05	3.946E+05
DIB column reboiler	3.097E+07	3.097E+07	-	3.100E+07	-	3.101E+07	-	3.094E+07	-	3.094E+07
Purge column reboiler	1.216E+07	1.216E+07	1.216E+07	-	1.216E+07	-	1.216E+07	-	1.216E+07	-
DIB column condenser	2.963E+07	2.964E+07	2.960E+07	2.977E+07	2.960E+07	2.978E+07	2.963E+07	2.964E+07	2.956E+07	2.968E+07
Purge column condenser	1.328E+07	1.328E+07	1.328E+07	1.321E+07	1.328E+07	1.321E+07	1.327E+07	1.328E+07	1.327E+07	1.328E+07
DIB auxiliary reboiler	-	-	2.503E+07	-	2.503E+07	-	2.499E+07	-	2.499E+07	-
Purge auxiliary reboiler	-	-	-	7.294E+06	-	7.294E+06	-	7.292E+06	-	7.292E+06
Total hot utilities	4.952E+07	4.953E+07	4.264E+07	4.268E+07	4.264E+07	4.268E+07	4.260E+07	4.261E+07	4.260E+07	4.261E+07
Total cold utilities	5.019E+07	5.020E+07	4.328E+07	4.338E+07	4.328E+07	4.338E+07	4.329E+07	4.331E+07	4.322E+07	4.335E+07
Total utilities	9.972E+07	9.973E+07	8.591E+07	8.606E+07	8.591E+07	8.607E+07	8.590E+07	8.592E+07	8.582E+07	8.596E+07

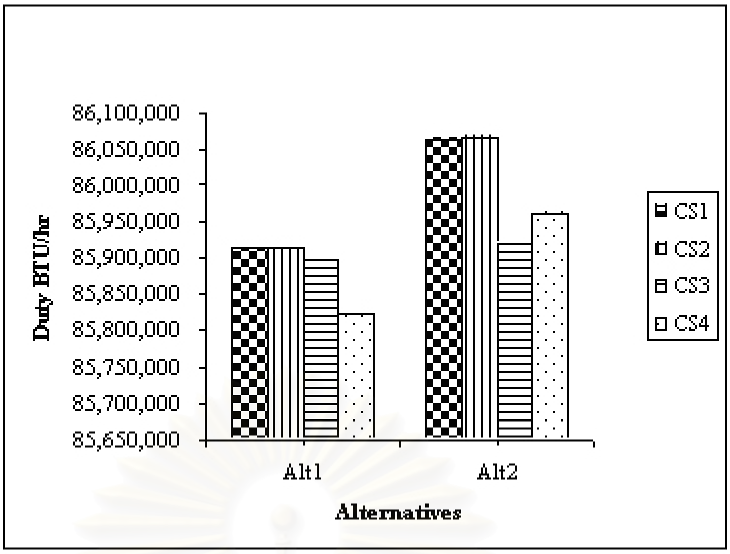


Figure 5.42: Comparison of the energy consumption of the four control structures before disturbance loads testing

For the utility consumptions of control structures in the butane isomerization process with different energy integration schemes (alternatives 1, 2 and base-case) from disturbance load changes are shown in figures 5.43 and 5.44.

As can be seen, when increase in the reactor inlet temperature and decrease in recycle flow, the utility consumptions of the new control structures (CS3 and CS4) are less than CS1 and CS2, since DIB column reboiler duty in the new control structures is manipulated to control the temperature on tray1 of DIB column, but CS1 and CS2 don't control the temperature on that.

However, when decrease in the reactor inlet temperature and increase in the recycle flow, the utility consumptions of Luyben's control structures (CS1 and CS2) are less than CS1 and CS2. Because when increase in recycle flow, the control structures CS3 and CS4 give more the product rate compared to CS1 and CS2 ,which causes the reboiler heat input to increase.

The energy consumption of the four control structures for Butane Isomerization process with different energy integration schemes from disturbance load changes are summarized in Table 5.6 and 5.7.

Table 5.6: The energy consumption of the four control structures to change in the setpoint of the reactor inlet temperature

Increase Reactor Inlet Temperature 10^{o}F										
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Utilities usage, E+06 (Btu/ hr)										
Furnace	6.5577	6.5577	5.8387	4.7746	5.8388	4.7747	5.8320	4.7621	5.8321	4.7622
cooler	7.5880	7.5882	0.3942	0.3941	0.3942	0.3941	0.3927	0.3932	0.3928	0.3933
DIB column reboiler	31.6177	31.6214	-	31.6691	-	31.6704	-	31.0247	-	31.0082
Purge column reboiler	12.1673	12.1676	12.1657	-	12.1658	-	12.1617	-	12.1618	-
DIB auxiliary reboiler	-	-	25.1366	-	25.1364	-	24.6079	-	24.5903	-
Purge auxiliary reboiler	-	-	-	6.7575	-	6.7576	-	6.7887	-	6.7881
Total hot utilities usage	50.3427	50.3467	43.1410	43.2011	43.1409	43.2027	42.6016	42.5755	42.5842	42.5586
Total cold utilities usage	7.5880	7.5882	3.9420	3.9412	0.3942	0.3941	0.3927	0.3932	0.3928	0.3933
Total utilities usage	57.9307	57.9349	47.0830	47.1423	43.5351	43.5969	42.9943	42.9687	42.9770	42.9518

Decrease Reactor Inlet Temperature 10^{o}F										
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Utilities usage, E+06 (Btu/ hr)										
Furnace	6.2295	6.2296	5.5268	4.4689	5.5270	4.4692	5.5288	4.4714	5.5288	4.4714
cooler	6.9820	6.9820	0.3972	0.3971	0.3972	0.3971	0.3972	0.3966	0.3972	0.3966
DIB column reboiler	30.3941	30.3997	-	30.4260	-	30.4297	-	30.4300	-	30.4272
Purge column reboiler	12.1589	12.1591	12.1573	-	12.1573	-	12.1567	-	12.1565	-
DIB auxiliary reboiler	-	-	24.5064	-	24.5073	-	24.5097	-	24.5099	-
Purge auxiliary reboiler	-	-	-	7..3362	-	7..3363	-	7..3346	-	7..3346
Total hot utilities usage	48.7825	48.7884	42.1905	42.2312	42.1916	42.2352	42.1952	42.2360	42.1952	42.2332
Total cold utilities usage	6.9820	6.9820	0.3972	0.3971	0.3972	0.3971	0.3972	0.3966	0.3972	0.3966
Total utilities usage	55.7645	55.7704	42.5877	42.6283	42.5888	42.6323	42.5924	42.6326	42.5925	42.6298

Table 5.7: The energy consumption of the four control structures to change in recycle flowrates

Increase recycle flow from 870.1 to 940.1lb.mol/h.										
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Utilities usage, E+06 (Btu/ hr)										
Furnace	7.2093	7.1836	5.9871	4.8303	5.9183	4.7622	5.9315	4.7764	5.9314	4.7763
cooler	7.9907	8.0485	0.3817	0.3806	0.4071	0.4063	0.4022	0.4009	0.4022	0.4009
DIB column reboiler	30.8293	33.1856	-	30.8792	-	33.2335	-	32.7602	-	32.7574
Purge column reboiler	12.6471	12.6639	12.6451	-	12.6617	-	12.6585	-	12.6585	-
DIB auxiliary reboiler	-	-	24.4447	-	26.7989	-	26.3640	-	26.3585	-
Purge auxiliary reboiler	-	-	-	7.4137	-	7.4413	-	7.4345	-	7.4345
Total hot utilities usage	50.6857	53.0330	43.0768	43.1232	45.3789	45.4370	44.9539	44.9711	44.9484	44.9682
Total cold utilities usage	7.9907	8.0485	0.3817	0.3806	0.4071	0.4063	0.4022	0.4009	0.4022	0.4009
Total utilities usage	58.6764	61.0815	43.4585	43.5038	45.7860	45.8433	45.3561	45.3720	45.3506	45.3691

Decrease recycle flow from 870.1 to 800.1lb.mol/h.										
	CS1-Base	CS2-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Utilities usage, E+06 (Btu/ hr)										
Furnace	5.6032	5.6340	5.0330	4.0464	5.0047	4.0010	5.0077	4.0046	5.0077	4.0046
cooler	6.5883	6.5291	0.3633	0.3632	0.3631	0.3630	0.3631	0.3630	0.3631	0.3630
DIB column reboiler	31.1301	28.7623	-	31.1611	-	28.7859	-	28.9435	-	28.9493
Purge column reboiler	11.6759	11.6586	11.6741	-	11.6564	-	11.6579	-	11.6580	-
DIB auxiliary reboiler	-	-	25.4669	-	23.2152	-	23.3976	-	23.4041	-
Purge auxiliary reboiler	-	-	-	7.0115	-	7.1289	-	7.1184	-	7.1186
Total hot utilities usage	48.4092	46.0549	42.1741	42.2190	39.8762	39.9157	40.0631	40.0664	40.0698	40.0724
Total cold utilities usage	50.1900	50.2000	43.2800	43.3800	43.2800	43.3800	43.2900	43.3100	43.2200	43.3500
Total utilities usage	99.7200	99.7300	85.9100	86.0600	85.9100	86.0700	85.9000	85.9200	85.8200	85.9600

The reactor outlet temperature data of the four control structures for Butane Isomerization process with different energy integration schemes from disturbance load changes are summarized in Table 5.8.

Table 5.8: The reactor outlet temperature from disturbance load changes

Reactor Outlet Temperature °F										
Type of Disturbances	CS1-base	CS2-base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Increase Reactor Inlet Temperature	439.28	439.28	439.25	440.14	439.25	440.14	438.76	439.58	438.77	439.59
Decrease Reactor Inlet Temperature	408.64	408.63	408.61	409.45	408.61	409.45	408.58	409.41	408.58	409.41
Increase recycle flow	420.04	421.68	420.03	420.93	421.68	422.58	421.37	422.26	421.37	422.26
Decrease recycle flow	428.31	426.09	428.27	429.08	426.05	426.84	426.29	427.05	426.28	427.04

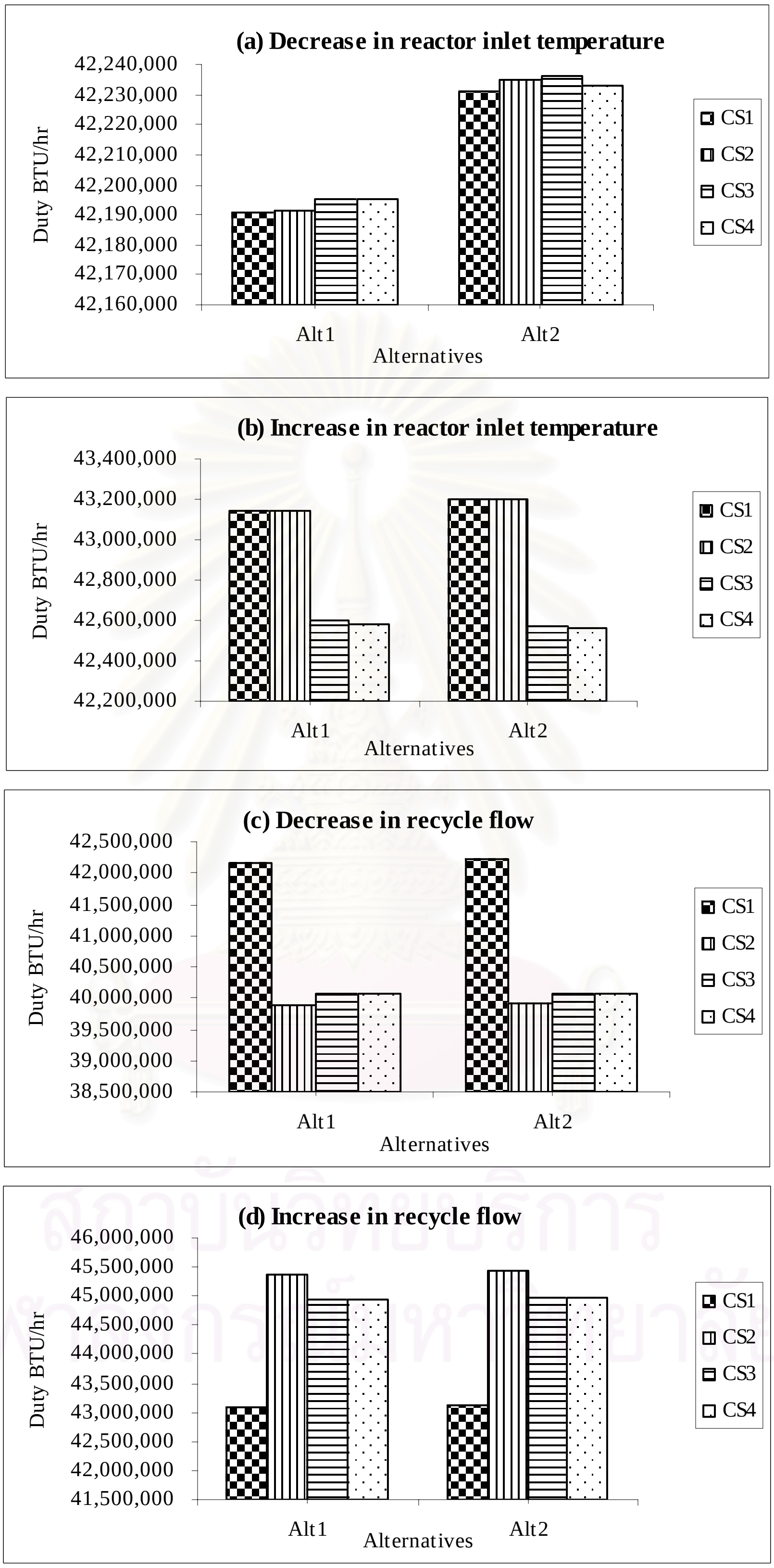


Figure 5.43: The hot utility consumptions of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1 and 2) from disturbance load changes, where (a) decrease in reactor inlet temperature, (b) increase in reactor inlet temperature, (c) decrease in recycle flow, (d) increase in recycle flow.

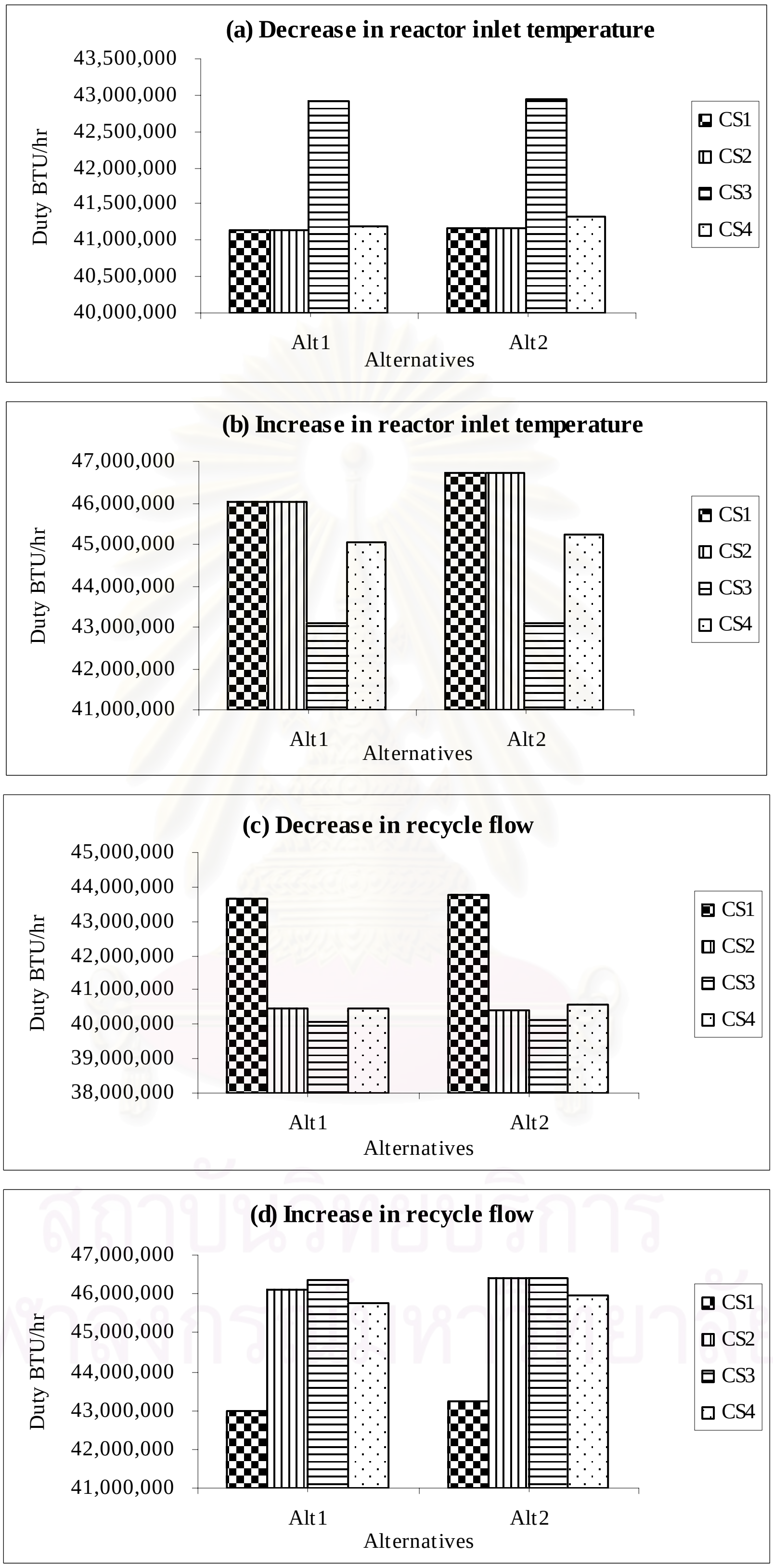


Figure 5.44: The cold utility consumptions of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1 and 2) from disturbance load changes, where (a) decrease in reactor inlet temperature, (b) increase in reactor inlet temperature, (c) decrease in recycle flow, (d) increase in recycle flow.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

In this work, the resilient heat exchanger networks to achieve maximum energy recovery and plantwide control strategies are studied and applied to Butane Isomerization plant. The control difficulties associated with heat integration are solved by adding auxiliary utilities which is kept minimal. Two alternatives of heat exchanger networks (HEN) designs of the Butane Isomerization plant are proposed, both used the heat from the reactor effluent stream to provide the heat for the column reboiler. The energy saved is 24.88 % from the design without heat integration.

The goal of this work is to presents two plantwide designed control structures for energy-integrated Butane Isomerization plant, the control results of these alternative structures are compared with reference structures (Poothanakul.; 2002, Luyben; 1998). The dynamic simulation of this process with various disturbances is made to evaluate performance of each control structures: increasing and decreasing the reactor inlet temperature, increasing and decreasing the recycle flowrates, increasing and decreasing the recycle stream temperature before entering the DIB column, decreasing the recycle flowrates before entering the DIB column.

Four plantwide control configurations of heat-integrated plant designed following Luyben's heuristic method. The first control structure (CS1) is the control structure of Luyben to control in the energy-integrated Butane Isomerization process. The second control structure (CS2) is the modification of the first control structure adding a ratio controller is used to increase the reflux flowrate in the DIB column as the recycle flowrate is increased. In the third control structure (CS3), the reflux flow can control the reflux drum level more effective than the distillate flow and we control the impurity of nC4 in product manipulating the distillate flowrate. In the fourth control structure (CS4), this control structure switches those two variables from the third control structure. The result shows the fourth control structure gives a smaller settling time and can reject disturbances better than other control structures and the utility consumption of the fourth control structure is less than those of the other control structures. In general, the control systems for CS1 to CS4 in the butane isomerization process alternative 1 are better than that in alternative 2. However, the control systems for CS1 to CS4 in the butane isomerization process without energy integration are the most effective one compared with the other two alternatives. Therefore, those results indicate that the dynamic performance of the Butane Isomerization process deteriorates when the process incorporates complex heat integration. However it can reduce energy cost and can be operated well by use plantwide methodology to design control structure. Various heat pathways throughout the network designed using Wongsri's disturbance propagation method to achieve DMER. The designed control structures are evaluated based on the rigorous dynamic simulation using the commercial software HYSYS.

The performance of these control structures can be arranged from the best to lowest performance (error of controllability point of view) as the following sequences: CS4, CS3, CS1 and CS2.

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.
3. Study the self-optimizing control structure of energy-integrated Butane Isomerization plant.

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APPENDICES

APPENDIX A

Table A.1: Data of Butane Isomerization process (Base Case) for simulation

Name	Rliquid	v1out	d1	b1	d2	b2	p1out	v4out
Vapour Fraction	0	0	0	0	0	0	0	0
Temperature [F]	124.9	90.44	121.2	143.87	108.92	173.76	117.37	117.67
Pressure [psia]	101.6	102.4	100	104	65	66	866	702
Molar Flow [lbmole/hr]	870.1	580	550.09	900	870.1	29.9	870.1	870.1
Heat Flow [Btu/hr]	-5.56E+07	-3.73E+07	-3.55E+07	-5.61E+07	-5.50E+07	-2.18E+06	-5.47E+07	-5.47E+07
Comp Mole Frac (Propane)	0	0.02	0.0211	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.7098	0.24	0.9589	0.2548	0.2635	0.0004	0.2635	0.2635
Comp Mole Frac (n-Butane)	0.2872	0.69	0.02	0.7101	0.7335	0.0295	0.7335	0.7335
Comp Mole Frac (i-Pantane)	0.003	0.05	0	0.0351	0.003	0.9701	0.003	0.003
Name	cHEin	cHEout	hHEin	hHEout	Rin	Rout	coolout	V6out
Vapour Fraction	0	0	1	0	1	1	0	0
Temperature [F]	117.67	285.46	424.1	298.6	390.1	424.1	125	124.94
Pressure [psia]	702	698.2	675	671	682	675	662.3	101.6
Molar Flow [lbmole/hr]	870.1	870.1	870.1	870.1	870.1	870.1	870.1	870.1
Heat Flow [Btu/hr]	-5.47E+07	-4.85E+07	-4.23E+07	-4.85E+07	-4.23E+07	-4.23E+07	-5.56E+07	-5.56E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.2635	0.2635	0.7098	0.7098	0.2635	0.7098	0.7098	0.7098
Comp Mole Frac (n-Butane)	0.7335	0.7335	0.2873	0.2873	0.7335	0.2873	0.2873	0.2873
Comp Mole Frac (i-Pantane)	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.003

Table A.1: Data of Butane Isomerization process (Base Case) for simulation (cont.)

Name	v3out	v5out	v2out	PFD
Vapour Fraction	0.1523	0.1158	0.1448	0
Temperature [F]	86.54	148.31	111.23	90
Pressure [psia]	60	46	65.47	300
Molar Flow [lbmole/hr]	550.09	29.9	900	580
Heat Flow [Btu/hr]	-3.55E+07	-2.18E+06	-5.61E+07	-3.73E+07
Comp Mole Frac (Propane)	0.0211	0	0	0.02
Comp Mole Frac (i-Butane)	0.9589	0.0004	0.2548	0.24
Comp Mole Frac (n-Butane)	0.02	0.0295	0.7101	0.69
Comp Mole Frac (i-Pantane)	0	0.9701	0.0351	0.05

Name	qc1	qr1	qc2	qr2	qp1	qfur	qcooler
Heat Flow [Btu/hr]	2.97E+07	3.10E+07	1.33E+07	1.22E+07	2.94E+05	6.22E+06	7.12E+06

Table A.2: Data of Butane Isomerization process (Base Case) for simulation (Poothanakul P., 2002)

Name	Rliquid	v1out	d1	b1	d2	b2	p1out	v4out
Vapour Fraction	0	0	0	0	0	0	0	0
Temperature [F]	124.9	90.44	121.2	143.9	108.9	173.8	117.37	117.67
Pressure [psia]	101.6	102.4	100	104	65	66	866	702
Molar Flow [lbmole/hr]	870.1	580	550.09	900	870.1	29.9	870.1	870.1
Heat Flow [Btu/hr]	-5.56E+07	-3.73E+07	-3.55E+07	-5.61E+07	-5.50E+07	-2.18E+06	-5.47E+07	-5.47E+07
Comp Mole Frac (Propane)	0	0.02	0.0211	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.7098	0.24	0.9589	0.2548	0.2635	0.0004	0.2635	0.2635
Comp Mole Frac (n-Butane)	0.2872	0.69	0.02	0.7101	0.7335	0.0295	0.7335	0.7335
Comp Mole Frac (i-Pantane)	0.003	0.05	0	0.0351	0.003	0.9701	0.003	0.003

Name	cHEin	cHEout	hHEin	hHEout	Rin	Rout	coolout	V6out
Vapour Fraction	0	0	1	0	1	1	0	0
Temperature [F]	117.67	285.46	424.1	298.6	390.1	424.1	125	124.94
Pressure [psia]	702	698.2	675	671	682	675	662.3	101.6
Molar Flow [lbmole/hr]	870.1	870.1	870.1	870.1	870.1	870.1	870.1	870.1
Heat Flow [Btu/hr]	-5.47E+07	-4.85E+07	-4.23E+07	-4.85E+07	-4.23E+07	-4.23E+07	-5.56E+07	-5.56E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.2635	0.2635	0.7098	0.7098	0.2635	0.7098	0.7098	0.7098
Comp Mole Frac (n-Butane)	0.7335	0.7335	0.2873	0.2873	0.7335	0.2873	0.2873	0.2873
Comp Mole Frac (i-Pantane)	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.003

Table A.2: Data of Butane Isomerization process (Base Case) for simulation (Poothanakul P., 2002) (cont.)

