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PLANTWIDE CONTROL STRUCTURE DESIGN FOR

AN AUTO-REFRIGERATED ALKYLATION PROCESS

Miss Safiya Benchavichien

A Thesis Submitted in Partial Fulfillment of the Requirements

for the Degree of Master of Engineering Program in Chemical Engineering

Department of Chemical Engineering

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Thesis Title   PLANTWIDE CONTROL STRUCTURE DESIGN FOR

AN AUTO-REFRIGERATED ALKYLATION PROCESS

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ซัฟฟียา เบญจวิเชียร : การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์สำหรับ
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กระบวนการอัลคิเลชั่นเป็นกระบวนการที่ใช้ในการผลิตไอโซออกเทนสำ รับการกลั่น
ผลิตภัณฑ์ปิโตรเลียม ไอโซออกเทนเป็นเชื้อเพลิงหลักที่ใช้ในเครื่องยนต์เบนซิน กระบวนการผลิต
ไอโซออกเทนได้จากการเกิดปฏิกิริยาระหว่างไอโซบิวเทนและบิวทีน โดยใช้กรดซัลฟิวริกเป็นตัวเร่ง
ปฏิกิริยา ปฏิกิริยาดังกล่าวเป็นปฏิกิริยาคายความร้อนซึ่งเกิดขึ้นในถังปฏิกรณ์ชนิดต่อเนื่องที่มีการ
กวนต่อแบบอนุกรม ภายในถังปฏิกรณ์มีการรักษาระดับอุณหภูมิให้ต่ำเพื่อควบคุมการ
เกิดปฏิกิริยาที่ไม่ต้องการ ในส่วนของกระบวนการแยกสาร ประกอบด้วยหอกลั่นจำนวน 2 หอ เพื่อ
แยกสารที่ต้องการและส่งส่วนที่เหลือที่เป็นประโยชน์ต่อกระบวนการกลับสู่กระแสรีไซเคิล

งานวิจัยนี้ได้ศึกษาและออกแบบโครงสร้างการควบคุมของกระบวนการอัลคิเลชั่น
โดยใช้ขั้นตอนการวิเคราะห์พฤติกรรมของวงศ์ศรีซึ่งมีความเหมาะสมในการกำจัดสิ่งรบกวนชนิด
มวลสารและพลังงานออกสู่ภายนอกร ะบบ โดยโปรแกรมพลวัตเชิงพาณิชย์ได้ถูกนำมาใช้เพื่อ
จำลองกระบวนการอัลคิเลชั่นที่สถานะคงตัวและที่เงื่อนไขแบบไดนามิก พบว่าวิธีการออกแบบ
โครงสร้างดังกล่าวมีสมรรถนะที่ดีเมื่อเปรียบเทียบกับโครงสร้างการควบคุมที่ออกแบบโดยไลเบน
เปรียบเทียบจากปริพันธ์ของค่าคลาดเคลื่อนส้ มบูรณ์และพลังงานที่ใช้ในระบบ ซึ่งสามารถกำจัด
ตัวรบกวนที่เข้าสู่ระบบและสามารถรักษาคุณภาพของผลิตภัณฑ์ได้

ภาควิชา : วิศวกรรมเคมี   ลายมือชื่อนิสิต...
สาขาวิชา: วิศวกรรมเคมี   ลายมือชื่อ อ.ที่ปรึกษาวิทยานิพนธ์หลัก.......................
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SAFIYA BENCHAVICHIEN : PLANTWIDE CONTROL STRUCTURE DESIGN FOR AN AUTO-REFRIGERATED ALKYLATION PROCESS. ADVISOR : ASST. PROF. MONTREE WONGSRI, D.Sc., 111 pp.

The alkylation process is widely used in oil refinery as a process to produce an alkylate product which is very useful for internal combustion engines. The process operated by reacting isobutene with olefins (primarily mixture of butane-butylene) and adding the sulfuric acid catalyst. The process is carried out in exothermic reactions in a series of agitated reactors. The separation sections with two distillations are then installed to extract the desirable products and return the useful remnant back to the recycled stream. This research has been developed by using plantwide control procedure of Wongsri (2012) to improve the control structure of an auto-refrigerated alkylation process which can be referred as multi-unit process containing several unit operations. The procedure used heuristics method to find the fixture plant which is appropriate in handing material and heat disturbances entering the process. Wherefore, a commercial dynamics simulator is used to design and simulate the alkylation process at steady state and dynamic conditions

Department   : Chemical Engineering   Student's Signature

Field of Study : Chemical Engineering   Advisor's Signature

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CHAPTER I

INTRODUCTION

1.1 Importance and Reasons for Research

In most industries, cost of production, products quality and environmental impact are very important issue. So the production process should approach its highest performance due to quality and efficiency by using less energy and meeting the products specification. The economics is the main focus of most process industries. Therefore to improve them, the recycle streams and energy integrations are included in the process. Hence, the strategies for plantwide control structure are used to operate the entire plant at the desired conditions in order to achieve the required products specification and assign the environmental impact.