Name	v3out	v5out	v2out	PFD
Vapour Fraction	0.1523	0.1158	0.1448	0
Temperature [F]	86.54	148.31	111.23	90
Pressure [psia]	60	46	65.47	300
Molar Flow [lbmole/hr]	550.09	29.9	900	580
Heat Flow [Btu/hr]	-3.55E+07	-2.18E+06	-5.61E+07	-3.73E+07
Comp Mole Frac (Propane)	0.0211	0	0	0.02
Comp Mole Frac (i-Butane)	0.9589	0.0004	0.2548	0.24
Comp Mole Frac (n-Butane)	0.02	0.0295	0.7101	0.69
Comp Mole Frac (i-Pantane)	0	0.9701	0.0351	0.05

Name	qc1	qr1	qc2	qr2	qp1	qfur	qcooler
Heat Flow [Btu/hr]	2.97E+07	3.10E+07	1.33E+07	1.22E+07	2.94E+05	6.22E+06	7.12E+06

Table A.3: Data of Butane Isomerization process (alt.1) for simulation

Name	Rliquid	v1out	d1	boil1	cHE3in	hHE2in	hHE1out	d2
Vapour Fraction	0	0	0	1	0	0	0	0
Temperature [F]	124.9	90.44	121.2	143.9	142.08	162	298.6	108.92
Pressure [psia]	101.6	102.4	100	104	104	667	671	65
Molar Flow [lbmole/hr]	870.1	580	550.1	3923	4823	870.1	870.1	870.1
Heat Flow [Btu/hr]	-5.56E+07	-3.73E+07	-3.55E+07	-2.14E+08	-3.01E+08	-5.44E+07	-4.85E+07	-5.50E+07
Comp Mole Frac (Propane)	0	0.02	0.0211	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.7098	0.24	0.9589	0.3105	0.3001	0.7098	0.7098	0.2635
Comp Mole Frac (n-Butane)	0.2872	0.69	0.02	0.673	0.6799	0.2873	0.2873	0.7335
Comp Mole Frac (i-Pantane)	0.003	0.05	0	0.0165	0.02	0.003	0.003	0.003

Name	cHE3out	toboil1	b1	b2	v2out	v5out	p1out	v4out
Vapour Fraction	0.1564	1	0	0	0.1448	0.1158	0	0
Temperature [F]	142.38	143.87	143.87	173.76	111.23	148.31	117.37	117.67
Pressure [psia]	104	104	104	66	65.47	46	866	702
Molar Flow [lbmole/hr]	4823	3923	900	29.9	900	29.9	870.1	870.1
Heat Flow [Btu/hr]	-2.95E+08	-2.14E+08	-5.61E+07	-2.18E+06	-5.61E+07	-2.18E+06	-5.47E+07	-5.47E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.3001	0.2548	0.3105	0.0004	0.2548	0.0004	0.2635	0.2635
Comp Mole Frac (n-Butane)	0.6799	0.7101	0.673	0.0295	0.7101	0.0295	0.7335	0.7335
Comp Mole Frac (i-Pantane)	0.02	0.0351	0.0165	0.9701	0.0351	0.9701	0.003	0.003

Table A.3: Data of Butane Isomerization process (alt.1) for simulation (cont.)

Name	cHE2in	cHE1in	hHE3out	hHE2out	v6out	cHE1out	hHE1in	hHE3in
Vapour Fraction	0	0	0	0	0	0	1	0
Temperature [F]	117.67	143.04	162	137.67	124.94	300.11	424.1	298.6
Pressure [psia]	702	701	667	666	101.6	698.2	675	671
Molar Flow [lbmole/hr]	870.1	870.1	870.1	870.1	870.1	870.1	870.1	870.1
Heat Flow [Btu/hr]	-5.47E+07	-5.39E+07	-5.44E+07	-5.52E+07	-5.56E+07	-4.77E+07	-4.23E+07	-4.85E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.2635	0.2635	0.7098	0.7098	0.7098	0.2635	0.7098	0.7098
Comp Mole Frac (n-Butane)	0.7335	0.7335	0.2873	0.2873	0.2873	0.7335	0.2873	0.2873
Comp Mole Frac (i-Pantane)	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.003

Name	Rout	Rin	coolout	v3out	PFD
Vapour Fraction	1	1	0	0.1523	0
Temperature [F]	424.1	390.1	125	86.54	90
Pressure [psia]	675	682	662.3	60	300
Molar Flow [lbmole/hr]	870.1	870.1	870.1	550.1	580
Heat Flow [Btu/hr]	-4.23E+07	-4.23E+07	-5.56E+07	-3.55E+07	-3.73E+07
Comp Mole Frac (Propane)	0	0	0	0.0211	0.02
Comp Mole Frac (i-Butane)	0.7098	0.2635	0.7098	0.9589	0.24
Comp Mole Frac (n-Butane)	0.2873	0.7335	0.2873	0.02	0.69
Comp Mole Frac (i-Pantane)	0.003	0.003	0.003	0	0.05

Name	qr1	auxiliary reboiler	qc2	qc1	qp1	qfur	qcooler
Heat Flow [Btu/hr]	1.22E+07	2.50E+07	2.97E+07	1.33E+07	2.94E+05	5.43E+06	3.98E+05

Table A.4: Data of Butane Isomerization process (alt.2) for simulation

Name	Rliquid	v1out	b1	d1	cHE3in	d2	cHE2in	PFD
Vapour Fraction	0	0	0	0	0	0	0	0
Temperature [F]	124.9	90.44	143.87	121.2	171.5	108.92	117.67	90
Pressure [psia]	101.6	102.4	104	100	66	65	702	300
Molar Flow [lbmole/hr]	870.1	580	900	550.1	1340.4	870.1	870.1	580
Heat Flow [Btu/hr]	-5.56E+07	-3.73E+07	-5.61E+07	-3.55E+07	-9.73E+07	-5.50E+07	-5.47E+07	-3.73E+07
Comp Mole Frac (Propane)	0	0.02	0.0211	0	0	0	0	0.02
Comp Mole Frac (i-Butane)	0.7098	0.24	0.9589	0.2548	0.0009	0.2635	0.2635	0.24
Comp Mole Frac (n-Butane)	0.2872	0.69	0.02	0.7101	0.0563	0.7335	0.7335	0.69
Comp Mole Frac (i-Pantane)	0.003	0.05	0	0.0351	0.9429	0.003	0.003	0.05

Name	toboil1	cHE3out	hHE1out	hHE2in	boil1	b2	p1out	hHE1in
Vapour Fraction	1	0.3934	0	0	1	0	0	1
Temperature [F]	173.76	172.75	298.6	191.5	173.76	173.76	117.37	424.1
Pressure [psia]	66	66	671	668	66	66	866	675
Molar Flow [lbmole/hr]	1310.5	1340.4	870.1	870.1	1310.5	29.9	870.1	870.1
Heat Flow [Btu/hr]	-8.29E+07	-9.23E+07	-4.85E+07	-5.34E+07	-8.29E+07	-2.18E+06	-5.47E+07	-4.23E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.0009	0.0009	0.7098	0.7098	0.0009	0.0004	0.2635	0.7098
Comp Mole Frac (n-Butane)	0.0569	0.0563	0.2873	0.2873	0.0569	0.0295	0.7335	0.2873
Comp Mole Frac (i-Pantane)	0.9422	0.9429	0.003	0.003	0.9422	0.9701	0.003	0.003

Table A.4: Data of Butane Isomerization process (alt.2) for simulation (cont.)

Name	v4out	coolout	hHE3out	hHE2out	cHE1in	cHE1out	hHE3in	v6out
Vapour Fraction	0	0	0	0	0	0	0	0
Temperature [F]	117.67	125	191.5	137.67	173.99	315.39	298.6	124.94
Pressure [psia]	702	662.3	668	666	701	698.2	671	101.6
Molar Flow [lbmole/hr]	870.1	870.1	870.1	870.1	870.1	870.1	870.1	870.1
Heat Flow [Btu/hr]	-5.47E+07	-5.56E+07	-5.34E+07	-5.52E+07	-5.29E+07	-4.67E+07	-4.85E+07	-5.56E+07
Comp Mole Frac (Propane)	0	0	0	0	0	0	0	0
Comp Mole Frac (i-Butane)	0.2635	0.7098	0.7098	0.7098	0.2635	0.2635	0.7098	0.7098
Comp Mole Frac (n-Butane)	0.7335	0.2873	0.2873	0.2873	0.7335	0.7335	0.2873	0.2873
Comp Mole Frac (i-Pantane)	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.003

Name	Rin	Rout	v5out	v3out	v2out
Vapour Fraction	1	1	0.1158	0.1523	0.1448
Temperature [F]	390.1	424.1	148.31	86.54	111.23
Pressure [psia]	682	675	46	60	65.47
Molar Flow [lbmole/hr]	870.1	870.1	29.9	550.1	900
Heat Flow [Btu/hr]	-4.23E+07	-4.23E+07	-2.18E+06	-3.55E+07	-5.61E+07
Comp Mole Frac (Propane)	0	0	0	0.0211	0
Comp Mole Frac (i-Butane)	0.2635	0.7098	0.0004	0.9589	0.2548
Comp Mole Frac (n-Butane)	0.7335	0.2873	0.0295	0.02	0.7101
Comp Mole Frac (i-Pantane)	0.003	0.003	0.9701	0	0.0351

Name	qc1	qr1	qc2	auxiliary reboiler	qp1	qcooler	qfur
Heat Flow [Btu/hr]	2.97E+07	3.10E+07	1.33E+07	7.28E+06	2.94E+05	3.98E+05	4.42E+06

Equipment data and specifications

Table A.5: Column specifications

Column specifications	DIB column	Purge column
Totaltrays	50	20
Feed tray	20/30	10
Diameter (ft)	16	6
Condenser volume (ft^3)	1700	370
Reboiler volume (ft^3)	2000	400
Reflux ratio	7.3	0.8
Specification 1	nC_4 fraction in overhead = 0.02	iC_5 fraction in overhead =0.0030
Specification 2	iC_4 fraction in bottom = 0.2548	nC_4 fraction in bottom = 0.0295

Table A.6: Equipment data

Butane Isomerization process (Base Case)

Kinetics	A_f (1/h)	$4x10^8$
	E_f (Btu/lb.mol)	$3x10^4$
Furnace	Tube volume(ft^3)	340
Fooded Condensor	volume(ft^3)	340
Reactor	Diameter (ft)	7
	Length (ft)	18
	volume(ft^3)	693
FEHE 1	UA (Btu/F-hr)	4.401E+04
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21

Butane Isomerization process (alt. 1)

Kinetics	A_f (1/h)	$4x10^8$
	E_f (Btu/lb.mol)	$3x10^4$
Furnace	Tube volume(ft^3)	340
Fooded Condensor	volume(ft^3)	340
Reactor	Diameter (ft)	7
	Length (ft)	18
	volume(ft^3)	693
FEHE 1	UA (Btu/F-hr)	6.50E+04
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21
FEHE 2	UA (Btu/F-hr)	1.20E+05
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21
EHE 3	UA (Btu/F-hr)	1.40E+05
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21

Butane Isomerization process (alt. 2)

Kinetics	A_f (1/h)	$4x10^8$
	E_f (Btu/lb.mol)	$3x10^4$
Furnace	Tube volume(ft^3)	340
Fooded Condensor	volume(ft^3)	340
Reactor	Diameter (ft)	7
	Length (ft)	18
	volume(ft^3)	693
FEHE 1	UA (Btu/F-hr)	9.50E+04
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21
FEHE 2	UA (Btu/F-hr)	5.60E+05
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21
EHE 3	UA (Btu/F-hr)	1.850E+05
	Shell volume(ft^3)	21
	Tube volume(ft^3)	21

Table A.7: Tray properties of DIB column (steady state profile)

Stage	Pressure [psia]	Temp [F]	Net Liquid [lbmole/hr]	i-Butane (Light Liq)	n-Butane (Light Liq)
Condenser	100.0	121.20	3373.82	0.95891	0.0200
50__Main TS	100.0	122.40	3376.04	0.96396	0.0260
49__Main TS	100.1	123.03	3376.54	0.96208	0.0324
48__Main TS	100.2	123.42	3375.75	0.95698	0.0394
47__Main TS	100.2	123.71	3374.31	0.95018	0.0469
46__Main TS	100.3	123.96	3372.50	0.94229	0.0551
45__Main TS	100.4	124.22	3370.42	0.93354	0.0640
44__Main TS	100.5	124.48	3368.13	0.92404	0.0736
43__Main TS	100.6	124.75	3365.65	0.91382	0.0838
42__Main TS	100.7	125.04	3362.99	0.90291	0.0948
41__Main TS	100.7	125.33	3360.16	0.89132	0.1064
40__Main TS	100.8	125.65	3357.18	0.87910	0.1186
39__Main TS	100.9	125.97	3354.06	0.86628	0.1314
38__Main TS	101.0	126.31	3350.83	0.85293	0.1448
37__Main TS	101.1	126.66	3347.49	0.83910	0.1586
36__Main TS	101.1	127.02	3344.08	0.82489	0.1728
35__Main TS	101.2	127.38	3340.62	0.81038	0.1873
34__Main TS	101.3	127.75	3337.12	0.79566	0.2020
33__Main TS	101.4	128.13	3333.60	0.78083	0.2168
32__Main TS	101.5	128.51	3330.02	0.76597	0.2316
31__Main TS	101.6	128.90	3326.32	0.75115	0.2462
30__Main TS	101.6	129.29	4217.08	0.73637	0.2604
29__Main TS	101.7	129.49	4215.22	0.72873	0.2678
28__Main TS	101.8	129.74	4212.91	0.71947	0.2770
27__Main TS	101.9	130.03	4209.99	0.70821	0.2882
26__Main TS	102.0	130.39	4206.35	0.69454	0.3018
25__Main TS	102.0	130.81	4201.84	0.67803	0.3183
24__Main TS	102.1	131.31	4196.29	0.65823	0.3380
23__Main TS	102.2	131.90	4189.41	0.63467	0.3612
22__Main TS	102.3	132.61	4180.66	0.60686	0.3882
21__Main TS	102.4	133.49	4168.82	0.57419	0.4188
20__Main TS	102.4	134.63	4886.93	0.53577	0.4518
19__Main TS	102.5	134.85	4888.43	0.53549	0.4533
18__Main TS	102.6	135.02	4889.39	0.53459	0.4548
17__Main TS	102.7	135.15	4889.99	0.53317	0.4566
16__Main TS	102.8	135.28	4890.33	0.53122	0.4587
15__Main TS	102.9	135.41	4890.43	0.52871	0.4613

Table A.7: Tray properties of DIB column (steady state profile) (cont.)

Stage	Pressure [psia]	Temp [F]	Net Liquid [lbmole/hr]	i-Butane (Light Liq)	n-Butane (Light Liq)
14__Main TS	102.9	135.55	4890.29	0.52551	0.4645
13__Main TS	103.0	135.70	4889.87	0.52149	0.4685
12__Main TS	103.1	135.88	4889.13	0.51646	0.4736
11__Main TS	103.2	136.08	4888.01	0.51020	0.4798
10__Main TS	103.3	136.32	4886.42	0.50242	0.4876
9__Main TS	103.3	136.61	4884.28	0.49282	0.4972
8__Main TS	103.4	136.94	4881.49	0.48102	0.5089
7__Main TS	103.5	137.33	4877.93	0.46660	0.5233
6__Main TS	103.6	137.81	4873.48	0.44913	0.5407
5__Main TS	103.7	138.36	4867.97	0.42813	0.5615
4__Main TS	103.8	139.03	4861.16	0.40316	0.5861
3__Main TS	103.8	139.83	4852.50	0.37378	0.6145
2__Main TS	103.9	140.81	4840.76	0.33958	0.6464
1__Main TS	104.0	142.70	4823.49	0.30013	0.6799
Reboiler	104.0	143.90	900.00	0.25478	0.7101

Table A.8: Tray properties of Purge column (steady state profile)

Stage	Pressure [psia]	Temp [F]	Net Liquid [lbmole/hr]	i-Butane (Light Liq)	n-Butane (Light Liq)
Condenser	65.00	108.90	699.39	0.26353	0.73349
20__Main TS	65.00	110.38	696.57	0.20969	0.78326
19__Main TS	65.05	111.11	695.05	0.18901	0.79978
18__Main TS	65.11	111.53	693.93	0.18096	0.80360
17__Main TS	65.16	111.84	692.96	0.17764	0.80266
16__Main TS	65.21	112.11	692.05	0.17605	0.79994
15__Main TS	65.26	112.36	691.16	0.17512	0.79657
14__Main TS	65.32	112.60	690.29	0.17443	0.79300
13__Main TS	65.37	112.84	689.44	0.17383	0.78938
12__Main TS	65.42	113.08	688.61	0.17328	0.78581
11__Main TS	65.47	113.31	1453.84	0.17275	0.78233
10__Main TS	65.53	114.84	1447.42	0.13373	0.80955
9__Main TS	65.58	116.77	1437.36	0.10119	0.81775
8__Main TS	65.63	119.64	1420.84	0.07405	0.79681
7__Main TS	65.68	124.29	1396.11	0.05138	0.73263
6__Main TS	65.74	131.54	1366.59	0.03286	0.61643
5__Main TS	65.79	141.30	1342.10	0.01892	0.46215
4__Main TS	65.84	151.89	1330.69	0.00976	0.30743
3__Main TS	65.89	161.00	1330.73	0.00460	0.18530
2__Main TS	65.95	167.48	1335.45	0.00204	0.10432
1__Main TS	66.00	171.50	1340.41	0.00087	0.05626
Reboiler	66.00	173.80	29.91	0.00036	0.02950

Criteria for selection of best temperature control tray

The procedure for selecting which tray to control is to look at steady-state temperature profile in the column at the base-case conditions, as illustrated in Fig.A.1. We find the control tray that is most sensitive to changes in the manipulated variable. A steady-state rating program is used too make small open-loop changes in the manipulated variable (heat input in this example).We look at the resulting changes in tray temperatures and select the tray that shows the largest changes. In numerical case shown in Fig A.1, tray 1 appears to be the location where changes in the heat input (Qr) produce the largest changes in tray temperature.

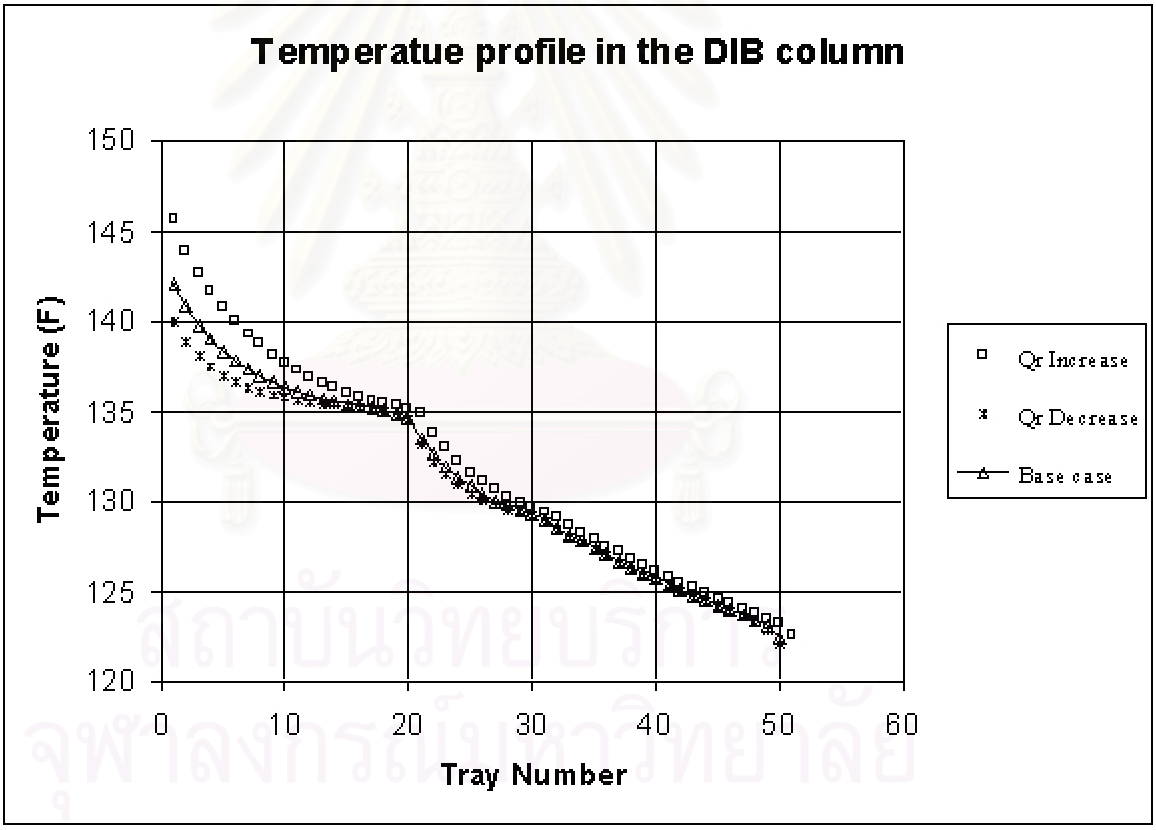


Figure A.1: Effect of changes in the column boilup on the temperature profile in the DIB column

For Effect of changes in the column boilup on the temperature profile in the Purge column is shown in Figure A.2. As can be seen, temperature profiles are very sharp (large temperature differences between trays) when the separation is easy (high relative volatility). This situation also can cause control problems. A very small change in the manipulated variable gives a very large change in temperature. A fairly easy solution to this problem is to use multiple temperature measurements over a section of the column in which the temperature profile moves and control an ”average temperature”.

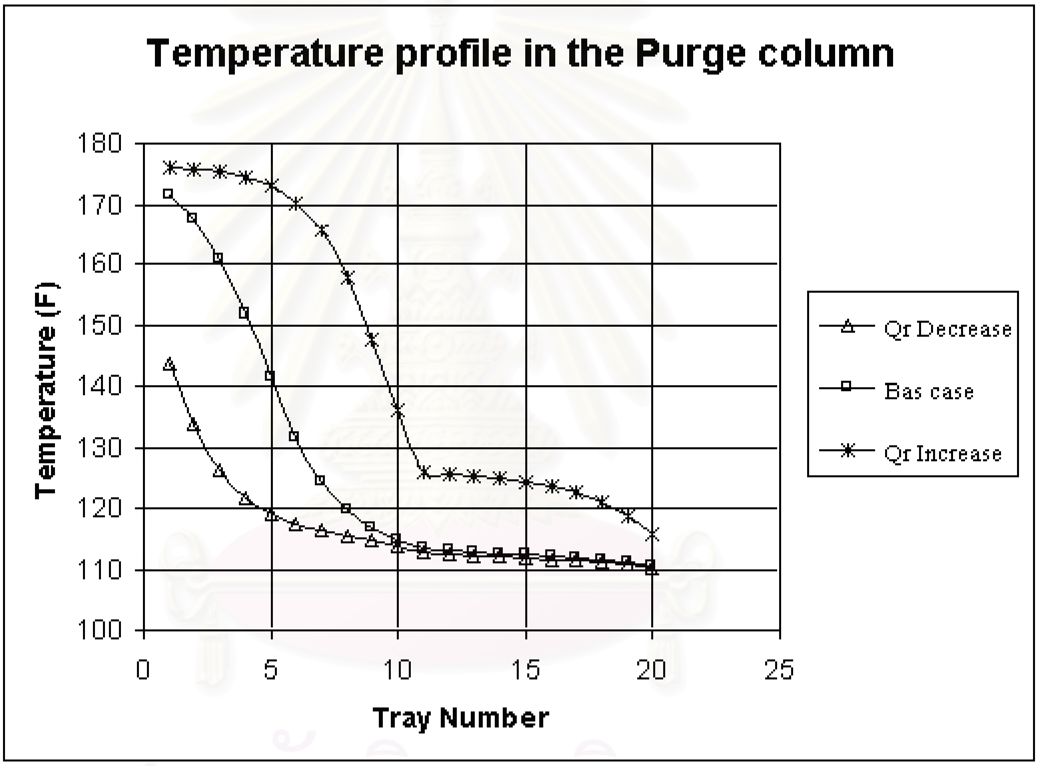


Figure A.2: Effect of changes in the column boilup on the temperature profile in the Purge column

APPENDIX B

PARAMETER TUNING OF CONTROL STRUCTERS

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 $K_C = 0.5$ 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 retuned 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 volumn. So the recommended tuning of a level controller is $K_C = 2$.

Pressure Controllers

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

Temperature Controllers

Temperature dynamic responses are generally slow, so PID control is used. Typically, the controller gain, K_C, 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 height of the relay h. This height is typically 5 to 10% of the controller-output scale. The loop starts to oscilate around the setpoint, with the controller output switching every time the process varisble (PV) signal crosses the setpoint.

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

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

The period of the output PV curve is the ultimate period P_u. From these two parameters, controller tunning 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

$$K_C = \frac{K_u}{2.2}$$

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

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

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 button. The loop will start to oscilate. After several cycles, the tuning is stopped and some recommended settings for a PID controller are suggested.

B.3 Inclusion of Lags

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

In this plant, A 3-minute deadtime is assumed in the product composition measurement (CC1). We include lags at temperature control loops of TC1, TC2, TCR and TC-cool. Some lags are recommended in table below:

Table B.1: Typical measurement lags

		Number	Time constant (minutes)	Type
Temperature	Liquid	2	0.5	First-Order Lag
	Gas	3	1	First-Order Lag
Composition	Chromatograph	1	3 to10	Deadtime

Table B.2: Parameter tuning of Butane Isomerization process (Base Case) for CS1and CS2 (reference, Luyben (1998))

Controller	controlled variable	manipulated variable	Control action	Set point		K_C	τ_i (min)	τ_d (min)
CC1	product composition	DIB reboiler duty (qr1)	Reverse	0.02	-	1	60	-
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	390.1	^{o}F	4.12	0.504	0.112
TC-cooler	cooler outlet temperature	cooler duty (qcooler)	Direct	125	^{o}F	10.8	0.597	0.133
LC11	DIB column base level	PFD feed valve (V1)	Direct	50.00	%	2	-	-
LC12	DIB column reflux drum level	DIB product valve (V3)	Reverse	50.00	%	2	-	-
LC21	Purge column reflux drum level	Purge reboiler duty (qr2)	Reverse	50.00	%	2	-	-
LC22	Purge column base level	Purge feed valve (V2)	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	Rliquid feed valve (V6)	Direct	671.0	psia	2	10	-
FC21	Purge column bottom flowrate	Purge column bottom flow valve (V5)	Reverse	29.90	kgmole/h	0.5	0.3	-
FC22	Recycle flowrate	Purge column distillate flow valve (V4)	Reverse	870.1	kgmole/h	0.5	0.3	-
FC-reflux	DIB column reflux flowrate	DIB column reflux valve (V1-reflux)	Reverse	3373.8	kgmole/h	0.5	0.3	-

Table B.3: Parameter tuning of Butane Isomerization process (Base Case) for CS3 and CS4

Controller	controlled variable	manipulated variable		Control action	Set point		K_C	τ_i (min)	τ_d (min)
CC1	DIB column top stage composition	CS3	DIB product valve (V3)	Reverse	0.25961	-	5.48	19.0	4.22
		CS4	DIB column reflux valve (V1-reflux)	Direct			1.03	12.1	2.69
TCR	reactor inlet temperature	furnace duty (qfur)		Reverse	390.1	^{o}F	4.12	0.504	0.112
TC-cooler	cooler outlet temperature	cooler duty (qcooler)		Direct	125	^{o}F	10.8	0.597	0.133
LC11	DIB column base level	PFD feed valve (V1)		Direct	50.00	%	2	-	-
LC12	DIB column reflux drum level	CS3	DIB column reflux valve (V1-reflux)	Reverse	50.00	%	2	-	-
		CS4	DIB product valve (V3)						
LC21	Purge column reflux drum level	TC2		Reverse	50.00	%	0.225	9.81	-
LC22	Purge column base level	Purge feed valve (V2)		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	Rliquid feed valve (V6)		Direct	671.0	psia	2	10	-
FC21	Purge column bottom flowrate	Purge column bottom flow valve (V5)		Reverse	29.90	kgmole/h	0.5	0.3	-
FC22	Recycle flowrate	Purge column distillate flow valve (V4)		Reverse	870.1	kgmole/h	0.5	0.3	-
TC1	DIB column stage1 temperature	DIB reboiler duty (qr1)		Reverse	142.7	^{o}F	11	2.76	0.612
TC2	Purge column average temperature	Purge reboiler duty (qr2)		Reverse	149.8578	^{o}F	5.12	3.34	0.743

Table B.4: Parameter tuning of Butane Isomerization process (Base Case) for S1, S2 and S3 (Poothanakul P., 2002)

Controller	controlled variable	manipulated variable		Control action	Set point		K_C	τ_i (min)	τ_d (min)
CC1	product composition	S1	DIB product valve (V3)	Reverse	0.02	-	2.68	70.3	15.6
		S2,S3	DIB reboiler duty (qr1)				1	60	-
TCR	reactor inlet temperature	furnace duty (qfur)		Reverse	390.1	^{o}F	4.12	0.504	0.112
TC-cooler	cooler outlet temperature	cooler duty (qcooler)		Direct	125	^{o}F	10.8	0.597	0.133
LC11	DIB column base level	PFD feed valve (V1)		Direct	50.00	%	2	-	-
LC12	DIB column reflux drum level	S1	DIB column reflux valve (V1-reflux)	Reverse	50.00	%	2	-	-
		S2,S3	DIB product valve (V3)						
LC21	Purge column reflux drum level	Purge reboiler duty (qr2)		Reverse	50.00	%	2	-	-
LC22	Purge column base level	Purge feed valve (V2)		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	Rliquid feed valve (V6)		Direct	671.0	psia	2	10	-
FC21	Purge column bottom flowrate	S1,S2	Purge column bottom flow valve (V5)	Reverse	29.90	kgmole/h	0.5	0.3	-
		S3	-						
FC22	Recycle flowrate	Purge column distillate flow valve (V4)		Reverse	870.1	kgmole/h	0.5	0.3	-
FC-reflux	DIB column reflux flowrate	DIB column reflux valve (V1-reflux)		Reverse	3373.8	kgmole/h	0.5	0.3	-
TC2-com	Purge column stage20 temperature	Purge column reflux valve (V2-reflux)		Reverse	110.35	^{o}F	4.67	96.8	-
TC2	Purge column stage2 temperature	Purge column bottom flow valve (V5)		Direct	167.447	^{o}F	13.5	39.2	8.72

Table B.5: Parameter tuning of control structures for Butane Isomerization process alternative 1

Controller	controlled variable	manipulated variable		Control action	Set point		K_C	τ_i (min)	τ_d (min)
CC1	product composition	CS1	DIB reboiler duty (qr1)	Reverse	0.02	-	1	60	-
		CS2	DIB reboiler duty (qr1)	Reverse			1	60	-
	DIB column top stage composition	CS3	DIB product valve (V3)	Reverse	0.25961	-	5.54	18.9	4.20
		CS4	DIB column reflux valve (V1-reflux)	Direct			1.04	12.1	2.68
TCR	reactor inlet temperature	furnace duty (qfur)		Reverse	390.1	^{o}F	5.67	0.442	0.0982
TC-cooler	cooler outlet temperature	cooler duty (qcooler)		Direct	125	^{o}F	14.8	2.67	0.459
LC11	DIB column base level	PFD feed valve (V1)		Direct	50.00	%	2	-	-
LC12	DIB column reflux drum level	CS1	DIB product valve (V3)	Reverse	50.00	%	2	-	-
		CS2	DIB product valve (V3)						
		CS3	DIB column reflux valve (V1-reflux)						
		CS4	DIB product valve (V3)						
LC21	Purge column reflux drum level	CS1,CS2	Purge reboiler duty (qr2)	Reverse	50.00	%	2	-	-
		CS3,CS4	TC2				0.225	9.81	-
LC22	Purge column base level	Purge feed valve (V2)		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	Rliquid feed valve (V6)		Direct	671.0	psia	2	10	-
FC21	Purge column bottom flowrate	Purge column bottom flow valve (V5)		Reverse	29.90	kgmole/h	0.5	0.3	-
FC22	Recycle flowrate	Purge column distillate flow valve (V4)		Reverse	870.1	kgmole/h	0.5	0.3	-
TC1	DIB column stage1 temperature	DIB reboiler duty (qr1)		Reverse	142.7	^{o}F	11.9	2.76	0.614
TC2	Purge column average temperature	Purge reboiler duty (qr2)		Reverse	149.8578	^{o}F	5.12	3.34	0.743

Table B.5: Parameter tuning of control structures for Butane Isomerization process alternative 1 (cont.)

Controller	controlled variable	manipulated variable	Control action	Set point	K_C	τ_i (min)	τ_d (min)
TC-hHE1	FEHE1 hot stream outlet temperature	valve bypass across FEHE1(VBP1)	Reverse	305.46 °F	3.09	0.271	0.0603
TC-cHE2	FEHE2 cold stream outlet temperature	valve bypass across FEHE2(VBP2)	Direct	285.46 °F	13.7	0.346	0.0769

Table B.6: Parameter tuning of control structures for Butane Isomerization process alternative 2

Controller	controlled variable	manipulated variable		Control action	Set point		K_C	τ_i (min)	τ_d (min)
CC1	product composition	CS1	DIB reboiler duty (qr1)	Reverse	0.02	-	1	60	-
		CS2	DIB reboiler duty (qr1)	Reverse			1	60	-
	DIB column top stage composition	CS3	DIB product valve (V3)	Reverse	0.25961	-	5.55	18.8	4.17
		CS4	DIB column reflux valve (V1-reflux)	Direct			1.04	12.1	2.68
TCR	reactor inlet temperature	furnace duty (qfur)		Reverse	390.1	^oF	3.93	0.641	0.142
TC-cooler	cooler outlet temperature	cooler duty (qcooler)		Direct	125	^oF	14.8	2.16	0.481
LC11	DIB column base level	PFD feed valve (V1)		Direct	50.00	%	2	-	-
LC12	DIB column reflux drum level	CS1	DIB product valve (V3)	Reverse	50.00	%	2	-	-
		CS2	DIB product valve (V3)						
		CS3	DIB column reflux valve (V1-reflux)						
		CS4	DIB product valve (V3)						
LC21	Purge column reflux drum level	CS1,CS2	Purge reboiler duty (qr2)	Reverse	50.00	%	2	-	-
		CS3,CS4	TC2				0.355	10.1	-
LC22	Purge column base level	Purge feed valve (V2)		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	Rliquid feed valve (V6)		Direct	671.0	psia	2	10	-
FC21	Purge column bottom flowrate	Purge column bottom flow valve (V5)		Reverse	29.90	kgmole/h	0.5	0.3	-
FC22	Recycle flowrate	Purge column distillate flow valve (V4)		Reverse	870.1	kgmole/h	0.5	0.3	-
TC1	DIB column stage1 temperature	DIB reboiler duty (qr1)		Reverse	142.7	^oF	11.1	2.65	0.589
TC2	Purge column average temperature	Purge reboiler duty (qr2)		Reverse	149.8578	^oF	7.74	3.04	0.676

Table B.6: Parameter tuning of control structures for Butane Isomerization process alternative 2 (cont.)

Controller	controlled variable	manipulated variable	Control action	Set point	K_C	τ_i (min)	τ_d (min)
TC-hHE1	FEHE1 hot stream outlet temperature	valve bypass across FEHE1(VBP1)	Reverse	305.46 °F	2.88	0.284	0.0632
TC-cHE2	FEHE2 cold stream outlet temperature	valve bypass across FEHE2(VBP2)	Direct	285.46 °F	13.6	0.346	0.0768

APPENDIX C

DYNAMIC RESPONSES

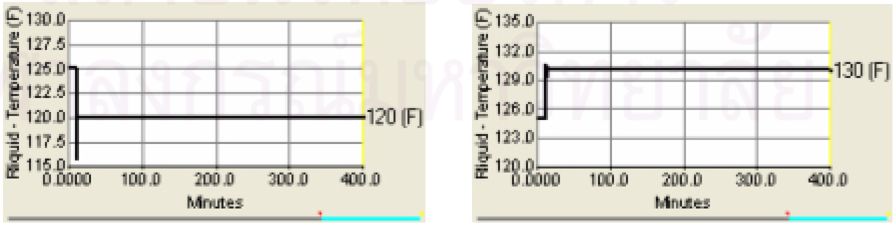
The dynamic responses and table of the IAE results of the control structures in the Butane Isomerization plant alternatives 1, 2 and base-case to changes in the recycle stream temperature and the recycle flowrates before entering the DIB column are shown in figures below.

These disturbances are made as follows:

- Step changes of +5 ^{0}F increasing and -5 ^{0}F decreasing at time 10 minute are made in the recycle stream temperature before entering the DIB column (The starting conditions is 125 ^{0}F)
- Step change of decreasing the recycle flowrates before entering the DIB column from 870 to 800.1lb.mol/h.

The disturbance testing is used to compare the dynamic response of this work's structures (CS3 and CS4) with Luyben's structures (CS1 and CS2), the result shows that performances of this work's structures are better than Luyben's structures.

C.1 Change in the recycle stream temperature before entering the DIB column



(a) Change of 5 °F decreasing (b) Change of 5 °F increasing

Figure C.1: Dynamic responses to 5 ^{0}F increase and 5 ^{0}F decrease in the recycle stream temperature before entering the DIB column.

C.1.1 Change in the recycle stream temperature before entering the DIB column for reference control structure I (CS1) in Butane Isomerization plant (Base Case)

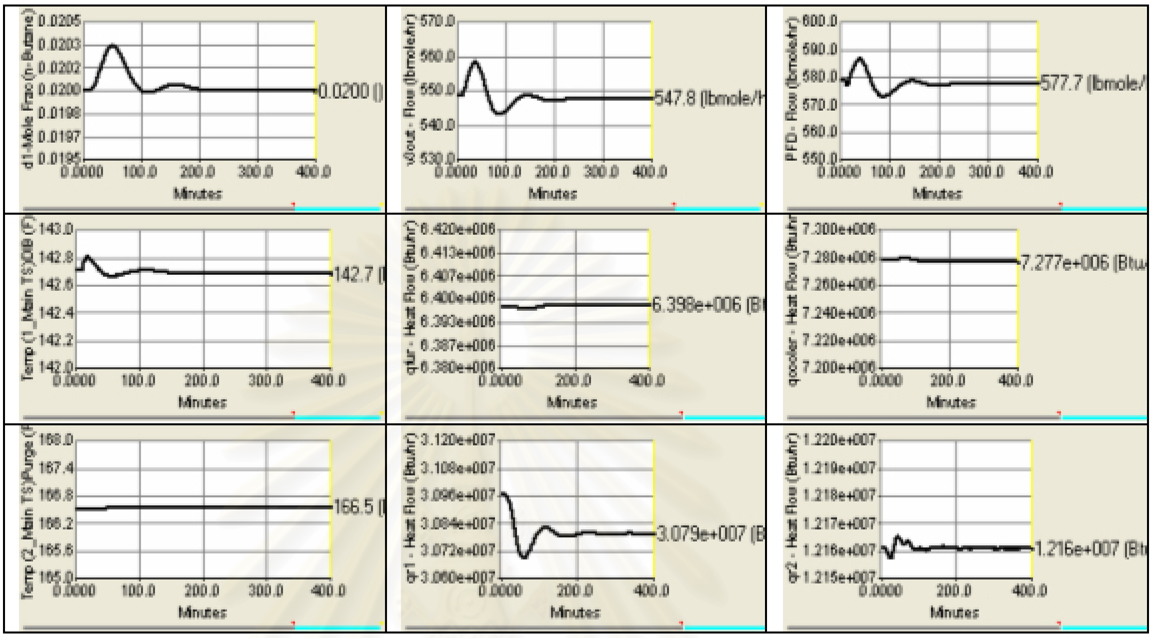


Figure C.2: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to 5 ^{0}F increase in the recycle stream temperature before entering the DIB column.

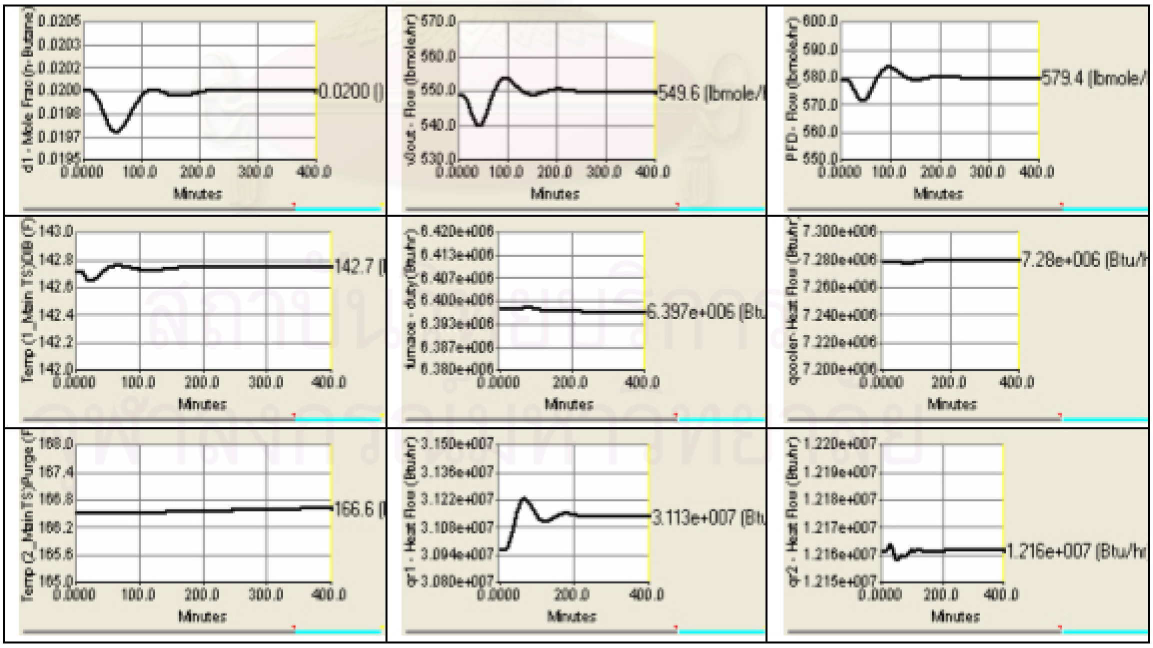


Figure C.3: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to 5 ^{0}F decrease in the recycle stream temperature before entering the DIB column.

C.1.2 Change in the recycle stream temperature before entering the DIB column for reference control structure II (CS2) in Butane Isomerization plant (Base Case)

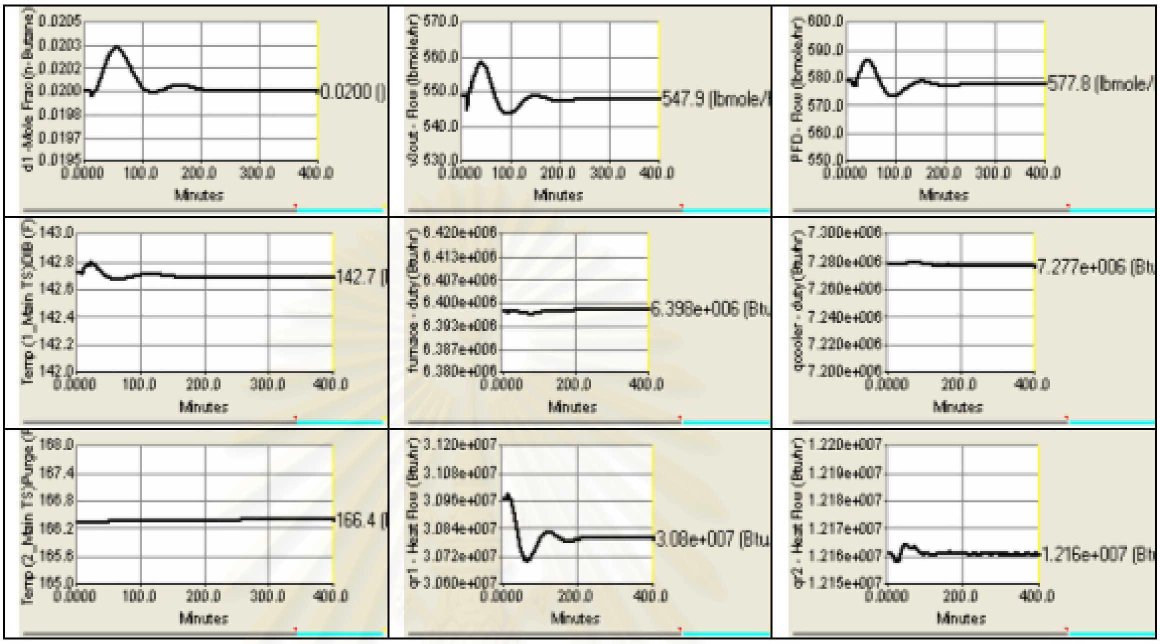


Figure C.4: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to 5 ^{0}F increase in the recycle stream temperature before entering the DIB column.

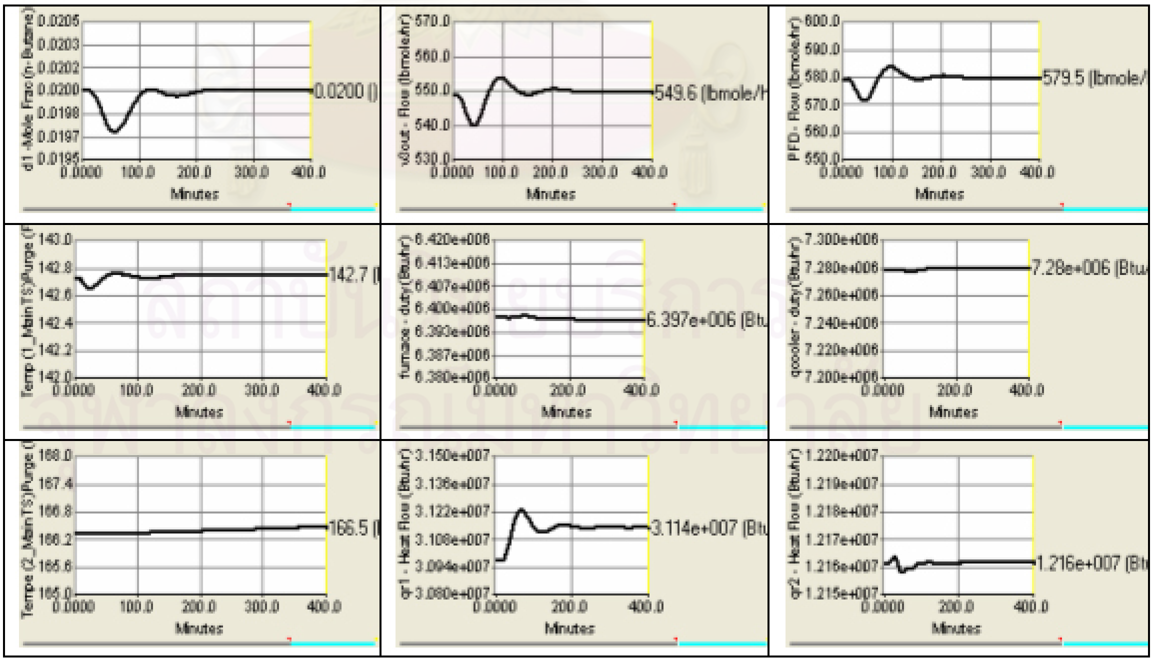


Figure C.5: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to 5 ^{0}F decrease in the recycle stream temperature before entering the DIB column.