Recently, the plantwide control structure has been used in chemical engineering process due to its advantages in optimizing multi-complex process control (considered highly integrated streams). Designing the plantwide control system is quite challenging task due to material and energy recycles streams in the process. The plantwide control structure can be categories in to two based, heuristic and mathematical. Luyben et al., 1998 have proposed 9-step heuristic procedure for moving the process from steady state to dynamic conditions. They have divided the overall plantwide control system into smaller task. Though, to set production rate and material supply steps, the decision is ad-hoc which hampers the usage of this methodology by less experience in a skill person. However, some generic description and specific guidelines are given. On the other hand, Wongsri, 2009 has proposed 8-step design procedure which is completely difference from Luyben et al. Wongsri procedure can be used for novices, the steps is not complicated and can be followed easily.

Alkylation process is employed to study the effect of the 8-step design procedure. The alkylate which is the product of the process is build up by reacting isobutane and olefins (primarily a mixture of propene and butene). The alkylate gasoline

is generally used in automobiles due to its anti-knocking properties. The octane number of alkylate rely on the kind of olefins used in the process and operating conditions. The alkylation process is carried out in exothermic reactions in series of continuous stirred tank reactors (CSTRs). It is very important to keep the temperature low in order to improve the selectivity, not to convert all of the products in to side reaction. The separation processes are then used to extract the desired product out of undesirable one. Therefore, the alkylation plant is chosen for current study to observed Wongsri procedure (2012).

1.2 Research Objectives

The objective of this research is:

To design the plantwide control structures for an auto-refrigerated alkylation process using Wongsri design procedure (2012).

1.3 Scopes of Research

The scopes of this research are:

1. Performed a dynamic simulation of an auto-refrigerated alkylation process using Aspen HYSYS dynamic simulator (version 7.0).

2. Two new plantwide control structures of an auto-refrigerated alkylation process are designed via Wongsri design procedure (2012).

3. Detailed and data are obtaining from Luyben (2009).

1.4 Contributions of Research

The contributions of this research are:

1. Simulated a flowsheet diagram of an auto-refrigerated alkylation process in both steady and dynamic state.

2. The new plantwide control structures of an auto-refrigerated alkylation process are designed using Wongsri design procedure (2012) and compared with the work given by Luyben (2009).

3. Evaluation of the new plantwide control structures design procedure.

1.5 Research Procedure

The research procedures are:

1. Study of the plantwide control structure theory, an auto-refrigerated alkylation process and the process relevant information.

2. Simulation of an auto-refrigerated alkylation process at steady state and dynamic modules via Aspen HYSYS.

3. Study of the new control structures design procedure.

4. Designing of new plantwide structures using Wongsri design procedure (2012).

5. Simulation and evaluation of new plantwide control structures at dynamic and compare with the base case.

6. Analyzation of the design and simulation results

7. Conclusion of the research studied

1.6 Research Framework

This thesis is divided into six chapters as followed:

Chapter I is an introduction of this research. This chapter consists of an importance and reason, objective, scopes, contributions and procedure of the research.

Chapter II Review the earlier worked carried out on plantwide control, control structure design, control structure procedure and the method of selection set of controlled variables.

Chapter III covers some background information of Luyben's plantwide control theory and plantwide control structure design procedure of Wongsri, 2012.

Chapter IV describes the auto-refrigerated alkylation process, process simulation via ASPEN HYSYS and the new control structures design procedure.

Chapter V describes the design of control structures, dynamic simulation results and the comparison of the control structure of Luyben to the new design control structures.

Chapter VI presents the conclusion of this research and gives out the recommendations

for future work.

This is follow by:

References

Appendix A: Process streams and equipments data

Appendix B: Tuning parameters of each control structure

CHAPTER II

LITERATURE REVIEWS

The Plantwide process control (PWC) deal with the control of an entire chemical plant consisting of a complex flowsheet with recycle streams, energy integration, and many interconnected unit operations. The methodologies of PWC structure range from pure mathematical programming based methods to heuristic-based methods. Many works has been considered on PWC structure, heuristic-based approach, and related works. This chapter would be presented in two main categories; Plantwide control and Control structure design.

2.1 Plantwide Control

Luyben, Tyreus and Luyben (1997) presented a general heuristic design procedure which creates a practical plantwide control structure for processes involving reaction and separation sections. The Nine steps procedure consists of:

Step 1 Establish control objectives.

Step 2 Determine control degree of freedom.

Step 3 Ensures that any heat production within the process is properly dissipated.

Step 4 Set the production rate and design constrains required for the production rate.

Step 5 Control products quality and handle safety, operational, and environmental constraints.

Step 6 Control inventories (pressures and levels) and fix a flow in every recycle loop.

Step 7 Check overall components balance for each chemical species in the process.

Step 8 Control individual unit operations.

Step 9 Optimize economics and improve controllability using the remains degree of freedom.

Applications of the procedure are illustrated in this article with three industrial process examples: the vinyl acetate monomer process, Eastman process, and the hydrodealkylation of toluene process.

Vasbinder and Hoo (2003) presented a flowsheet development methodology for synthesizing plantwide control structures. The technique is based on a modification version of the decision-making methodology of the analytical hierarchical process (AHP). The control structures of each modules was developed using the nine-step approach of Luyben. The decomposition provides easy ways to deal with the plantwide control problem by reducing the size of the problem, while the modified AHP (mAHP) guarantees consistency. The modular decomposition approach was applied to the dimethyl ether (DME) process, and the results were compared to a traditional plantwide design approach. Both methods produced similar control structure which was adequate for the process. An acceptable disturbance rejection was demonstrated on the integrated flowsheet.

Skogestad (2004) proposed two main systematic procedures for control structure design of complete chemical plants (plantwide control); top-down analysis and bottom-up analysis. Top-down analysis is used to identify degree of freedom and primary control variable. While, bottom-up analysis is used to determine secondary controlled variables and pairing the structure of control system. The studied also presented inventory and production rate control, decentralized versus multivariable control, loss in performance by bottom-up design and a definition of a "complexity number" which can then proceed to find the optimal controller for regulatory and supervisory control layers.

2.2 Control Structure Design

Luyben (1994) presented a mathematical analysis of the problems for some typical kinetic systems. In the binary first-order system with reaction A⟶B, an analytical solution for the recycle flow rate can be determined as a function of the fresh feed flow rate and fresh feed composition. Two control structures have been considered for this system. It is shown analytically why the control structure proposed by Luyben prevents the snowball problems and why the usual structure results in severe snowballing. The results confirm that the problems can be prevented by fixing the flow rate of a stream in a recycle loop.

Luyben (1996) presented the number of parameters or variables that must be specified to complete the defined steady-state process, called design degree of freedom (DOF). DOF can be calculated by subtracting the number of equations from the number of the number of variables. For complex process DOF equal to the number of manipulated variables (the number of control valves in the process). The complexity of the phase equilibrium and the physical properties does not affect DOF.

Luyben (1999) presented a significant study of temperature control of boiling-liquid reactors. The effects of conversion and activation energy are analyzed. The principal contribution of this paper is an illustration of the condenser heat-transfer area required for dynamic stability which can be an order of magnitude larger than suggested by standard steady-state heat-transfer design heuristics. Control problem are infrequently encountered for endothermic and reversible exothermic reactions because of their temperature self regulating term. If the reactions are endothermic, adding sufficient heat to the reactor at the desired temperature results in a decrease in conversion. If the reactions are reversible exothermic, remove sufficient heat from the rector results in increasing in temperature which leads to decline in the equilibrium constant. Despite, if the reaction are irreversible exothermic, which means that there is no reaction runaways and self regulation. In order to improve the control system the

heat-transfer area must be larger than suggested by common heuristic to makes the process more self-regulatory.

Mahajanam, Zheng and Douglas (2001) presented a shortcut method for selecting controlled variables for plantwide control problems, in order to eliminate poor choices and to generate and rank attractive alternatives without solving optimizations problems. The method is based on scaling of all the candidate controlled variables so that they would have similar impacts on the steady-state profit. The procedure demonstrated on a simplified butane alkylation process.

Larson, Govatsmark, Skogestad and Yu (2003) considered a selection of a control structure for simple plant with a liquid-phase reactor, a distillation column and recycle of an unreacted reactant. The study starts with a clear definition of the operation objectives, constraints, and degree of freedom. The procedure of Skogestad (2000) is used to find self-optimizing control structure to search for a constant setpoint strategy with an acceptable economic loss. For case of minimizing costs (case I) and maximizing production rate (case II), the reactor hold up is fixed at it maximum. The reflux ratio is here considered as self-optimizing variable. Moreover, the snowball effect is avoided by fixing a flow in a liquid recycle loop, although the rules are limited to only small feed-rate changes or reactor with large variations of holdup.

Konda, Rangaiah and Krishnaswamy (2005) proposed an integrated framework of simulation and heuristics methodology which can handle plantwide control problems well and practically. The methodology and its application are applied to Hydrodealkylation of toluene (HDA) process. The results come out that a viable control system can be generated by the proposed framework that can retain both simulation and heuristics. The general idea of this work is that the control system design cannot be accomplished by only heuristics or quantitative techniques lacking the aid of rigorous nonlinear simulation tools.