C.1.3 Change in the recycle stream temperature before entering the DIB column for Butane Isomerization plant alternatives 1 and 2

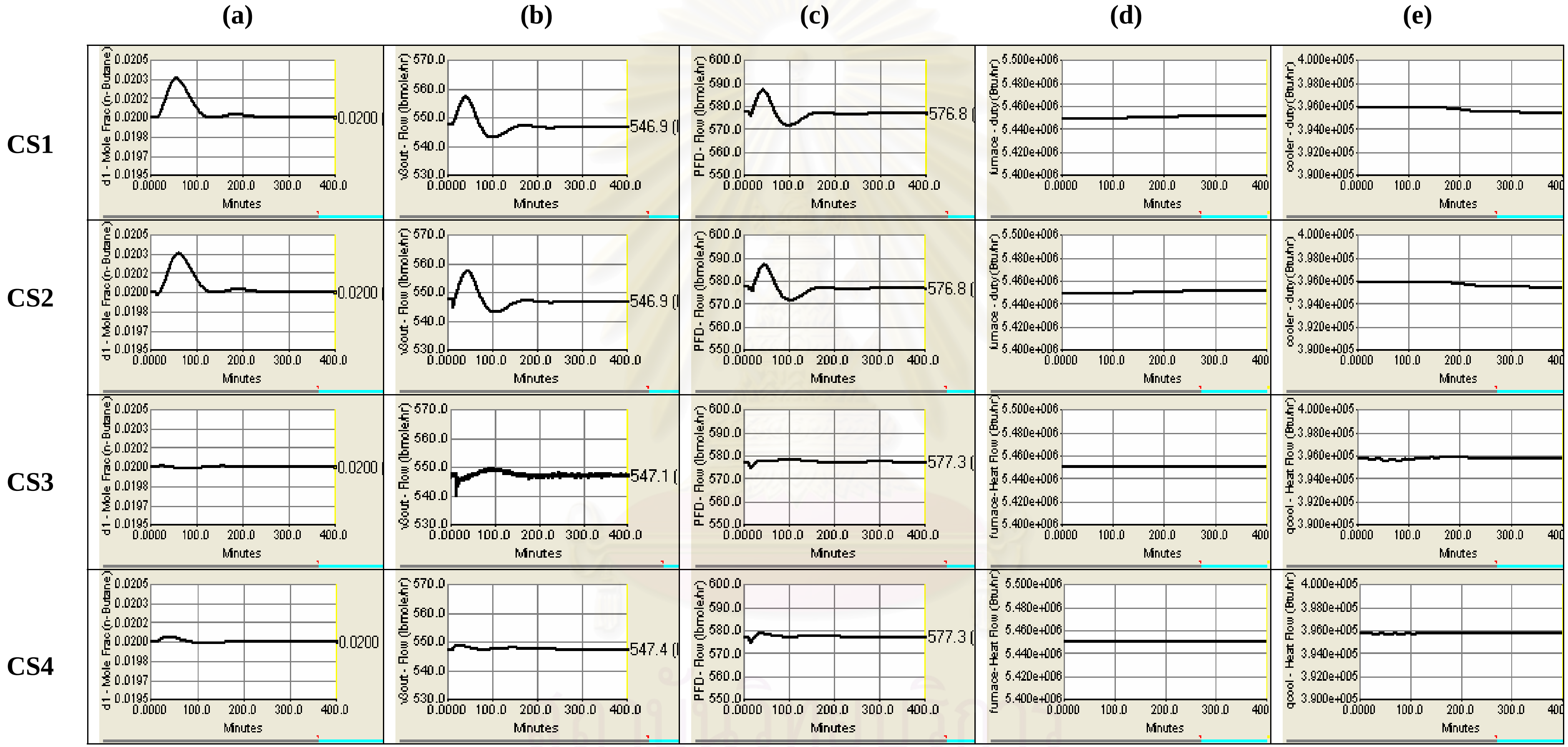


Figure C.6: Dynamic responses of the Butane Isomerization plant alternative 1 to 5 ^{o}F increase in the recycle stream temperature before entering the DIB column, where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (e) cooler duty; comparison between CS1,CS2,CS3 and CS4.

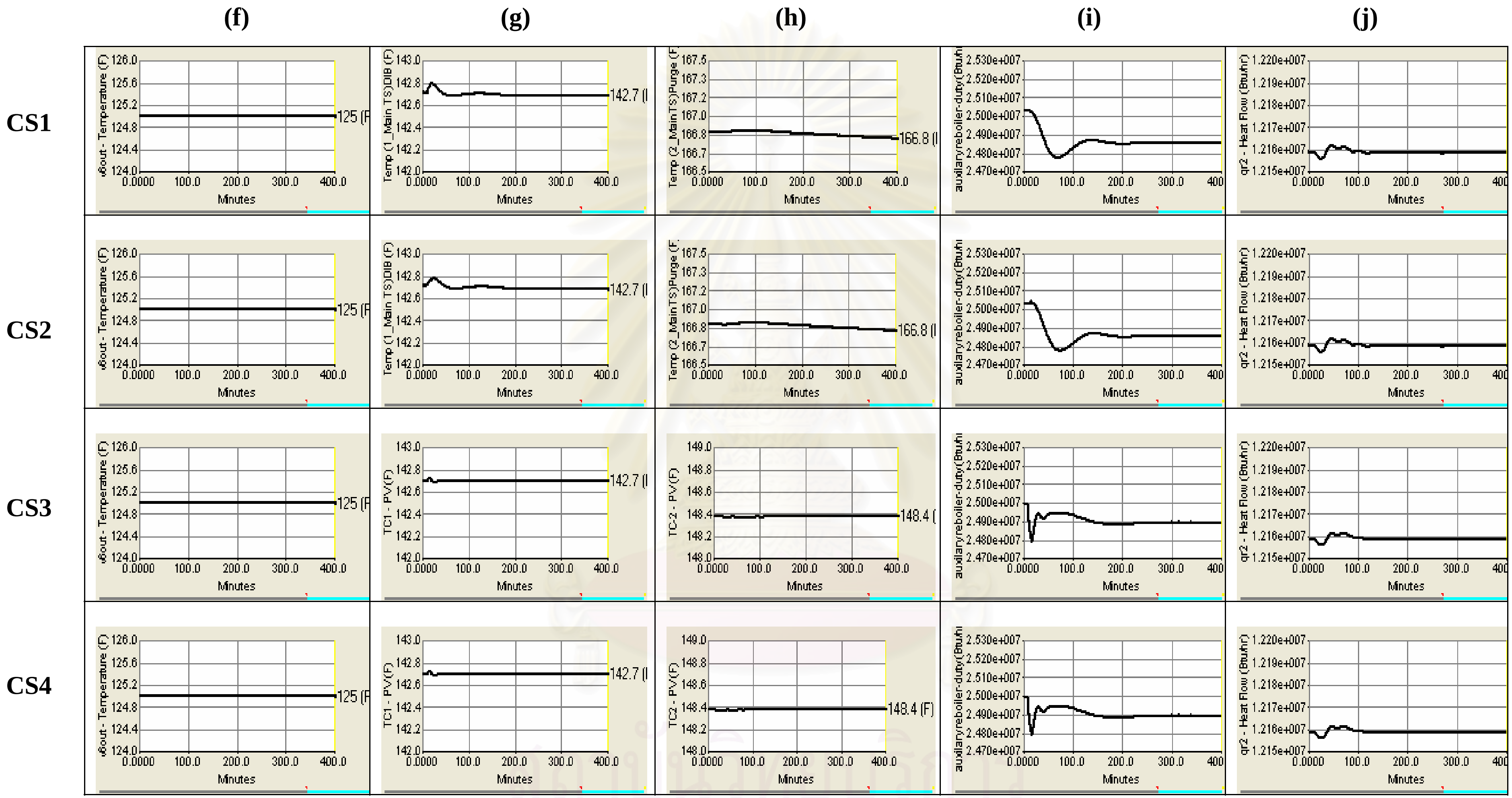


Figure C.6: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

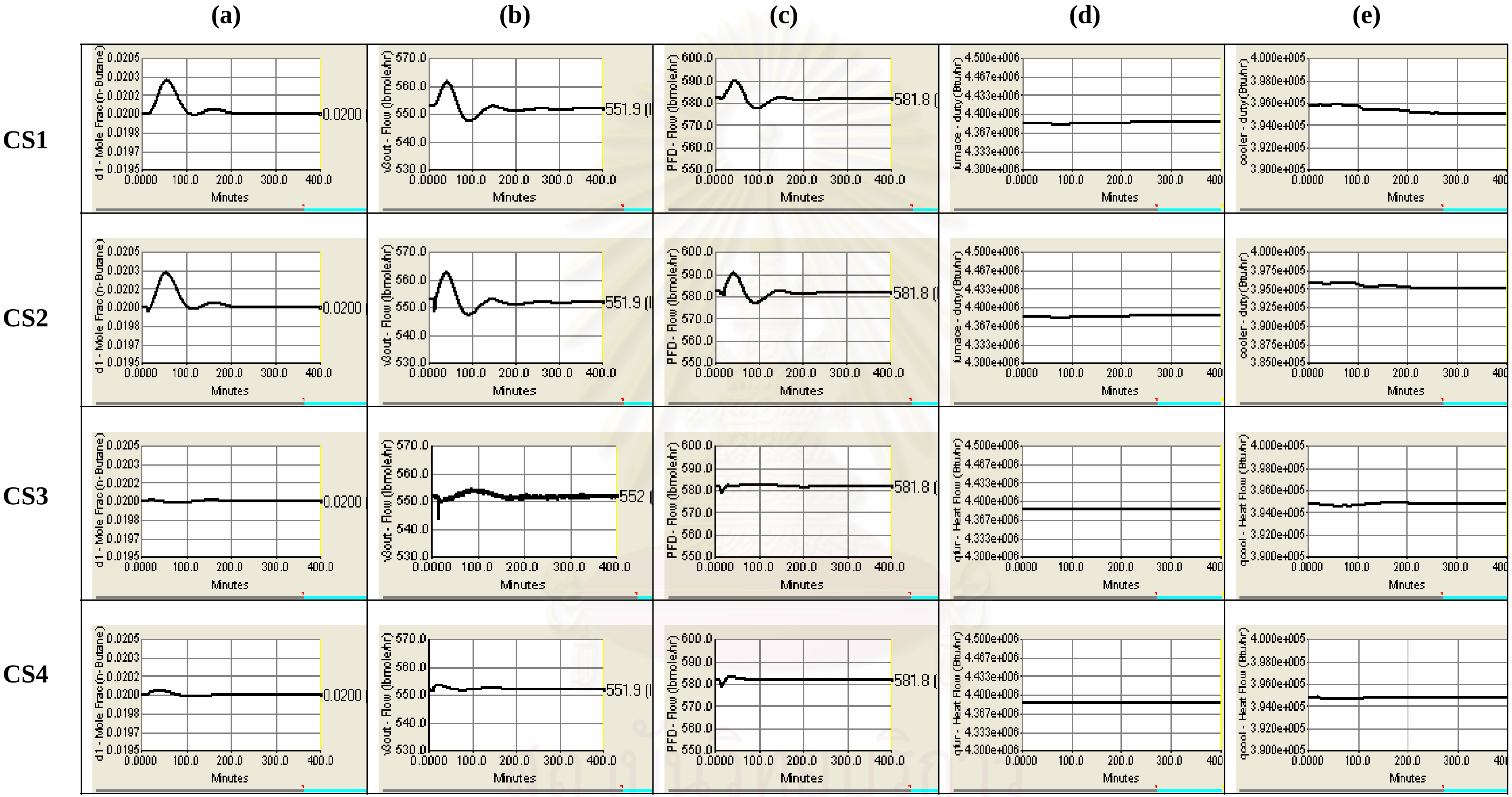


Figure C.7: Dynamic responses of the Butane Isomerization plant alternative 2 to 5 ^{o}F increase in the recycle stream temperature before entering the DIB column, where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1,CS2,CS3 and CS4.

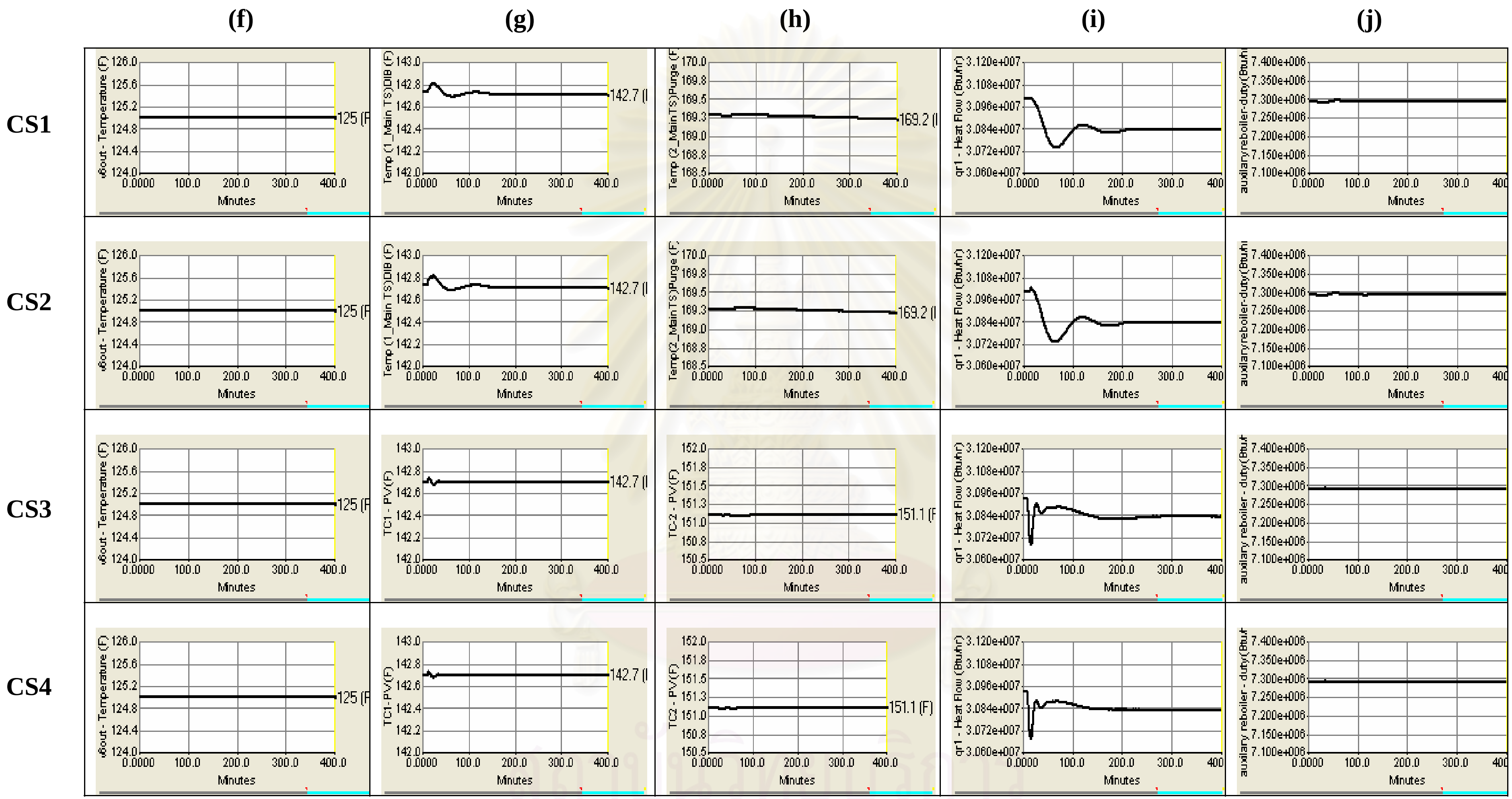


Figure C.7: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

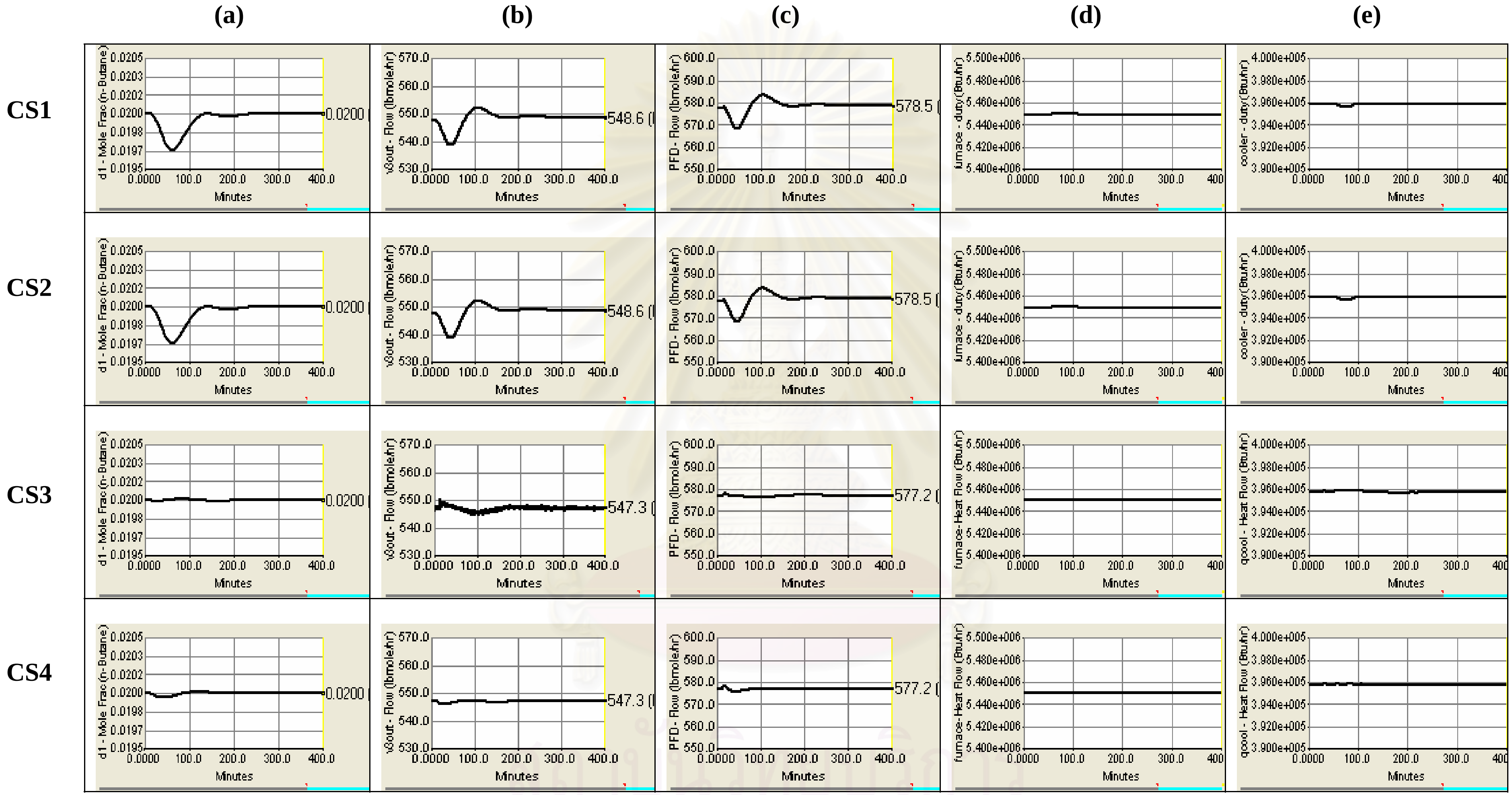


Figure C.8: Dynamic responses of the Butane Isomerization plant alternative 1 to 5 °F decrease in the recycle stream temperature before entering the DIB column, where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1,CS2,CS3 and CS4.

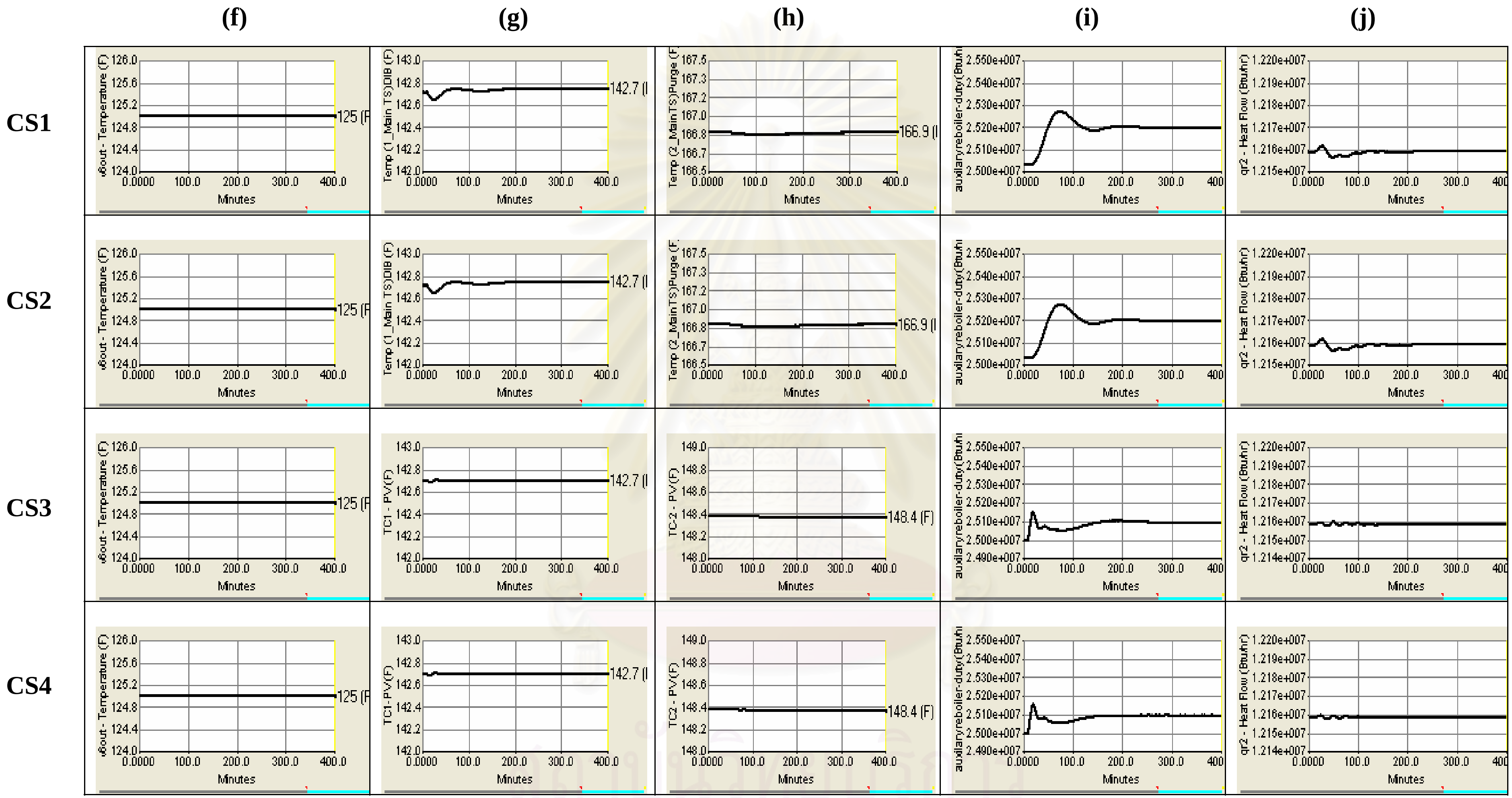


Figure C.8: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

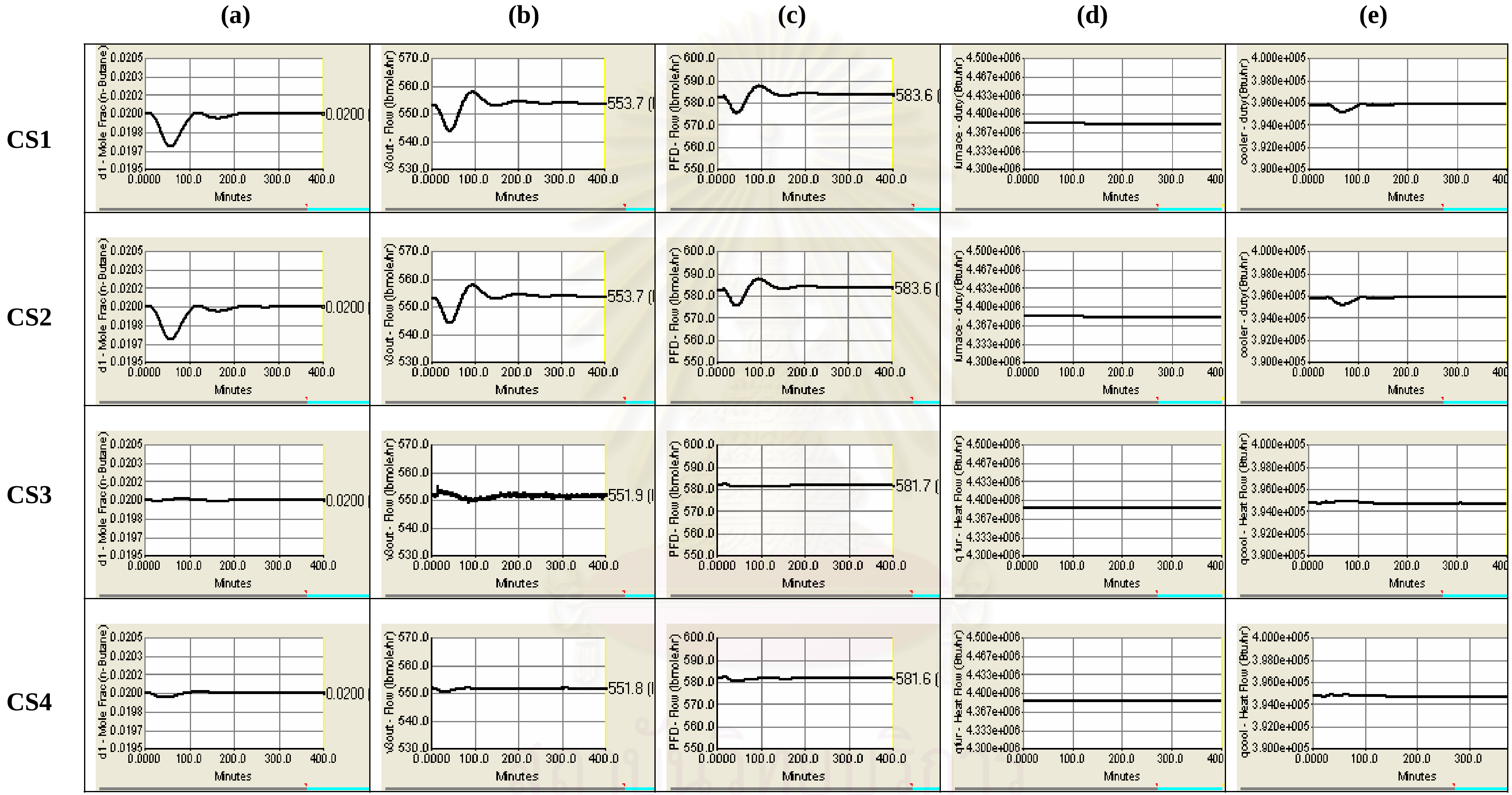


Figure C.9: Dynamic responses of the Butane Isomerization plant alternative 2 to 5 °F decrease in the recycle stream temperature before entering the DIB column, where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty; comparison between CS1,CS2,CS3 and CS4.