Konda, Rangaiah and Lim (2006) presented a simulation-based heuristic approach for optimal process design and effective plantwide control of industrial

process. A sequential approach and combining rigorous nonlinear simulation with heuristics is proposed for integrated design and control of the hydrodealkylation of toluene (HDA) process. The conflicts between steady-state and dynamic operability and the importance of integration of design and control from a plantwide perspective are highlights. Dynamic disturbance sensitivity is proposed and used to observe the dynamic performance of difference process preferences and control structures.

Suntisrikomol (2008) proposed the "Fixture Point Theorem" for Hydrodealkylation process (HDA) to select suitable set of controlled variables from candidate outputs. The theorem states that the most disturbed points must be controlled before other controlled variables. The maximum gain is used to selected and paired controlled variables with manipulated variables. Therefore, three sets of controlled variables and five controlled structures are set, designed and compared to work done by Luyben(1998) to interpret the dynamic behaviors of the control structures with economic disturbance load. The performance of designed control structures were presented in the IAE values and compared with the reference structure which responded faster and more effective than the reference structure 1 (Araujo et al, 2006) and the reference structure 2 (Luyben, 1998).

Dimian and Bildea (2008) proposed the design of an isobutene/butane alkylation plant. The plantwide control structures of this process are created based on degree of freedom analysis. A robust design ensures that the plant remain operable with large disturbances or design parameter uncertainties. It is also proposed heat-integration issues, such as heat transfer between the feed and the effluent of the chemical reactor. The effectiveness of the approach has been proven by rigorous design and closed-loop dynamic simulation.

Dorneau, Bildea and Grievink (2009) proposed a new approach exploiting advantage of fundamental structure that fit in a chemical plant in the form of units or groups of units connected together via material and energy streams. The recommended procedure is to employ model reduction, then to link these reduced-order models. The

procedure is flexible and accurate due to its algorithm and variation from one unit to another. The time for solving solution is drastically reduced. The performance of the approach is verified by means of a case study.

Vasudevan, Rangaiah, Konda and Tay (2009) presented the development of a PWC structure for styrene monomer plant using three methodologies, namely, an integrated framework of heuristic and simulation, heuristic procedure and self-optimizing control procedure. The control structures are developed employing the nine-step procedure of Luyben. All methodologies are then analyzed for their performance in the presence of adequate disturbance and test for their stability, which appoints that all structures are workable. The integrated framework and self-optimizing control structures perform better and are more or less equally robust. The Luyben control structure behaves poorer for the more important feed rate disturbances.

Detjareansri (2009) proposed the control structures development for alkylation process by designing eight new control structures using Wongsri (2009) procedure. The dynamic performance of the design control structures are then evaluated and compared to Luyben (2002) by inserting two types of disturbances; material and thermal disturbances. The designed control structures has good performance which presented by number of IAE and total energy used.

Luyben (2009) proposed a clarify version study of the autorifrigerated alkylation process and illustrated the design trade-offs between reactor size and recycle flow rate, also interaction among design optimization variables. The study has mentioned that the economic design must be optimized by balancing the capital costs of reactors and distillation columns with the energy cost of compression and reboiler heat inputs. The design effects by the location of the fresh feed stream entering the process. An effective plantwide control structure is developed to handles large disturbances in throughput and feed compositions. The structure has some uncommon control features: control of two compositions and one temperature in the side stream column and a proportional temperature control in the other column.

CHAPTER III

THEORIES

The flowsheet of chemical plants composed of many interconnected unit operations linked together by material and energy recycle streams. Therefore Plantwide Process Control strategies are necessary to control the entire chemical plant and obtain satisfactory performance, stability, and products.

3.1 Integrated Process

Three fundamental characteristic of integrated chemical processes are necessary to be considered for control system of the entire plant:

1. the effect of material recycle,

2. the effect of energy integration,

3. the need to account for chemical component inventories.

These issues are concerned if we have to deal with a complex plantwide control.
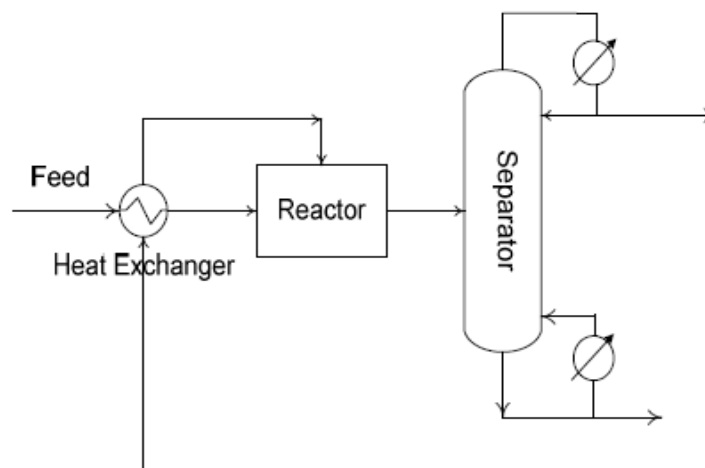
Figure 3.1 Integrated Process Flowsheet

3.1.1 Material Recycle

The effects of material recycle are important for six fundamental issues.

1. Increase conversion

For chemical processes involving reversible reactions, conversion of reactants to products is bounded by thermodynamics equilibrium constraints. Consequently the reactor effluent by the essential contains both reactants and products. To obtain economical viable, separation and recycle of reactants are necessary.

2. Improve economics

In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than to reach the necessary conversion in one reactor or several in series. A reactor followed by a stripping column with recycle streams is much reasonable in price than using one large reactor or three reactors in series.

3. Improve yields

In reaction systems such as, A$\longrightarrow$B$\longrightarrow$C, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much undesirable product C. Hence the concentration of B is kept moderately low in the reactor and a large recycle of A is required.

4. Provide thermal sink

In adiabatic reactors or reactors where cooling is difficult and exothermic heat effects are large, it is often essential to feed excess material to the reactor to prevent large amount of temperature increase in the reactor. High temperature can cause several unpleasant events: it can lead to thermal runaways, it can deactivate catalysts, it can create undesirable side reactions, it can cause mechanical failure of equipment, etc. Therefore the heat of reaction is absorbed by the sensible heat required to raise the temperature of the excess material in the stream flowing through the reactor.

5. Prevent side reactions

A large excess of one the reactant is often used in order to keep the concentration of the other reactant low. If a limiting reactant is not kept in low concentration, it could react to produce undesirable products. Therefore the excess

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

3.1.2 Energy Integration

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

3.1.3 Chemical Component Inventories

The Chemical species in plants can be characterized into three types: reactants, products and inerts. A material balance for each of these components must be satisfied. The actual problem typically appears when reactants are considered (because of recycle) and accounted for their inventories within the entire process. Because of their value, it is necessary to minimize the loss of reactants exiting the process since this represents a yield penalty. So reactants are prevented from leaving. This means we must ensure that every mole of reactant fed to the process is consumed by the reactions.

3.2 Effects of Recycle

In most actual processes, recycle streams are enclosed. Here, the plantwide control problem becomes much more complex. Two basic effect of recycle is: (1) an impact on the dynamics of the process. The overall time constant can be much different than the sum of the constants of the time constants of the individuals units. (2) Recycle

can cause the "snowball" effect; though a small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates.

3.2.1 Snowball Effects

Snowball effects exhibit with large variations in the magnitude of the recycle flows. This high sensitivity of the recycle flowrates to small disturbances is called the snowball effect. It is important to note that this is a steady- state phenomenon not a dynamic effect. But it does have dynamic implications for disturbance propagation and for inventory control. It has nothing to do with closed-loop stability. Nevertheless, this does not imply that it is independent of the plant's control structure. On the contrary, the extent of the snowball effect is very strongly dependent upon the control structure used.

The large fluctuations in recycle flowrates are undesirable in a plant because they can overload the capacity of the separation section or move the separation section into a flow region below its minimum turndown. So a plantwide control structure should be selected to that prevents this effect.

3.3 Plantwide Control Procedures

Two fundamentals of chemical engineering principles are necessary to be satisfied in plantwide control design procedure, which are over all conservation of mass and energy. Additionally, the procedure accounts for non-conserved entities within a plant such as chemical components (produced and consumed) and entropy (produced).

The goals for an effective plantwide process control system include:

1. Safe and smooth process operation.

2. Tight control of product quality in the face of disturbances.

3. Avoidance of unsafe process conditions.

4. A control system runs in automatic, not manual, requiring minimal operator attention.

5. Rapid rate and product quality transitions.

6. Zero unexpected environmental releases.

3.3.1 Basic Concepts of Plantwide Control

3.3.1.1 Buckley Basic

Page Buckley (1964) was the first to suggest the idea of separating the plantwide control 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. Note that most level controllers should be proportional-only (P) to achieve flow smoothing. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated. He tries to make these as small as possible so that good, tight control is achieved, but stability constraints impose limitations on the achievable performance.

3.3.1.2 Douglas doctrines

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

1. Minimize losses of reactants and products.

2. Maximize flowrates through gas recycle systems.

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

3.3.1.3 Downs drill

Jim Downs (1992) indicated 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. 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 raw material costs and maintain high-purity products must be minimized, most of the reactant 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 flowrates so that exactly the right amounts of the two reactants are fed in.

3.3.1.4 Luyben laws

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

1. To prevent the snowball effect, all recycle loops should be flow controlled.

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

3. If the final product from process comes out at 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. Changes in feed flowrate or feed composition have less of a dynamic effect on distillate composition than

they do on bottoms composition if the feed is saturated liquid. The reverse is true
if the feed is saturated vapor: bottom is less affected than distillate.