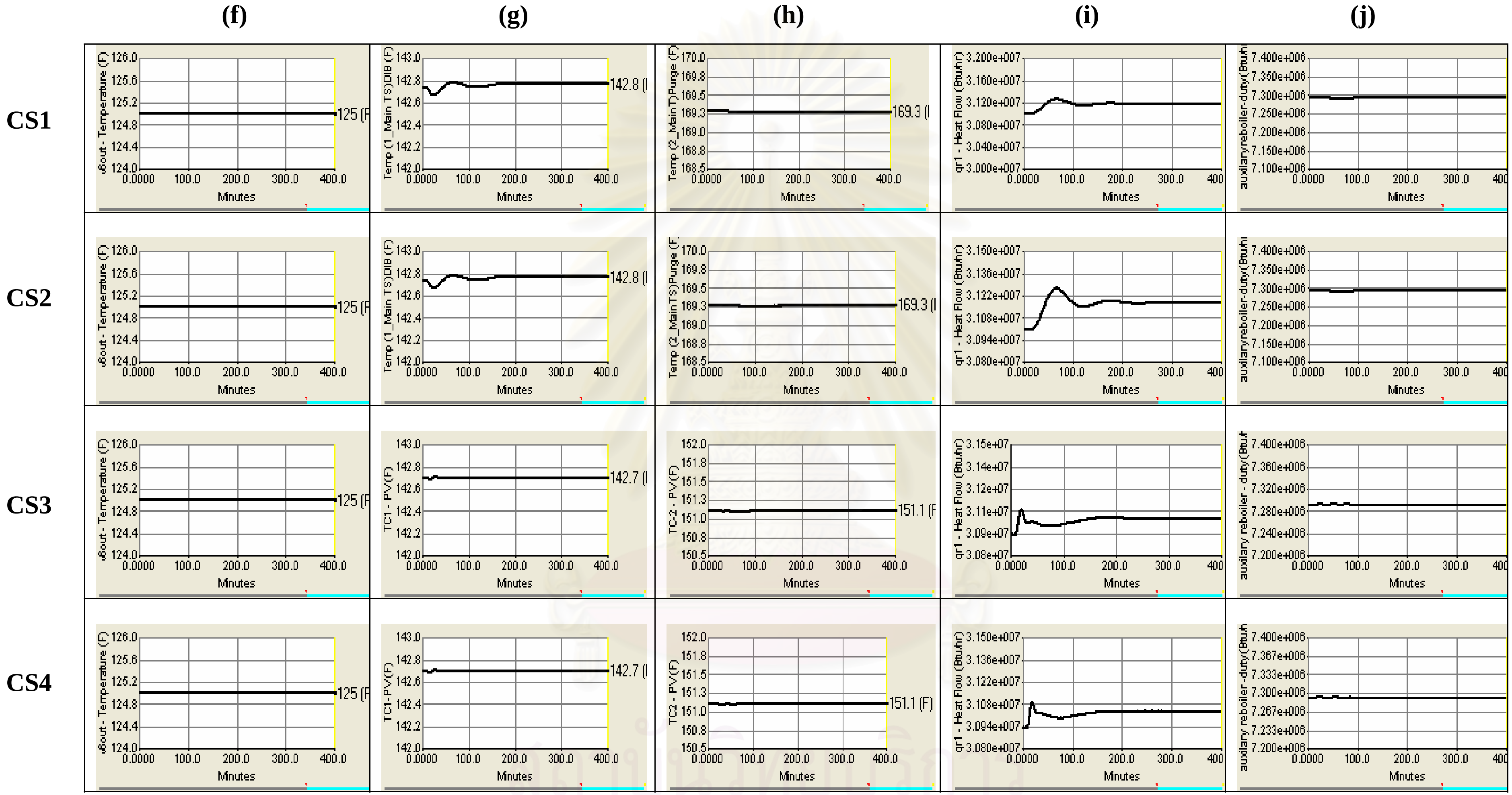


Figure C.9: Continued, where (f) the flooded condenser outlet temperature, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column auxiliary reboiler duty, (j) the Purge column reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

C.2 Change in the recycle flowrates before entering the DIB column

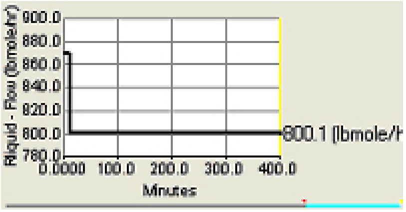


Figure C.10: Dynamic responses to decrease in the recycle flowrates before entering the DIB column from 870 to 800.1lb.mol/h.

C.2.1 Change in the recycle flowrates before entering the DIB column for reference control structure I (CS1) in Butane Isomerization plant (Base Case)

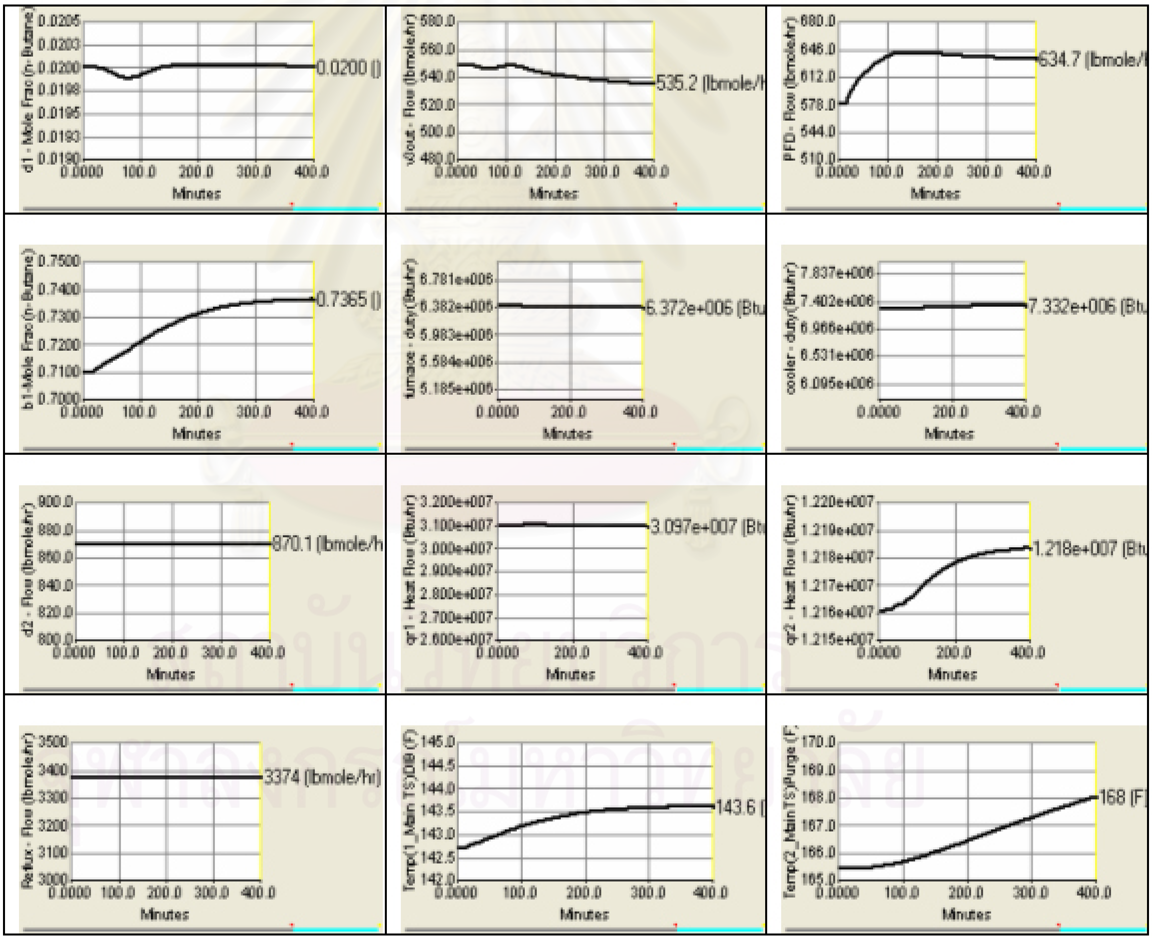


Figure C.11: Dynamic responses of CS1 in Butane Isomerization plant (Base Case) to decrease in the recycle flowrates before entering the DIB column from 870 to 800.1 lb.mol/h.

C.2.2 Change in the recycle flowrates before entering the DIB column for reference control structure II (CS2) in Butane Isomerization plant (Base Case)

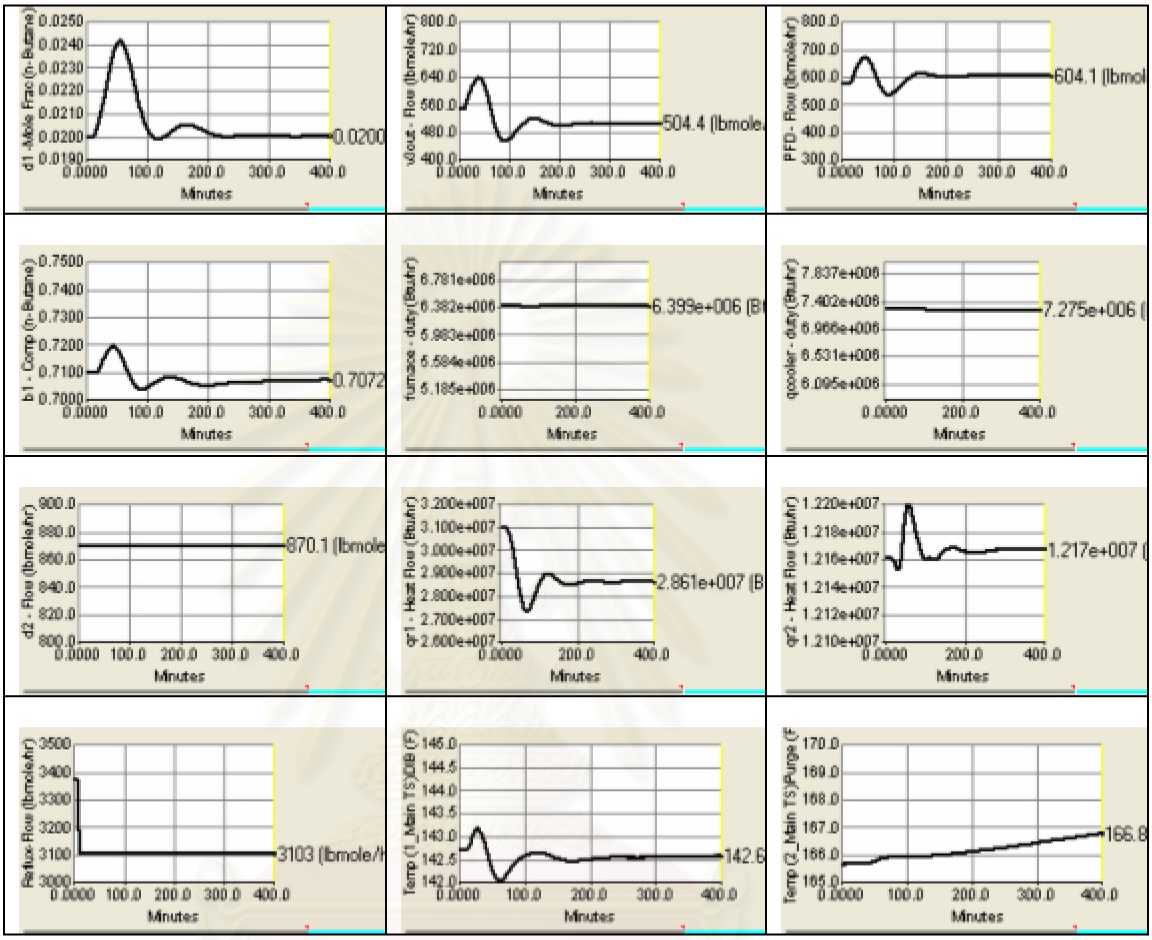


Figure C.12: Dynamic responses of CS2 in Butane Isomerization plant (Base Case) to decrease in the recycle flowrates before entering the DIB column from 870 to 800.1 lb.mol/h.

C.2.3 Change in the recycle flowrates before entering the DIB column for Butane Isomerization plant alternatives 1 and 2

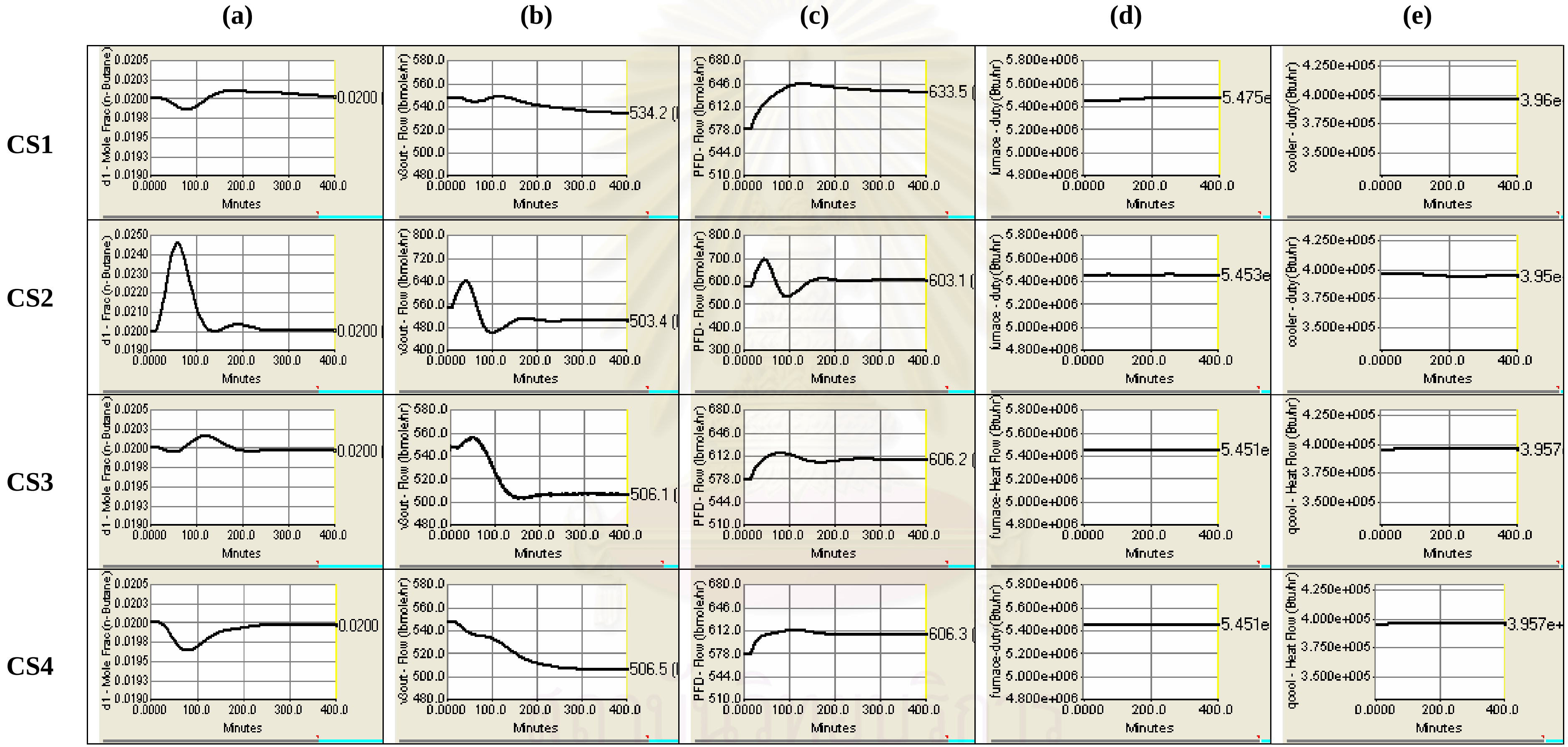


Figure C.13: Dynamic responses of the Butane Isomerization plant alternative 1 to decrease in recycle flowrates before entering the DIB column from 870 to 800.1lb.mol/h., where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty;comparison between CS1, CS2, CS3 and CS4.

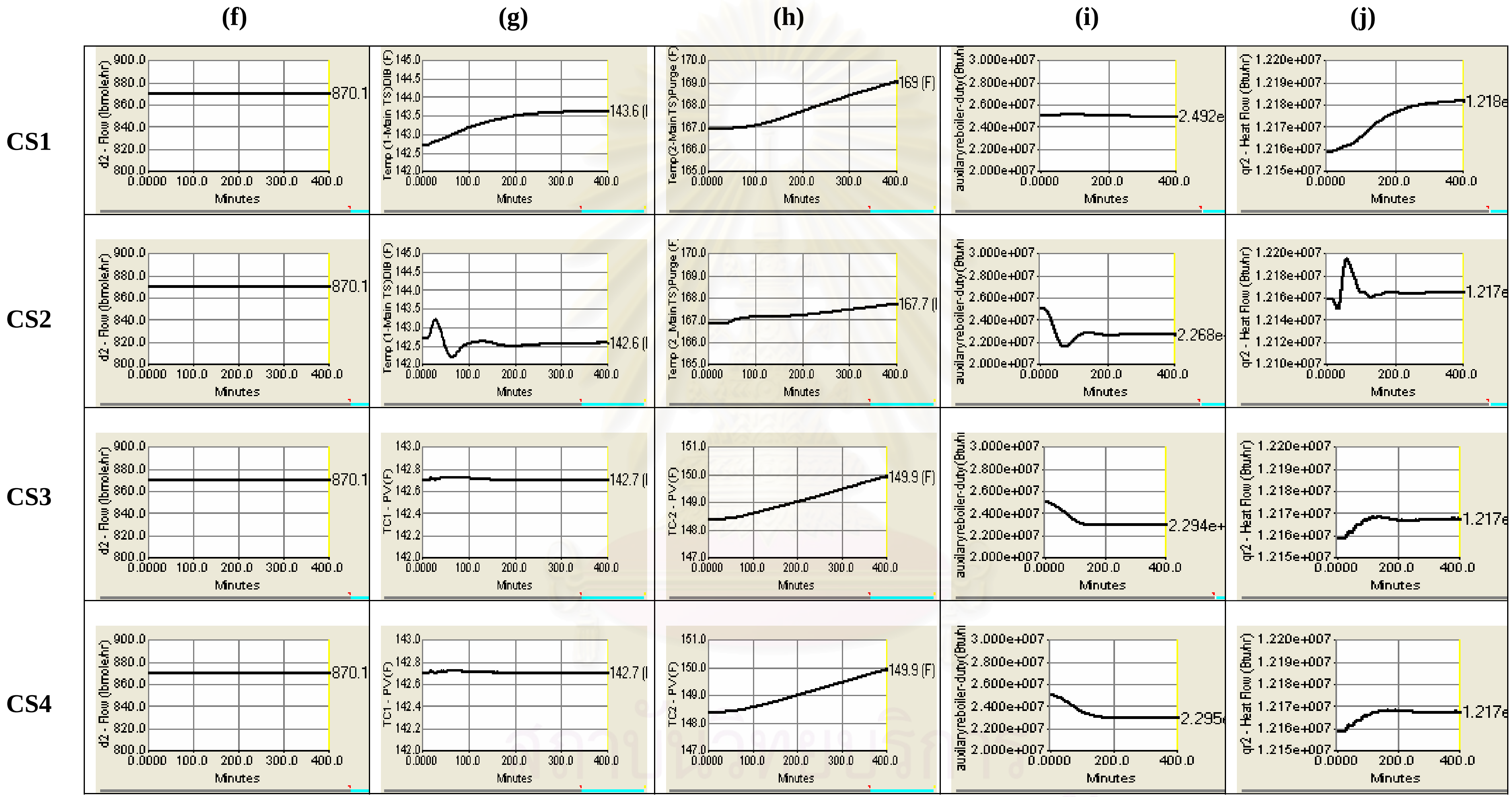


Figure C.13: Continued, where (f) the distillate flowrates of the purge column, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

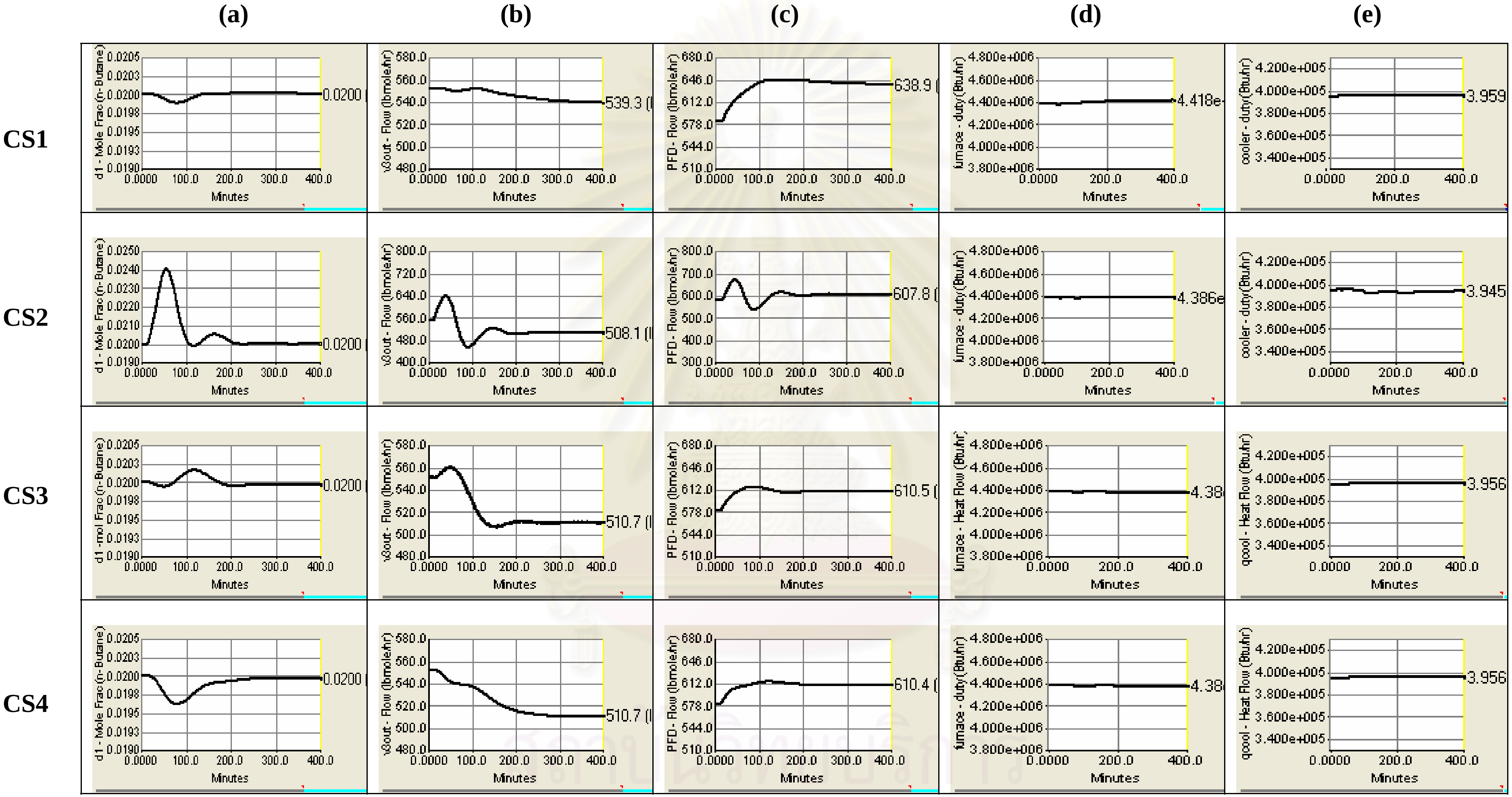


Figure C.14: Dynamic responses of the Butane Isomerization plant alternative 2 to decrease in recycle flowrates before entering the DIB column from 870 to 800.1lb.mol/h., where (a) the impurity of nC_4 in the product, (b) the iC_4 product flowrate, (c) the fresh feed flowrate, (d) furnace duty, (e) cooler duty;comparison between CS1, CS2, CS3 and CS4.