3.3.1.5 Richardson rule

Bob Richardson (1988) proposed 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. An analogy is that it is
much easier to maneuver a large barge with a tugboat than with a life. The point is that
the bigger the handle you have to affect a process, the better you can control it. This is
why there are often fundamental conflicts between steady-state design and dynamic
controllability.

3.3.1.6 Shinskey schemes

Greg Shinskey (1988) proposed a number of "advanced control" structures that
permit improvements in dynamic performance. These schemes are not only effective,
but they are simple to implement in basic control instrumentation. Liberal use should be
made of ratio control, cascade control, override control, and valve-position (optimizing)
control.

3.3.1.7 Tyreus tuning

The use of P-only controllers for liquid levels, tuning of a 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
settings 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 should be limited to those loops where two criteria are
both satisfied: (1) the controlled variable should have a very large signal-to-noise ratio
and (2) tight dynamic control from a feedback control stability aspect is very crucial. The

classical example of the latter is temperature control in an irreversible exothermic chemical.

3.3.2 Step of Plantwide Process Control Procedure

The nine steps of the design procedure was proposed by Luyben et al., (1997), the procedure focus on the fundamental principles of plantwide control: production rate; product quality; energy management; operational, environmental, and safety constraints; liquid level and gas pressure inventories; makeup of reactants; component balances; and economic or process optimization.

Step 1: Establish Control Objectives

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

Step 2: Determine Control Degree of Freedom (CDOF)

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

Step 3: Establish Energy Management System

Term energy management is used to describe two functions. (1) A control system that removes exothermic heats of reaction from the process is supplied. 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 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 propagation of the thermal disturbances and assures that the exothermic reactor heat is dissipated and not

recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

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

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

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, the overall reaction rates must be increased. This can be accomplished by raising temperature, increasing reactant concentrations, increasing reactor holdup, or increasing reactor pressure. The selected variable must be dominant for the reactor.

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 must be selected.

The choice of production-rate control cannot be made arbitrarily because of the implications for component balances examined in Step 7.

Step 5: Control Product Quality and Handle Safety, Operational, and Environmental Constraints

The best manipulators (valves) should be selected to achieve tight control of the product quality, safety, and environmental variables which requisites economic and operational reasons. The selection should be made such that the dynamic relationships between controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants, and the latter prevents problems with the range-ability of the manipulated variable (control-valve saturation).

Step 6: Control Inventories (Pressure and Level) and Fix a Flow in Every Recycle Loop

Flow in every recycle loop is to be fixed. Then, the best available manipulate variables (valves) are chosen to control the liquid and gas inventories based on Richardson's Rule, which state that an inventory variable should be controlled with he manipulated variable that exerts the large effect on it within that unit.

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

Step 7: Check Component Balances

Assure that the overall material balance for each and every component is satisfied at steady-state. Light, intermediate, and heavy inert components must have an exit path from the system. Reactant must be consumed in the reaction section or leave as impurities in the product streams. Fresh reactant makeup feed streams can be manipulated to control reactor feed composition or a recycle stream composition (or to hold pressure or level as noted in the previous step). Purge streams can also be used to control the amount of high- or low-boiling impurities in a recycle stream.

Step 8: Control Individual Unit Operations

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

Step 9: Optimize Economics or Improve Dynamic Controllability

After all of the basic regulatory requirements are satisfied, the remaining control degrees of freedom should be used in the best possible manner either to optimize steady-state economics or to improve dynamic performance. The setpoints of some controllers can also be adjusted.

3.4 New Plantwide Control Structure Design Procedure

New design procedure of Wongsri (2009) presented the eight step of plantwide control design procedure which analyzed by mathematical-based and heuristic-based. The priority of control variables is established in the procedure. The major disturbance are handled explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method) to cover the material disturbances. The propose procedure for selection the best set of control structure is perceptive, simple and straightforward. The new design procedures of Wongsri (2009) are:

Step1: *Establish of Control Objectives.*

Step2: *Selection of Controlled Variables (CVs) to achieve Product Quality, Safety, Operational and Environmental Constrains using The Fixture Point Theorem.*

Step3: *Selection of Manipulated Variables and Measurements by DOF Analysis.*

Step4: *Energy Management via Heat Exchanger Networks (HENs).*

Step5: *Selection of Control Configuration using Various Tools available.*

Step6: *Completing Control Structure Design by Checking the Component Balances.*

Step7: *Selection of Controller Type: Single loops or MPC.*

Step8: *Validation via Rigorous Dynamic Simulation.*

Wongsri (2008) propose the fixture point theorem that used to define the most sensitive CV. The steps of theorem analysis are:

1. Consider the process at dynamic mode until its responses are at steady-state.

2. CVs are arranged to follow the most sensibility of the process variable by step change of the MV in open loop control (change only one MV, the other should be fixed than alternate to other until complete).