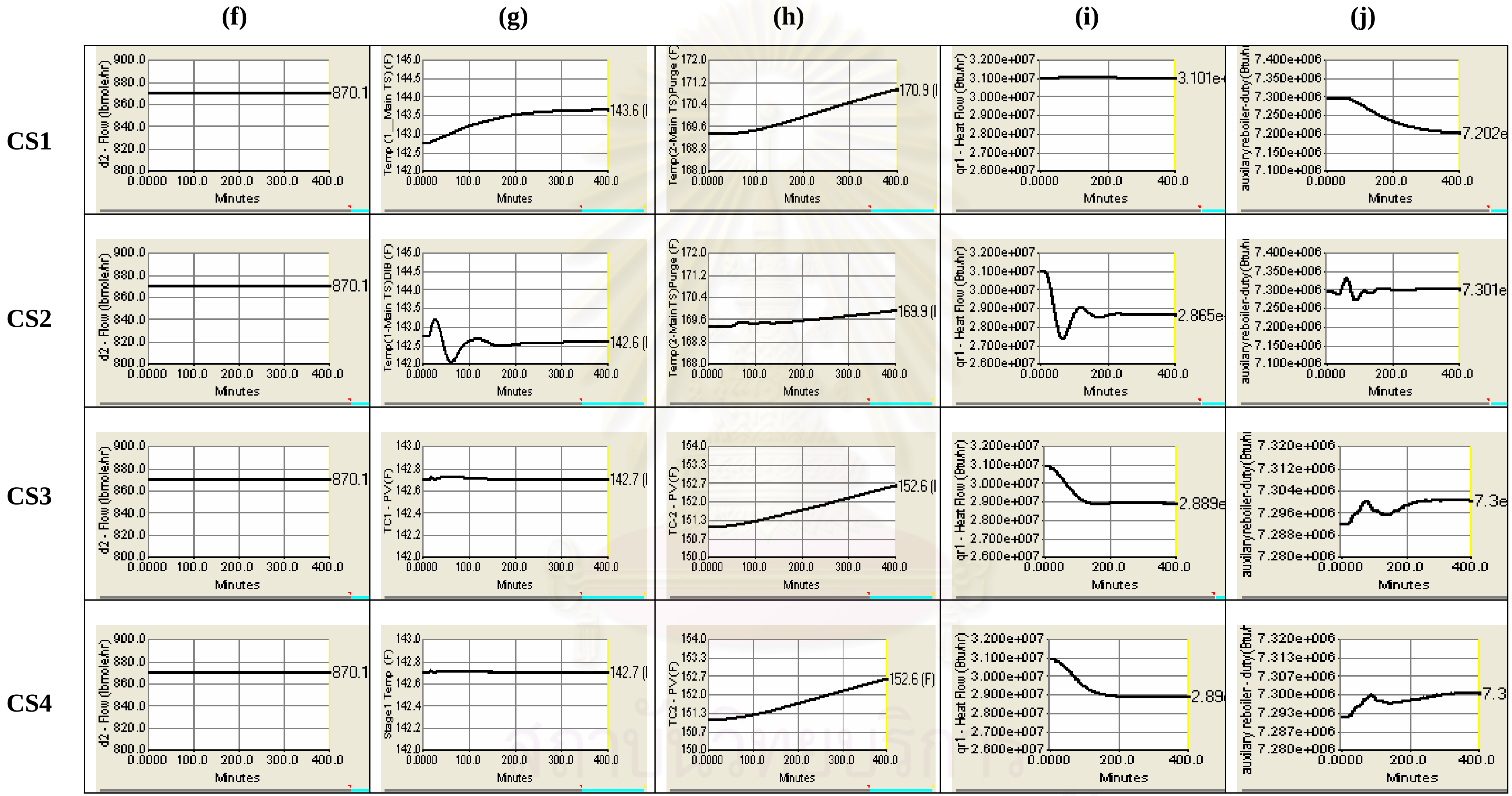


Figure C.14: Continued, where (f) the distillate flowrates of the purge column, (g) the temperature on tray1of DIB column, (h) the tray temperature of Purge column, (i) the DIB column reboiler duty, (j) the Purge column auxiliary reboiler duty ;comparison between CS1, CS2, CS3 and CS4.

Table C.1: The IAE results of the control systems to change in the recycle stream temperature before entering the DIB column.

Decrease in the recycle stream temperature 5 ^{o}F (before entering the DIB column)												
A	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.017258	0.017188	0.001797	0.0032492	0.020395	0.016724	0.020411	0.016667	0.001748	0.001718	0.003288	0.003367
TCR	0	0	0	0	0	0	0	0	0	0	0	0
TC-cool	0	0	0	0	0.011417	0.0445	0.011167	0.043417	0	0	0	0
PC1	4.1869	4.1682	0.73127	0.51890	3.7507	4.2433	3.7572	4.2581	0.80245	0.76139	0.57143	0.53922
PC2	0.1004	0.095033	0.06505	0.07178	0.082258	0.11185	0.088475	0.11751	0.086683	0.06565	0.07615	0.061942
Total A	4.304558	4.280421	0.798117	0.593924*	3.86477	4.416374	3.877253	4.435694	0.890881	0.828758	0.650868	0.604529
B	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1					0.19508	0.73792	0.19283	0.68692	1.6642	0	1.6967	0
TC-cHE2					0.03825	0	0.038083	0	0.012083	0	0.011667	0
Total B					0.23333	0.73792	0.230913	0.68692	1.676283	0	1.708367	0
	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B					6.6277	5.154294	6.598066	5.122614	0.902964	0.828758	0.663368	0.604529*
C	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1			0.23167	0.21758					0.2895	0.2415	0.25925	0.20025
TC2			0.062072	0.062083					0.07725	0.066833	0.0775	0.034917
ToltalA+B+C									1.269714	1.137091	1.000118	0.839696*

Note * = Minimum IAE value

Table C.1: Continued, the IAE results of the control systems to change in the recycle stream temperature before entering the DIB column.

Increase in the recycle stream temperature 5 °F (before entering the DIB column)												
A	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.017711	0.017834	0.0022133	0.0037569	0.020776	0.01687	0.020984	0.017486	0.001981	0.00218	0.003683	0.00375
TCR	0	0	0	0	0	0	0	0	0	0	0	0
TC-cool	0	0	0	0	0	0.013417	0	0.023667	0.004417	0.006	0	0.006667
PC1	4.8635	4.5905	1.1042	0.88133	4.0548	4.3597	3.979	4.8633	1.0003	1.1805	0.74464	0.86165
PC2	0.16097	0.11238	0.12832	0.12433	0.11158	0.1172	0.085417	0.13179	0.12287	0.084175	0.10257	0.087692
Total A	5.042181	4.720714	1.234733	1.009417	4.187156	4.507187	4.085401	5.036243	1.129568	1.272855	0.850893*	0.959759
B	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1					0.041	0	0.04225	0	0.0195	0	0.016083	0
TC-cHE2					1.0733	0	1.2033	0	0	0	0	0
Total B					1.1143	0	1.24555	0	0.0195	0	0.016083	0
	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B					7.043756	4.949517	7.244451	5.526243	1.154151	1.272855	0.872142*	0.960592
C	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1			0.44667	0.41892					0.39383	0.46208	0.35808	0.3955
TC2			0.10751	0.10733					0.10183	0.0865	0.088417	0.071
ToltalA+B+C									1.649811	1.821435	1.318639*	1.427092

Note * = Minimum IAE value

Table C.2: The IAE results of the control systems to decrease in the recycle flowrates before entering the DIB column from 870 to 800.1lb.mol/h.

Decrease recycle flow from 870.1 to 800.1 lb.mol/h. (before entering the DIB column)												
A	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
CC1	0.012088	0.23752	0.020223	0.042265	0.026526	0.011436	0.28246	0.23066	0.019028	0.01957	0.042365	0.041811
TCR	0	0.0348	0	0	0	0.14017	0	0.13992	0	0.027417	0	0.025083
TC-cool	0	0.011167	0	0	0	0	0.062333	0.25708	0.007833	0.0365	0.007917	0.036667
PC1	2.244	42.081	8.9297	10.316	2.6892	2.2511	36.532	42.84	9.7623	9.338	10.342	10.369
PC2	0.071	0.49512	0.16812	0.15878	0.07065	0.67637	0.43238	1.316	0.16303	0.41708	0.16183	0.45452
Total A	2.32709*	42.85964	9.118043	10.517045	2.786376	3.079076	37.30917	44.78366	9.952191	9.838567	10.55411	10.92708
B	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC-hHE1					0.28183	0.67475	11.083	19.385	0.1915	1.4957	0.17125	1.4803
TC-cHE2					0.29817	0.33908	0.44033	0.096167	0.01275	0.008667	0.013083	0.002583
Total B					0.58000	1.01383	11.52333	19.48117	0.20425	1.50437	0.18433	1.48288
	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
Toltal A+B					3.872456	8.491706	68.2555	64.81143	11.84464*	20.06613	12.40974	21.33686
C	CS1-Base	CS2-Base	CS3-Base	CS4-Base	CS1-alt1	CS1-alt2	CS2-alt1	CS2-alt2	CS3-alt1	CS3-alt2	CS4-alt1	CS4-alt2
TC1			1.6772	1.7398					2.0537	1.7485	1.973	1.6094
TC2			0.0768	0.077					0.095667	0.12408	0.078083	0.10142
ToltalA+B+C									13.99401*	21.93871	14.46083	23.04768

Note * = Minimum IAE value

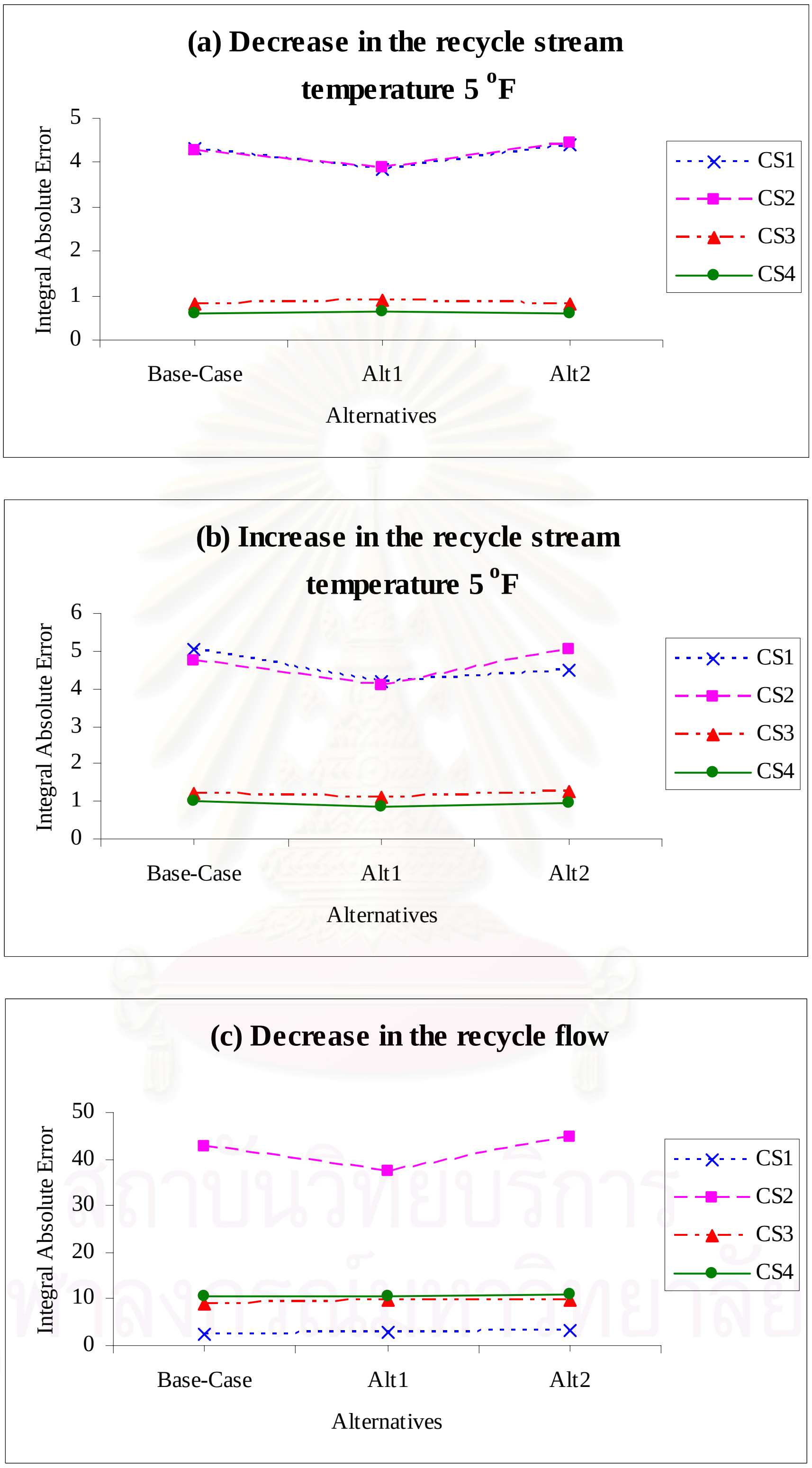
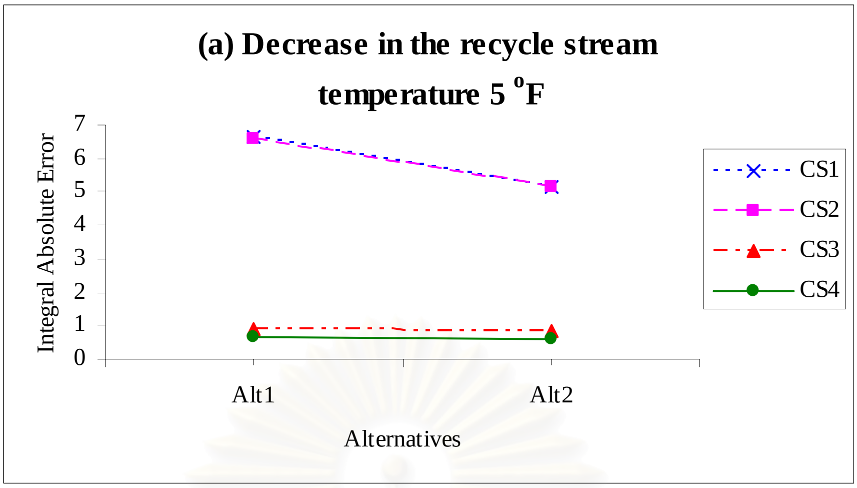
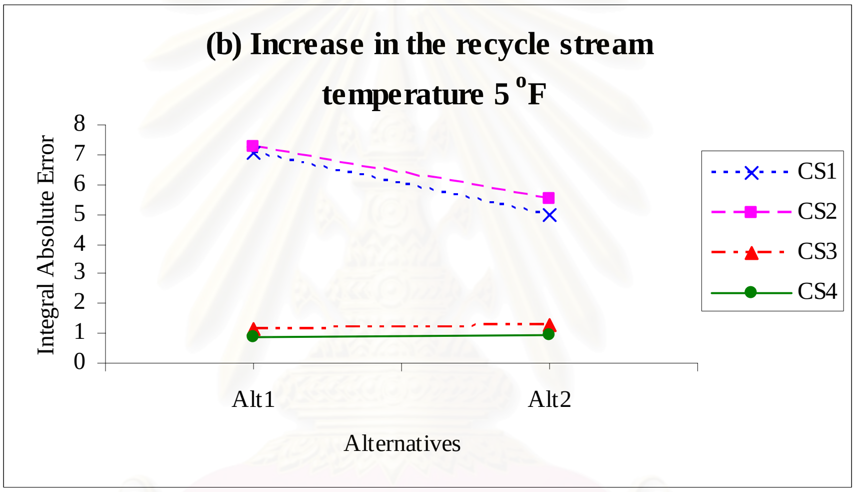


Figure C.15: The IAE results of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1, 2 and base-case) from disturbance load changes, where (a) Decrease in the recycle stream temperature 5 °F, (b) Increase in the recycle stream temperature 5 °F, (c) Decrease recycle flow from 870.1 to 800.1 lb.mol/h. (before entering the DIB column).





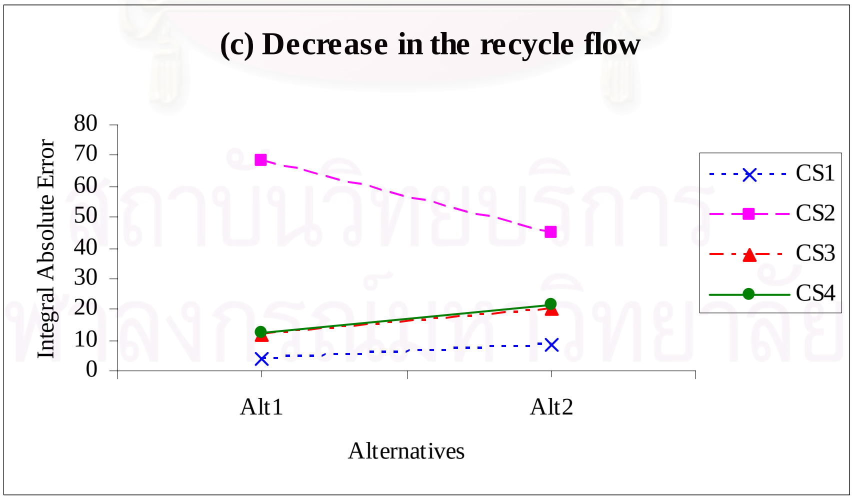


Figure C.16: The IAE results of CS1 to CS 4 in the butane isomerization process with different energy integration schemes (alternatives 1, 2 and base-case) from disturbance load changes, where (a) Decrease in the recycle stream temperature 5 °F, (b) Increase in the recycle stream temperature 5 °F, (c) Decrease recycle flow from 870.1 to 800.1 lb.mol/h. (before entering the DIB column).

APPENDIX D

POOTHANAKUL'S CONTROL STRUCTURES

For Butane Isomerization process with no energy integration, Poothanakul P.(2002) designed 3 control structures to reduce the effects of disturbances in order to achieved impurity of normal butane in product and desired production rate. The first control structure (S1) was modified from CS1 by controlled quality of product with fix product flow. The second control structure and the third control structure was modified from CS2. The second control structure (S2) concerned about reduction of effected of recycle by controlled temperature inside the distillation which could be controlled by adjusted reflux flow rate of column. And the last (S3) wanted to reduce effect of recycle indirectly by controlled temperature inside the distillation with outlet flow of bottom as shown in Figures D.1 to D.3.

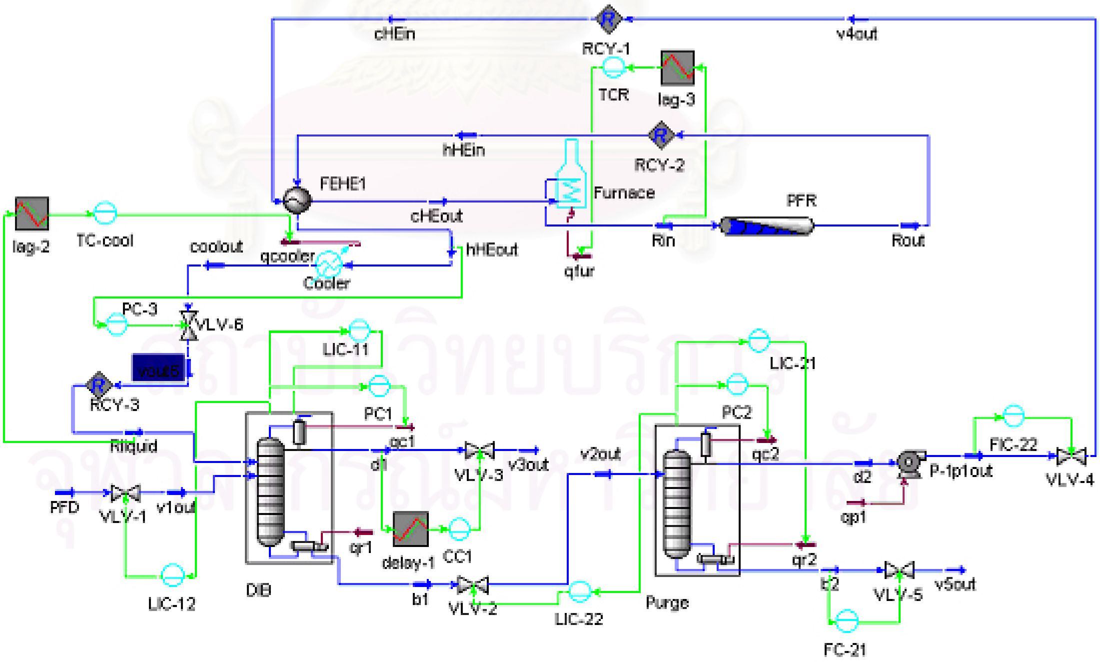


Figure D.1: The first control scheme of Poothanakul P.(S1).

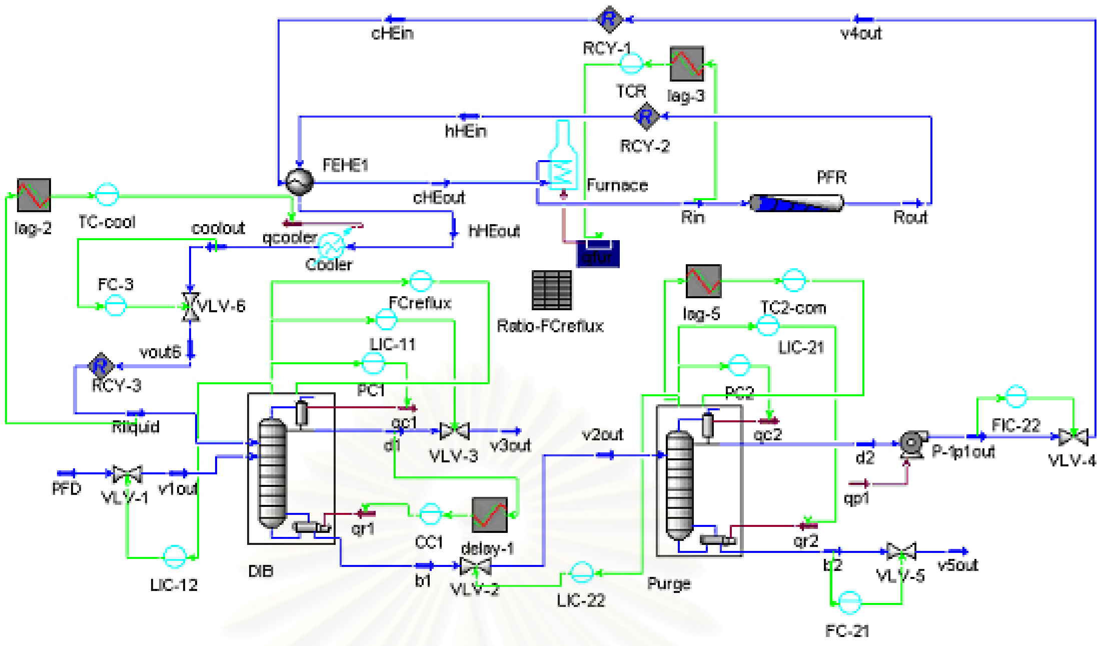


Figure D.2: The second control scheme of Poothanakul P. (S2).

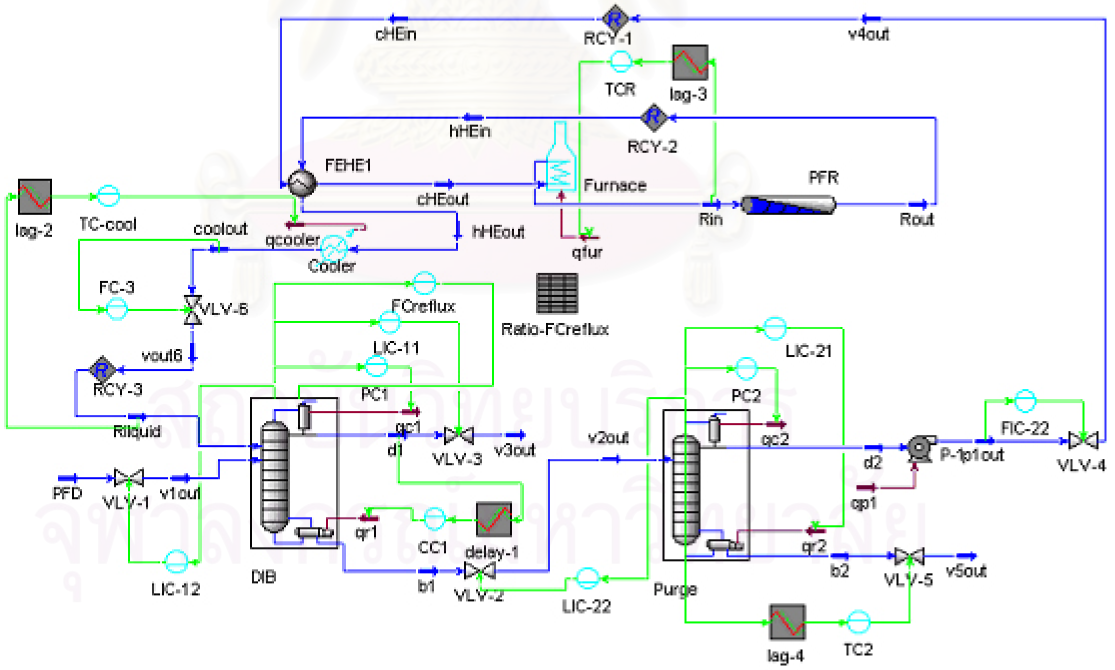


Figure D.3: The third control scheme of Poothanakul P. (S3).

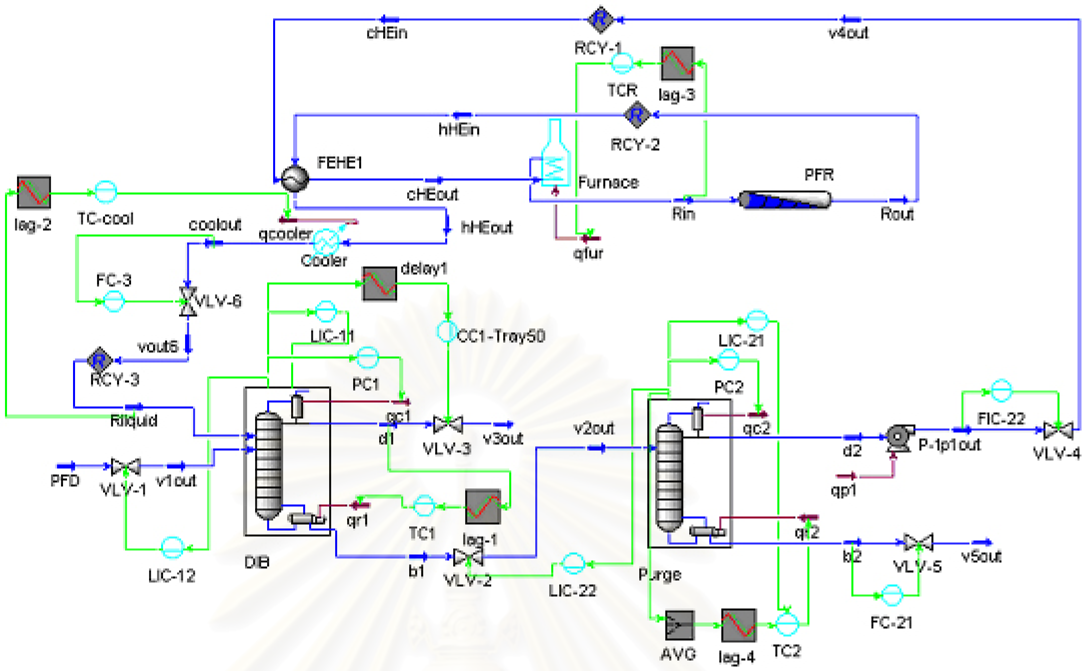


Figure D.4: Designed control structure (CS3) of Butane Isomerization plant.

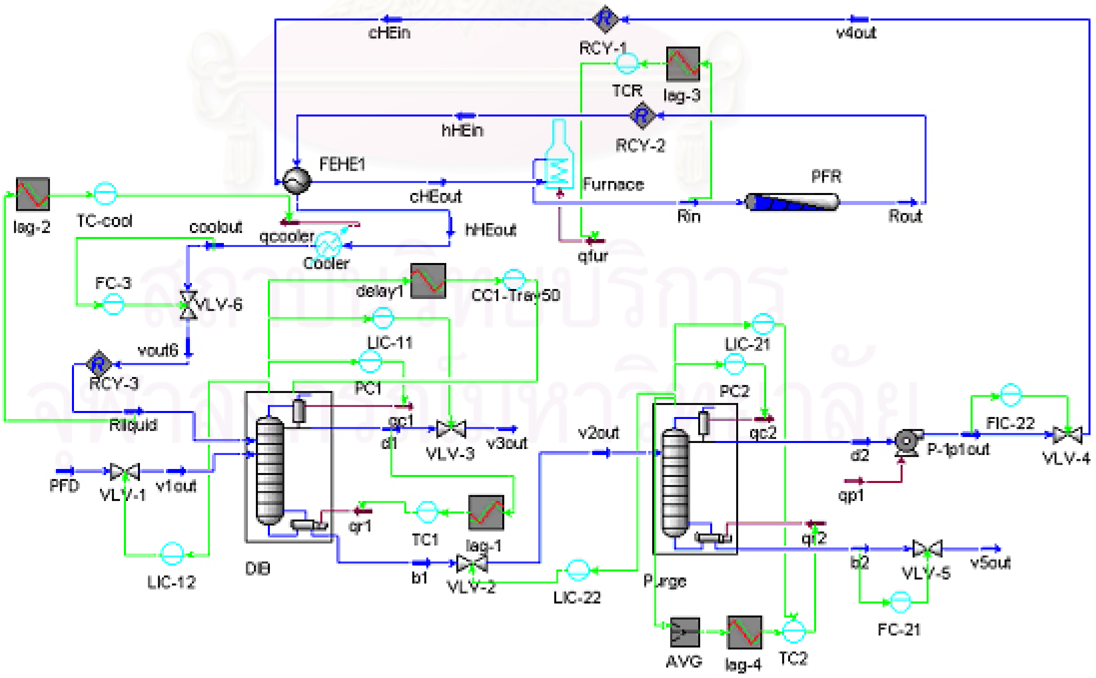


Figure D.5: Designed control structure (CS4) of Butane Isomerization plant.

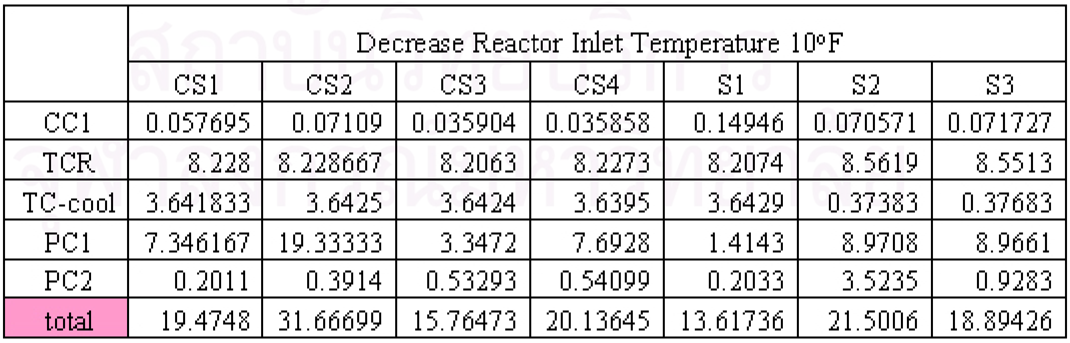
To guarantee this work, all of Poothanakul's control structures are compared with our control structures. In this work, we apply two plantwide designed control structures (CS3 and CS4) to the Butane Isomerization process (Base Case) as shown in. Figures D.4 to D.5. These two control structures are compared with reference structures, (Poothanakul; 2002 (S1, S2, S3) and Luyben; 1998 (CS1, CS2)), the result shows that performances of this work's structures are better than reference structures.

Result of her study showed performance of control structure S1 was the best (minimum total IAE) because of control product quality by fix product flow instead of reboiler duty could reduce effect of disturbance from recycle stream.

The performance of these control structures can be arranged from the best to lowest performance (error of controllability point of view) as the following sequences: CS3, CS4, CS1 and CS2. For Poothanakul's control structures performance of her structures are S1, S3, and S2 respectively.

The dynamic responses and table integral absolute error results of Poothanakul's control structures to change 10% in the recycle flowrate and change 10^0F in the reactor inlet temperature are shown in figures below.

Table D.1: The IAE results of the control systems to 10^0F decrease in the reactor inlet temperature



	Decrease Reactor Inlet Temperature 10°F						
	CS1	CS2	CS3	CS4	S1	S2	S3
CC1	0.057695	0.07109	0.035904	0.035858	0.14946	0.070571	0.071727
TCR	8.228	8.228667	8.2063	8.2273	8.2074	8.5619	8.5513
TC-cool	3.641833	3.6425	3.6424	3.6395	3.6429	0.37383	0.37683
PC1	7.346167	19.33333	3.3472	7.6928	1.4143	8.9708	8.9661
PC2	0.2011	0.3914	0.53293	0.54099	0.2033	3.5235	0.9283
total	19.4748	31.66699	15.76473	20.13645	13.61736	21.5006	18.89426

Table D.2: The IAE results of the control systems to 10^0F increase in the reactor inlet temperature.

	Increase Reactor Inlet Temperature 10°F						
	CS1	CS2	CS3	CS4	S1	S2	S3
CC1	0.065815	0.065783	0.03851	0.034039	0.17663	0.046833	0.061824
TCR	7.933833	7.933833	7.9626	7.9517	7.9646	8.7171	8.3805
TC-cool	3.073833	3.073833	3.3878	3.1628	3.3898	0.2825	0.25092
PC1	10.09167	15.169	2.1555	8.0329	1.5884	6.9873	9.2858
PC2	0.146825	0.282617	0.51919	0.5212	0.16968	1.5872	1.0822
total	21.31197	26.52507	14.0636	19.70264	13.28911	17.62093	19.06124

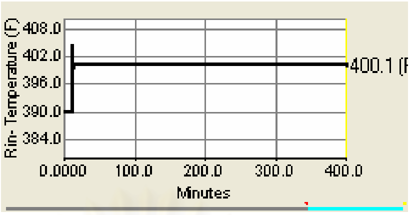
TableD.3: The IAE results of the control systems to decrease the recycle flowrates from 870.1 to 800.1lb.mol/h.

	Decrease recycle flow from 870.1 to 800.1 lb.mol/h.						
	CS1	CS2	CS3	CS4	S1	S2	S3
CC1	0.021682	0.236083	0.028511	0.055619	0.072113	0.23614	0.23638
TCR	1.538167	1.533333	1.4892	1.4894	1.5366	1.5552	1.5333
TC-cool	0.658167	0.666167	0.64017	0.643	0.65775	0.68042	0.6685
PC1	4.213167	44.735	12.286	7.3166	0.74341	44.665	44.838
PC2	10.74817	10.6035	5.3643	5.3997	10.808	15.618	11.74
total	17.17935	57.77408	19.80818	14.90432	13.81787	62.75476	59.01618

Table D.4: The IAE results of the control systems to increase the recycle flowrates from 870.1 to 940.1lb.mol/h.

	Increase recycle flow from 870.1 to 940.1 lb.mol/h.						
	CS1	CS2	CS3	CS4	S1	S2	S3
CC1	0.020062	0.2358	0.029694	0.056472	0.066747	0.080583	0.081895
TCR	1.577333	1.577583	1.539	1.5387	1.5763	3.102	3.0992
TC-cool	0.645667	0.650417	0.62625	0.62375	0.64125	0.26425	0.26575
PC1	3.837333	46.01	12.138	6.647	0.71048	12.555	12.531
PC2	7.926	7.793667	5.2323	5.277	7.9731	9.0682	7.1479
total	14.0064	56.26747	19.56524	14.14292	10.96788	25.07003	23.12575

- **The dynamic responses of increase 10°F in the reactor inlet temperature are as follow:**



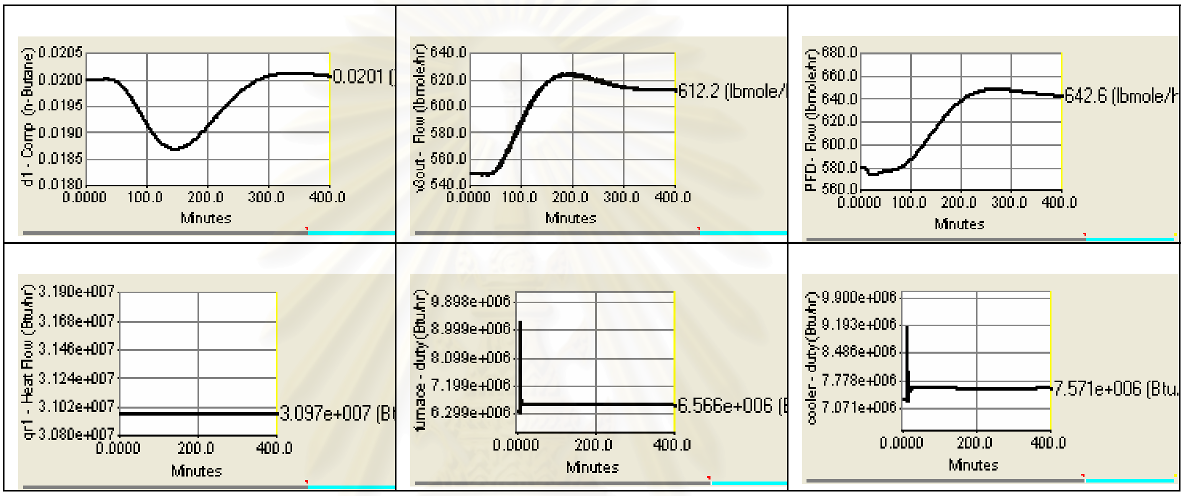


Figure D.6: Dynamic responses of the first control scheme of Poothanakul P. (S1) in Butane Isomerization plant (Base Case) to 10 °F increase in reactor inlet temperature.

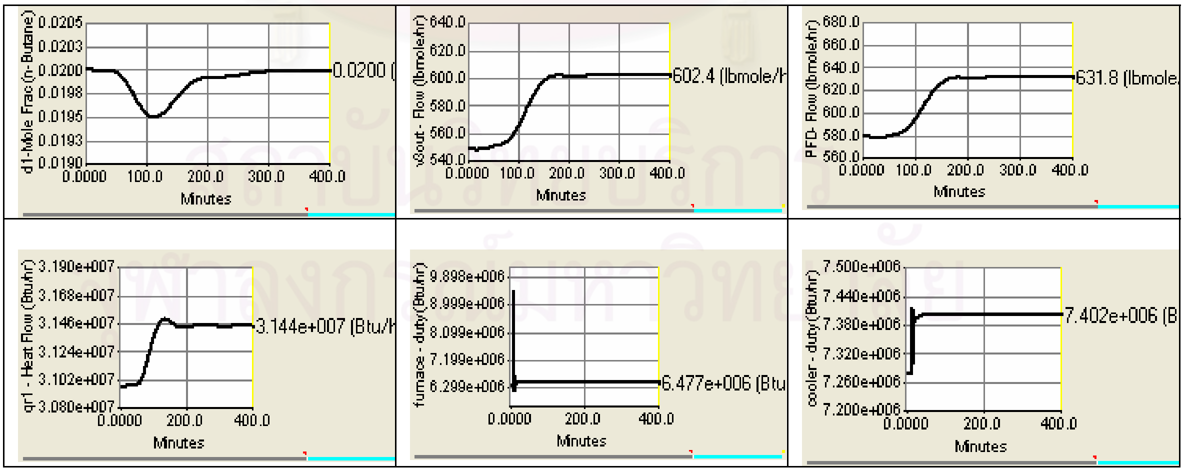


Figure D.7: Dynamic responses of the second control scheme of Poothanakul P. (S2) in Butane Isomerization plant (Base Case) to 10 °F increase in reactor inlet temperature

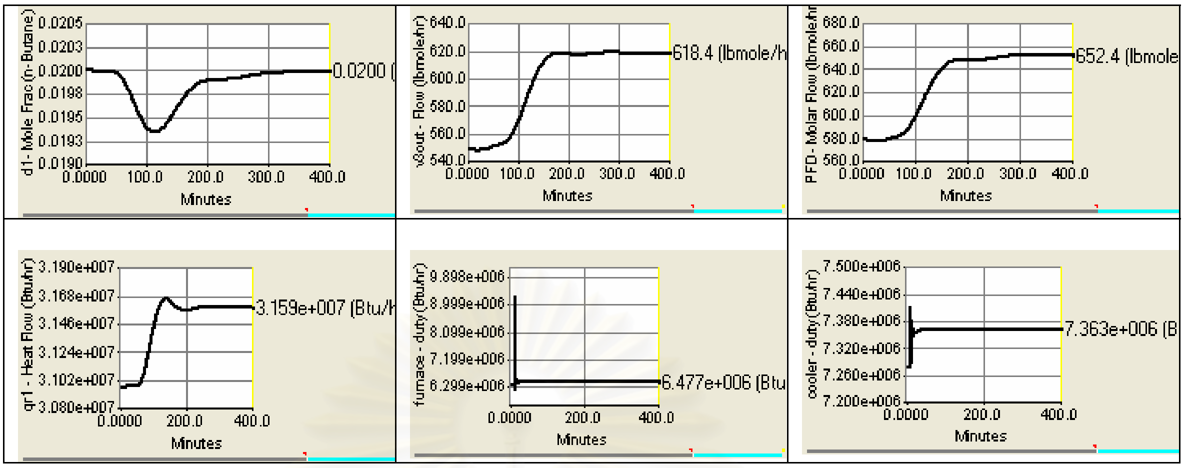


Figure D.8: Dynamic responses of the third control scheme of Poothanakul P. (S3) in Butane Isomerization plant (Base Case) to 10 °F increase in reactor inlet temperature.

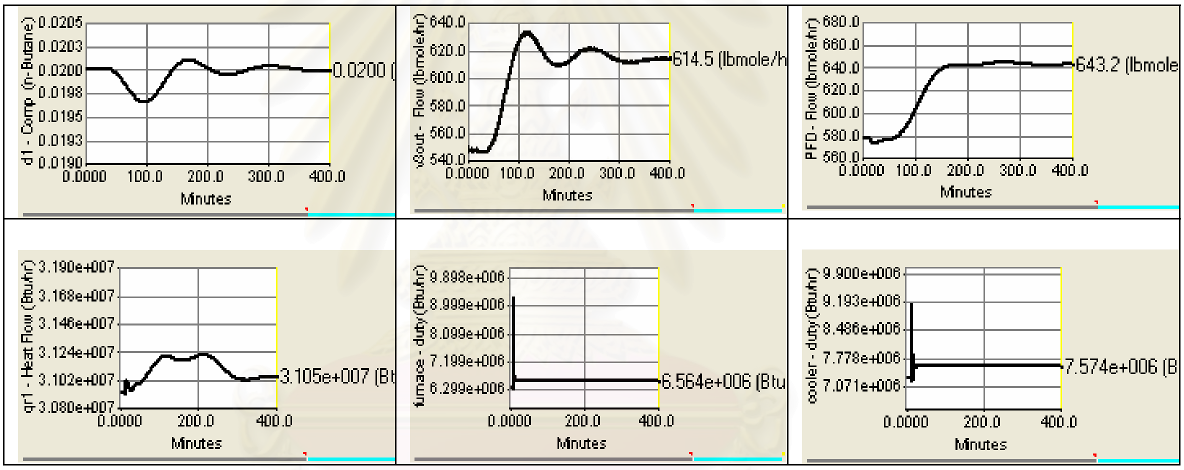


Figure D.9: Dynamic responses of CS3 in Butane Isomerization plant (Base Case) to 10 °F increase in reactor inlet temperature.

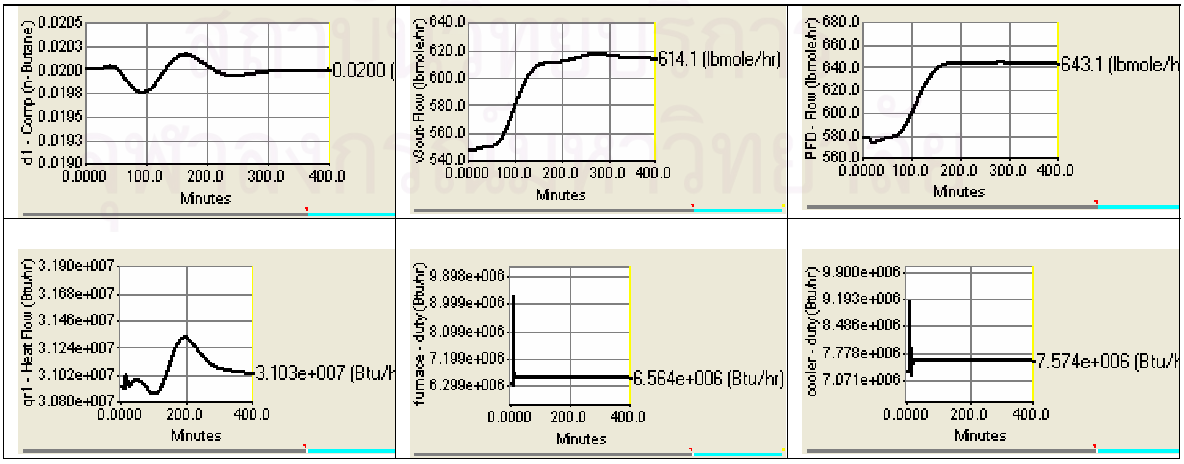
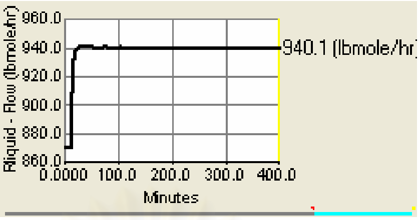


Figure D.10: Dynamic responses of CS4 in Butane Isomerization plant (Base Case) to 10 °F increase in reactor inlet temperature.

- **The dynamic responses of increase 10% in the recycle flowrate are as follow:**



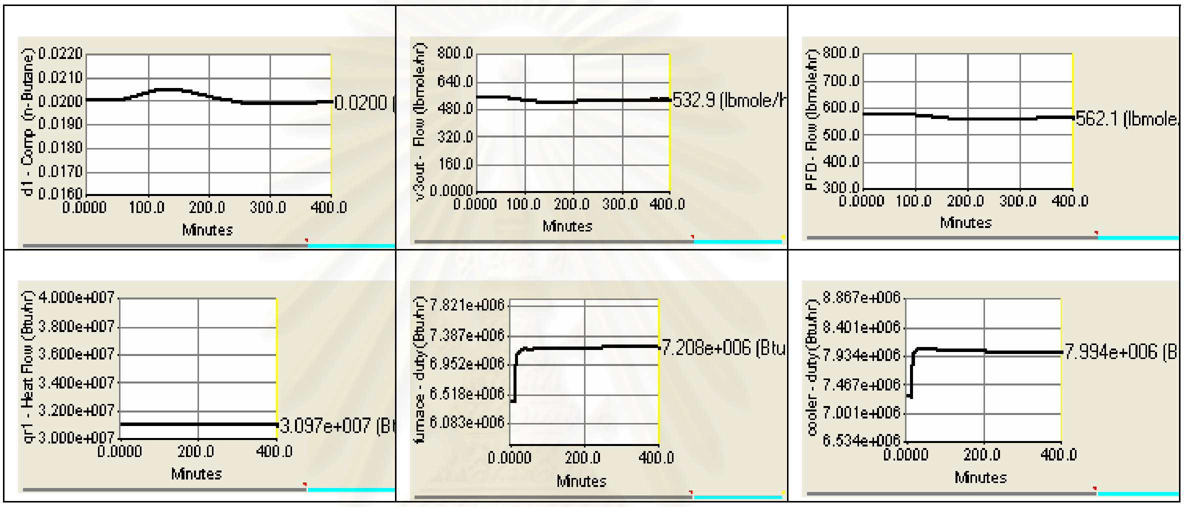


Figure D.11: Dynamic responses of the first control scheme of Poothanakul P. (S1) in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1 lb.mol/h.

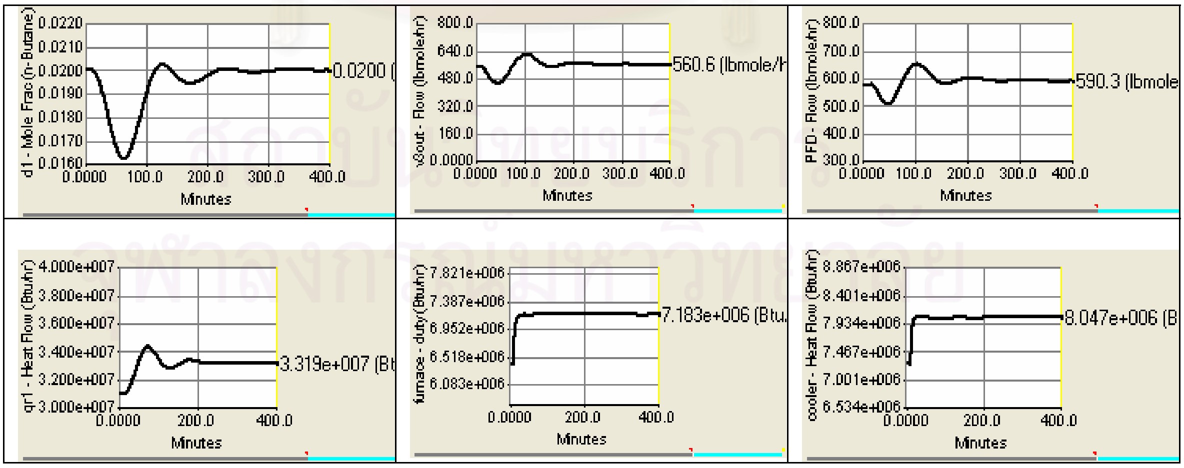


Figure D.12: Dynamic responses of the second control scheme of Poothanakul P. (S2) in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1lb.mol/h.