3. Evaluate the magnitude of integral absolute error (IAE) of all process variables that deviates from steady state.

4. Select CV by considering CV that gave the most deviation from steady state (high value score).

3.5 Heat Exchanger and Plantwide Energy Management

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

3.5.1 Heat Exchanger Dynamics

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

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

3.5.2 Heat Pathway

In the process, the most energy required for heating certain streams are matched by similar amount of energy required for cooling other streams. Heat recover from cooling a stream could be recycling back to the process to heat another stream. This is the proposed of heat integration and heat exchanger networks (HENs).

From a plantwide perspective, the heat pathways in the process can be separated to three different paths as illustrate in Figure 3.2. The first pathway dissipates to the environment heat generated by exothermic reaction and by degradation of mechanical work. This pathway is from inside the process and flows out. It is also possible to convert some of the heat to work as it is removed from high temperature in the process.
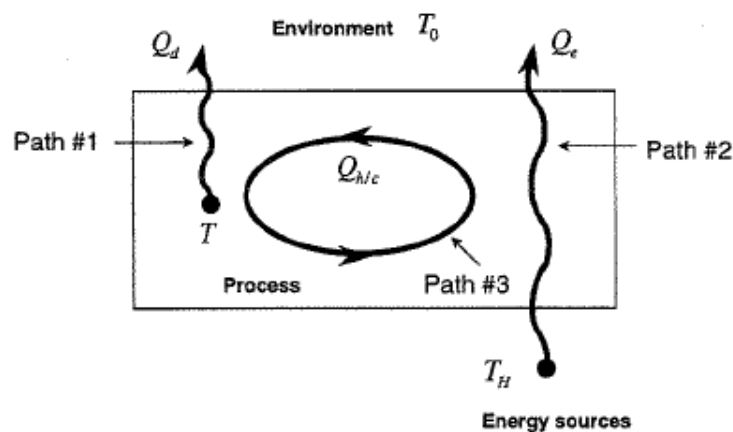
Figure 3.2 Heat Pathways.

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

from the heat stream to overcome process inefficiencies with stream mixing and heat transfer.

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

3.5.3 Heat Recovery

The great improvements in the plant's thermal efficiency are made by recycling much of the energy needed for heating and cooling process streams. There is of course a capital expense associated with improved efficiency but it can usually be justified when the energy savings are accounted for during the lifetime of the project. The current context draws attention on how heat integration affects the dynamics and control of a plant and how energy in plants can be managed with a high degree of heat recovery.

3.6 Control of Process-to-Process Exchangers

Process-to-process (P/P) exchangers are employed for heat recover within the process. Two exit temperatures can be controlled provided that the two inlet flowrates can be manipulated separately. Though, these flowrates are normally unavailable to manipulate. Therefore two degrees of freedom are given up fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Figure 3.3a. It is possible to combine the P/P exchanger with a utility exchanger as in Figure 3.3b.
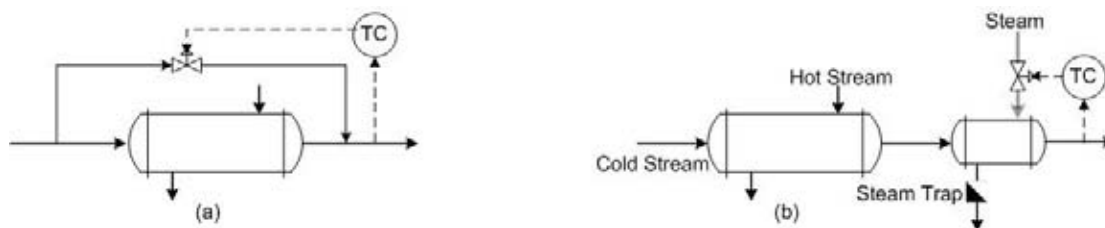
Figure 3.3 Control of P/P heat exchangers

(a) use of bypass; (b) use of auxiliary utility exchanger

3.6.1 Bypass Control

When the bypass method is employed for unit operation control, several choices about the bypass location and the control point are considered. Figure 3.4 shows the most common options. The question like "Which option is best?" may arise. The best alternative depends on how "best" is defined. As many other examples, it reduce the trade-off between design and control. Design considerations might suggest that the cold side is measured and bypass since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high temperature service. Cost consideration would also suggest a small bypass flow to minimize the exchanger and control valve sizes.