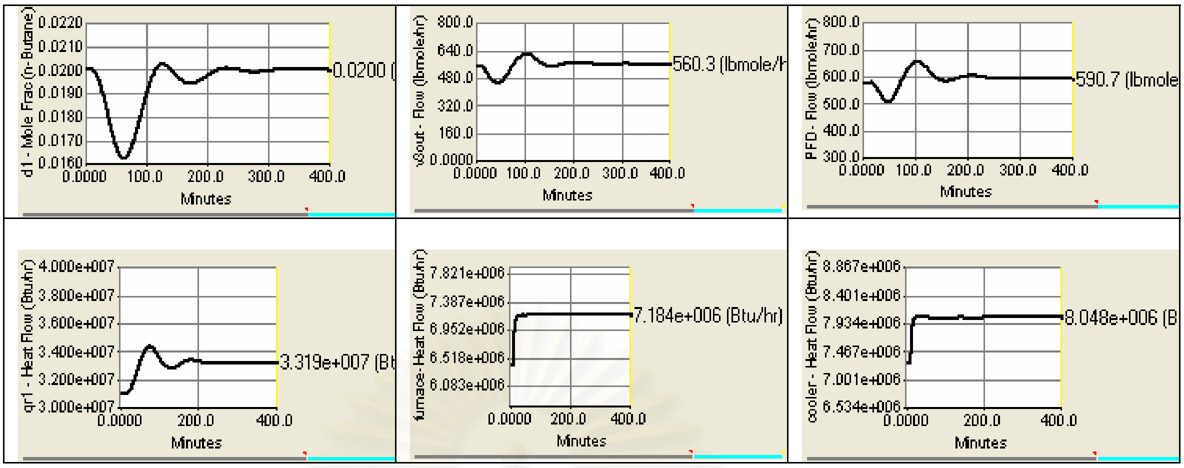


Figure D.13: Dynamic responses of the third control scheme of Poothanakul P. (S3) in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1 lb.mol/h.

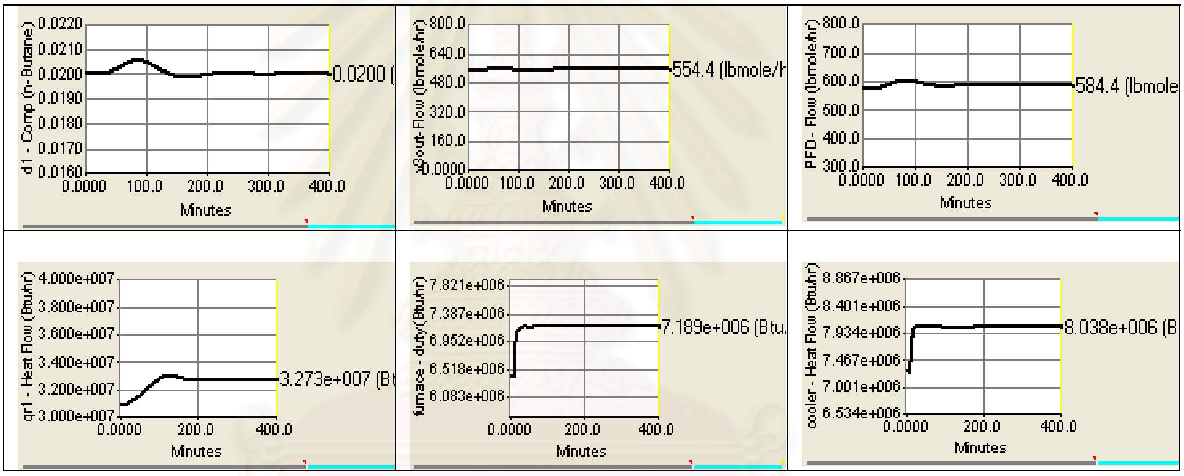


Figure D.14: Dynamic responses of CS3 in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1lb.mol/h.

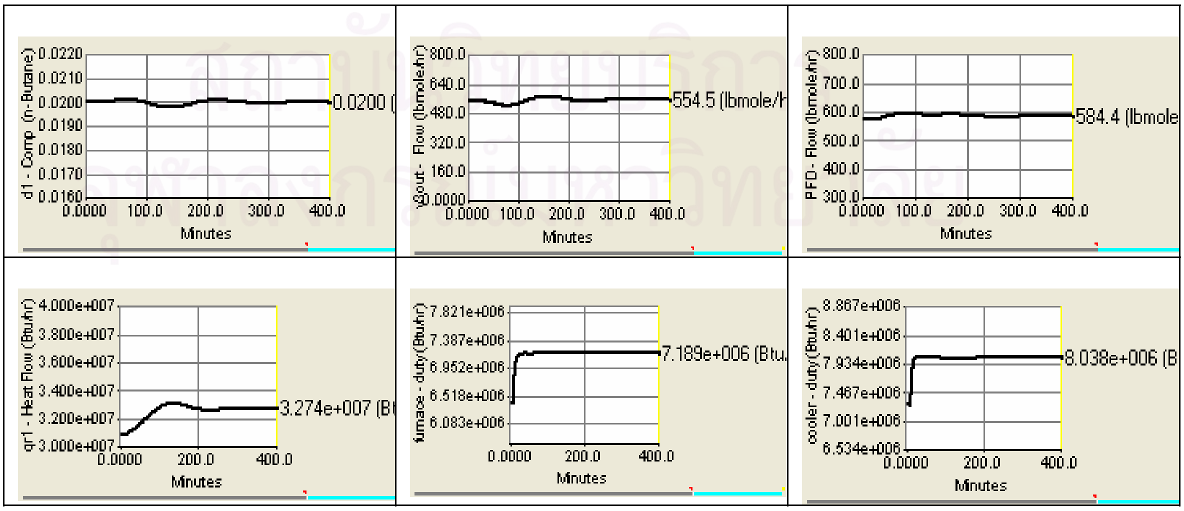


Figure D.15: Dynamic responses of CS4 in Butane Isomerization plant (Base Case) to increase in recycle flow from 870 to 940.1lb.mol/h.

APPENDIX E

THE CAPITAL COST ESTIMATION

E.1 Estimating the Total Capital Cost of a Plant

The capital cost for a chemical plant must take into consideration many costs other than the purchased cost of the equipment. As an analogy, consider the costs associated with building a new home.

A summary of the costs that must be considered in the evaluation of the total capital cost of a chemical plant is presented. The estimating procedures to obtain the full capital cost of the plant are described in this section. If an estimate of the capital cost for a process plant is needed and access to a previous estimate for a similar plant with a different capacity is available, then the principles already introduced for the scaling of purchased costs of equipment can be used, namely:

1. The six-tenths-rule may be used to scale up/down to a new capacity.
2. The Chemical Engineering Plant Cost Index should be used to update the capital costs.

The Chemical Engineering Plant Cost Index (CEPCI) can be used to account for change that result from inflation. The CEPCI values are composite value that reflect the inflation of a mix of goods and services associated with the chemical process industries (CPI)

E.2 Module Costing Technique

The equipment module costing technique is a common technique to estimate the cost of a new chemical plant. It is generally accepted as the best for making preliminary cost estimates and is used extensively. This approach, introduce by Guthrie, forms the basis of many of the equipment module techniques in use today. This costing technique relates all costs back to the purchased cost of equipment evaluated for some base conditions. Deviations form these base conditions are handled by using multiplying factors that depend on the following:

1. The specific equipment type
2. The specific system pressure
3. The specific materials of construction

Equation E.1 is used to calculate the bare module cost for each piece of equipment.

$$C_{BM} = C_p^0 F_{BM} = C_p^0(B_1 + B_2 F_M F_p) \qquad (1)$$

Where C_{BM} is bare module equipment cost: direct and indirect costs for each unit.

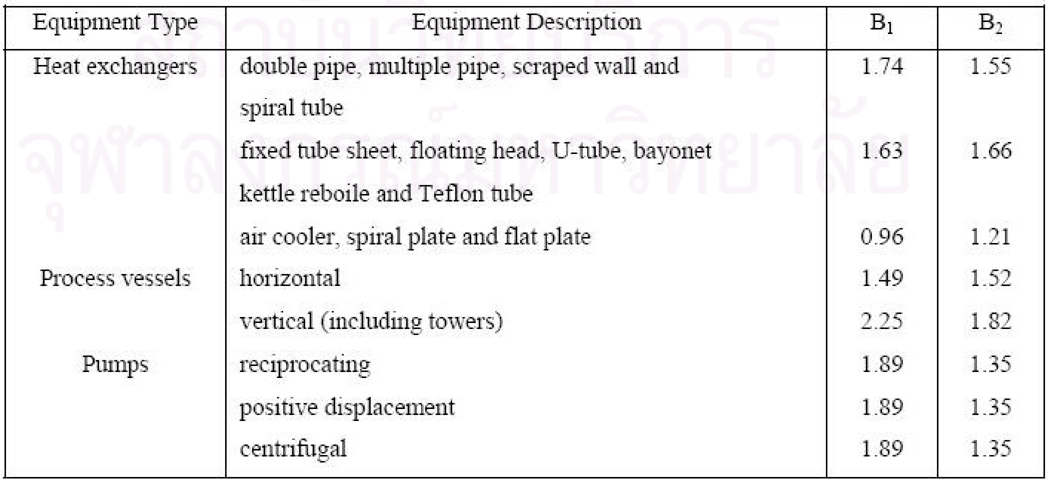
F_{BM} is bare module cost factor: multiplication factor to account for the items that are the specific materials of construction (F_M) and operating pressure (F_P).

The values of the constants B_1 and B_2 are given in Table E.1.

C_P^o the purchased cost at Base Conditions.

For the remaining equipment, the bare modules costs are related to the material and pressure factors by equations different from Equation (1). The form of these equations is given in Table E.2.

Table E.1 Constant for Bare Module Factor to be used in Equation E.1



Equipment Type	Equipment Description	B_1	B_2
Heat exchangers	double pipe, multiple pipe, scraped wall and spiral tube	1.74	1.55
	fixed tube sheet, floating head, U-tube, bayonet kettle reboile and Teflon tube	1.63	1.66
	air cooler, spiral plate and flat plate	0.96	1.21
Process vessels	horizontal	1.49	1.52
	vertical (including towers)	2.25	1.82
Pumps	reciprocating	1.89	1.35
	positive displacement	1.89	1.35
	centrifugal	1.89	1.35

Table E.2 Equations for Bare Module Cost

Equipment Type	Equation for Bare module Cost
Compressors and blowers without drives	$C_{BM} = C_p^0 F_{BM}$
Drives for compressors and blowers	$C_{BM} = C_p^0 F_{BM}$
Evaporators and vaporizers	$C_{BM} = C_p^0 F_{BM} F_p$
Fans with electric drives	$C_{BM} = C_p^0 F_{BM} F_p$
Fired heaters and furnaces	$C_{BM} = C_p^0 F_{BM} F_p F_T$ F_T is the superheat correlation factor for steam boilers (F_T=1 for other heaters and furnaces) and is given by $F_T = 1 + 0.00184\Delta T - 0.00000335(\Delta T)^2$ where ΔT is the amount of superheat (°C)
Power recovery equipment	$C_{BM} = C_p^0 F_{BM}$
Sieve trays, valve trays and demister pads	$C_{BM} = C_p^0 N F_{BM} F_q$ Where N is the number of trays and F_q is a quantity factor trays only given by $\log_{10} F_q = 0.4771 + 0.08516 \log_{10} N - 0.3473(\log_{10} N)^2$ for N<20 F_q=1 for $N \geq 20$
Tower packing	$C_{BM} = C_p^0 F_{BM}$

E.2.1 Bare Module Cost for Equipment at Base Conditions

The bare module equipment cost represents the sum of direct and indirect costs the conditions specified for the base case are

1. Unit fabricated from most common material, usually carbon steel (CS)
2. Unit operated at near-ambient pressure

Equation (1) is used to obtain the bare module cost for the base conditions. For these base conditions, a superscript "0" is added to the bare module cost factor and the bare module equipment cost.

E.2.2 Bare Module Cost for Nonbase Case Conditions

For equipment made from other materials of construction and/or operating at non-ambient pressure, the values for F_{BM} and F_P are greater than 1.0. In the equipment module technique, these additional costs are incorporated into the bare module cost factor,F_{BM} . The bare module factor used for the base case,F_{BM} , is replace with an actual bare module cost factor, F_{BM} in Equation (1) . The information needed to determine this actual bare module factor is provided in Appendix A. The effect of pressure on the cost of equipment is considered first.

Pressure Factors. As the pressure at which a piece of equipment operates increase. As an example, consider the design of a process vessel. Such vessels, when subjected to internal pressure (or external pressure when operating at vacuum) are subject to rigorous mechanic design procedures. For the simple case of a cylindrical vessel operating at above ambient pressure, the relationship between design pressure and wall thickness required to withstand the radial stress in the cylindrical portion of the vessel, as recommended by the ASME

For operating pressures less than -0.5 barg, the vessel must be designed to withstand full vacuum, that is, 1 bar of external pressure. For such operations, strengthening rings must be installed into the vessels to stop the vessel wall from buckling. A pressure factor of 1.25 should be used for such conditions. These pressure factors are presented in the general form given by Equation (2).

$$F_{p,vessel} = \frac{\frac{(P+1)D}{2[850-0.6(P+1)]}+0.00315}{0.0063} \tag{2}$$

The value predicted by this equation (using the appropriate constants) gives values of Fp much smaller than those for vessels at the same pressure. This difference arises from the fact that for other equipment, the internals of the equipment make up the major portion of the cost. Therefore, the cost of a thicker outer shell is a much smaller fraction of the equipment cost than for a process vessel, which is nearly totally dependent on the weight of the metal.

The pressure factors, F_p for the remaining process equipment are given by the following general form:

$$log_{10}F_P = C_1 + C_2log_{10}P + C_3(log_{10})^2 \quad (3)$$

The units of pressure, P, are bar gauge or barg unless stated otherwise. The pressure factors are always greater than unity; the values of constants depend on type of equipment. The values for the constants were regressed from data in Guthrie and Ulrich.

Materials of Construction (MOC). The choice of what MOC to use depends on the chemicals that will contact the walls of the equipment. However, the interaction between process streams and MOCs can be very complex and the compatibility of the MOC with the process stream must be investigated fully before the final design is completed.

Many polymeric compounds are nonreactive in both acidic and alkaline environments. However, polymers generally lack the structural strength and resilience of metals. Nevertheless, for operations below about 120 ^{0}C in corrosive environments the use of polymers as liners for steel equipment or incorporate into fiberglass structures (at moderate operating pressures) often give the most economical solution. The most common MOCs are still ferrous alloys, in particular carbon steel. Carbon steels are distinguished from other ferrous alloys such as wrought and cast iron by the amount of carbon in them. Carbon steel has less than 1.5 wt % carbon, and it can be given varying amounts of hardness or ductility, it is easy to weld, and it is cheap. It is still the material of choice in the CPI when corrosion is not a concern.

- Low-alloy steels are produced in the same way as carbon steel except amounts of chromium and molybdenum are added (chromium between 4, and 9 wt%). The molybdenum increases the strength of the steel at high temperatures while the addition of chromium makes the steel resistant to mildly acidic and oxidizing atmospheres and to sulfur containing streams

- Stainless steels are so called high-alloy steels containing greater than 12 wt% chromium and possessing a corrosion resistant surface coating, also known as a passive coating. At chromium levels above about 12%, the corrosion of steel to rusting is reduced by over a factor of 10. Chemical resistance is also increased dramatically.

- Nonferrous Alloys are characterized by higher cost and difficulty in machining. Nevertheless, they possess improved corrosion resistance.
- Nickel and its alloys are alloys in which nickel is the major component.
- Titanium and its alloys have good strength-to-weight ratios and very good corrosion resistance to oxidizing agents. However, it is attacked by reducing agents, it is relatively expensive, and it is difficult to weld.

Table E.3: Results of the capital cost estimation for Butane Isomerization plant

	Base case	Alternatives	
		1	2
Furnace	282,000.00	282,000.00	282,000.00
heat exchangers	192,000.00	384,000.00	384,000.00
reboiler DIB	1,120,000.00	-	1,120,000.00
reboiler Purge	502,000.00	502,000.00	-
Auxiliary reboiler DIB	-	942,000.00	-
Auxiliary reboiler Purge	-	-	324,000.00
Total capital cost ($)	2,096,000.00	2,110,000.00	2,110,000.00
Investment %	-	0.67	0.67

APPENDIX F

DESIGN THE RESILIENT HEN WITH THREE HEAT EXCHANGERS

F.1 RHEN Designs

With the stream information in Table 4.1, we deign 2 resilient heat exchanger network, called them alternative 1 and alternative 2, using the RHEN design (disturbance propagation) method, the design procedure is summarized Chapter 3. The variation of inlet temperature is arbitrarily selected to be 20 deg F. The minimum temperature difference in the process-to-process-heat-exchangers, ΔT_{min} is set to 20 ^{o}F. The resulting RHEN structures are shown in Figures F.1 and F.2. At the minimum heat load condition, the pinch temperature occurs at 137.67/117.67 ^{o}F. The minimum utility requirements have been predicted 42.816 x 10^6 Btu/hr of hot utilities and 5.655 x 10^5 Btu/hr of cold utilities.

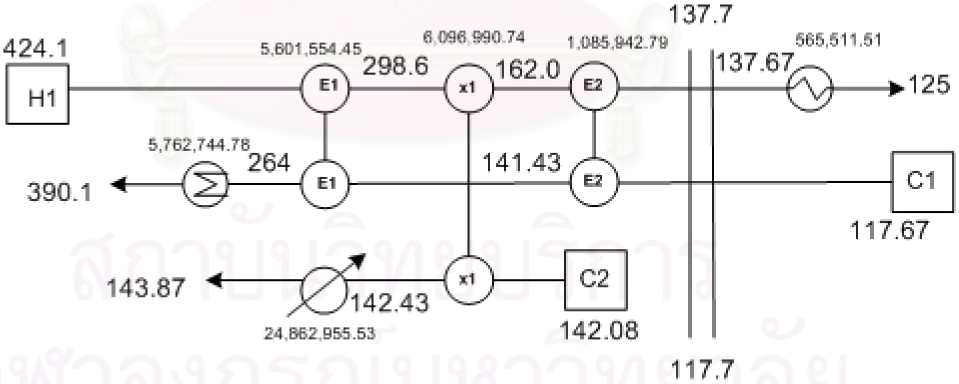


Figure F.1: The resilient heat exchanger network, alternative 1

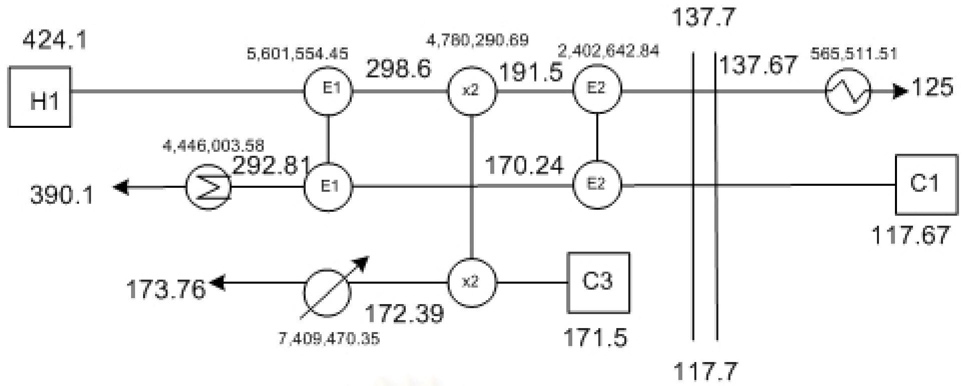


Figure F.2: The resilient heat exchanger network, alternative 2

From Table F.1, we see that when we install the various heat-exchanger network alternatives on the base-case design for the Butane Isomerization processes we obtain 24.88% energy savings and 13.54% savings in the annual utility costs.

Table F.1: Results of energy integration and cost estimation for Butane Isomerization process

	Base case	**Alternative 1**	**Alternative 2**
1. Utilities usage (Btu/ hr)			
Furnace	6,848,434.93	5,762,744.78	4,446,003.58
cooler	7,748,445.04	565,511.51	565,511.51
DIB reboiler	30,960,000	-	30,960,000
Purge reboiler	12,190,000	12,190,000	-
DIB auxiliary reboiler	-	24,862,955.53	-
Purge auxiliary reboiler	-	-	7,409,470.35
Total hot utilities	49,998,434.93	42,815,508.45	42,815,508.45
Total cold utilities	7,748,445.04	565,511.51	565,511.51
2. Energy savings %	-	24.88	24.88
3.Total capital cost ($)	2,096,000.00	2,259,000.00	2,227,000.00
Investment %	-	7.78	6.25
4. Utilities costs ($/year)	2,880,000.00	2,490,000.00	2,498,000.00
Cost savings %	-	13.54	13.26

F.2 HEN control configuration design using HPH

The HEN of Butane Isomerization Plant alternatives 1 and 2 as shown in Figure F.3 is used to explain how an appropriate heat pathway should be activated to carry associated load to the utility unit (Wongsri, 1990). For instance, when the inlet temperature of a disturbed cold stream decreases, path 1 (Fig.F.3a) should be activated by controlling the cold outlet temperature of FEHE2. This will have the effect of shifting the positive disturbance load to the cooler. Thus, the positive disturbance load of a cold stream will result in decrease of the cooler duty. Consider the case when the inlet temperature of a disturbed cold stream increases, path 2 (Fig.F.3b) should be activated by controlling the hot outlet temperature of FEHE2 to shift its negative disturbance load to heater. Thus, the negative disturbance load of a cold stream will result in decrease of the furnace duty. On the other hand, when the inlet temperature of a disturbed hot stream increases, path 3 (Fig.F.3c) should be activated by controlling the cold outlet temperature of FEHE1 to shift its positive disturbance load to auxiliary reboiler. As a result, the auxiliary reboiler duty of path 3 will be decreased. Consider the case when the inlet temperature of a disturbed hot stream decreases, path 4 (Fig.F.3d) should be activated by controlling the hot inlet temperature of EHE3 to shift its negative disturbance load to furnace. As a result, the furnace duty will be increased but, the auxiliary reboiler duty will be kept in the same as duty in the condition without disturbance.

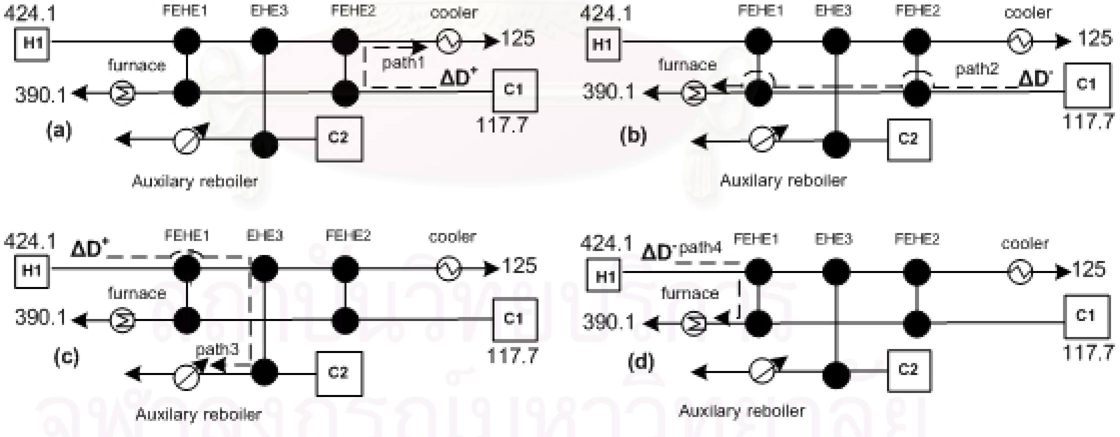


Figure F.3: Heat Pathways through HEN in the energy-integrated Butane Isomerization Plant to achieve the highest possible dynamic MER, where:(a) path1 is used to shift the positive disturbance load of the cold stream C_1 to the cooler, (b) path 2 is used to shift the negative disturbance load of the cold stream C_1 to the furnace, (c) path 3 is used to shift the positive disturbance load of the hot stream H_1 to the auxiliary reboiler, (d) path 4 is used to shift the negative disturbance load of the hot stream H_1 to the furnace.

VITA

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