From a control perspective the most important stream should be measured, regardless of temperature, and bypass on the same side. This minimizes the effects of heat exchanger dynamics in the loop. A large fraction of the controlled stream should be bypass as it improves control range. Hence a large heat exchanger is required.
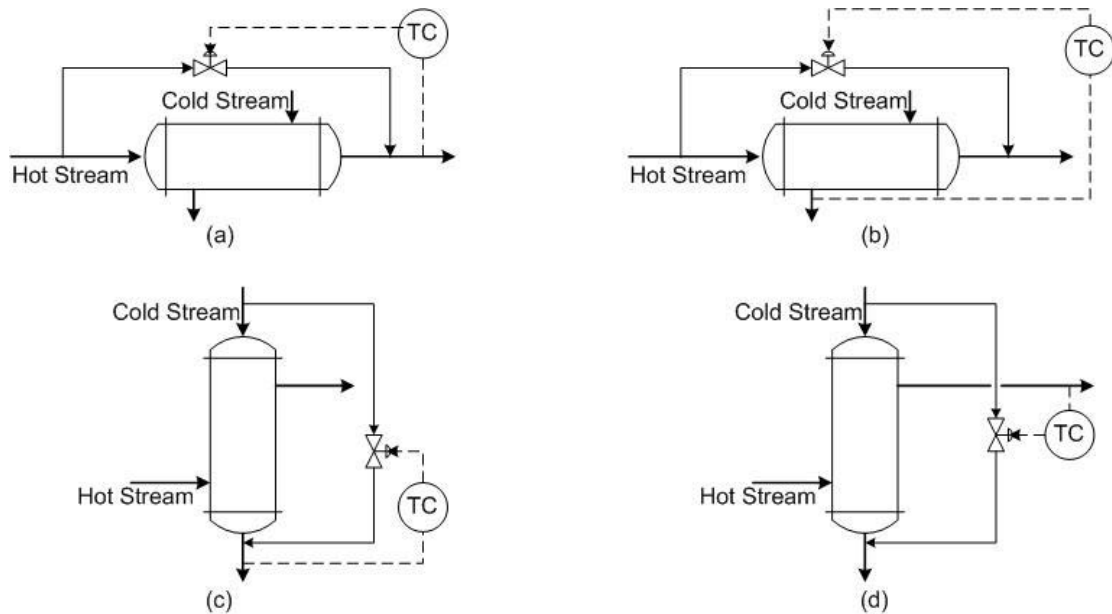
Figure 3.4 Bypass control of process-to-process heat exchangers.

(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.

3.6.2 Use of Auxiliary Utility Exchangers

There are a few design decisions to make, when the P/P exchanger is combined with a utility exchanger. First, the relative sizes between the recovery and the utility exchangers have to be established. From a design perspective, it is needed to make the recovery exchanger large and the utility exchanger small. This leads to the most heat recovery, and it is also the least expensive option from an investment standpoint. Though, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control standpoint.

Second, decision on how to combine the utility exchanger with the P/P exchanger must be made. This could be done either in a series or parallel arrangement. Physical implementation issues may dictate this choice but it could affect controllability. Finally, decision on how to control the utility exchanger for best overall control performance must be made.

Consider a distillation column that uses a large amount of high-pressure stream in its thermosiphon reboiler. Heat-integrate this column with the reactor is applied to reduce operating costs. A virtual way of doing this is to generate stream in a waste heat boiler connected to the reactor as suggested. Some or all of this steam can be used to help reboil the column by condensing the stream in the tubes of a stab-in reboiler. Nevertheless, the total heat from the reactor may not be enough to reboil the column, so the remaining heat must come from the thermosiphon reboiler which serves as an auxiliary reboiler. The column tray temperature controller would manipulate the stream to the thermosiphon reboiler.

CHAPTER IV

AUTO-REFRIGERATED ALKYLATION PROCESS

AND NEW CONTROL STRUCTURES DESIGN PROCEDURE

4.1 Introduction

Most chemical reactors (especially continuous stirred tanks, CSTRs) which operate the exothermic reaction needs to removed the heat of reactions generally by cooling jacket or cooling coils. In this study, the reactors removed the generated heat by evaporative cooling (auto-refrigeration), which generally operated at the liquid's bubble point. The examples of process that involves these types of heat generation are alkylation of olefins, polymerization of vinyl acetate and production of tetraethyl lead. The company whom provided the process licensed of sulfuric acid alkylation technologies are such as Exxon Mobil, MW Kellogg, DuPont STRATCO®, Chicago Bridge & Iron Company (CB&I), VNIPIneft Company, etc.

4.2 Process Description

The production of iso-octane (iC_8) from isobutane (iC_4) and 1-butene ($C_4^=$) is arranged into a series-parallel of reaction sequence in the liquid phase held by the continuous stirred tanks (CSTRs). The agitated reactors are operating at low temperature where sulfuric acid in liquid phase is used as a catalyst. The fresh olefin (butane-1-butene, BB) is feed into the process as a reactant which undergoes two reactions, main and side reaction. The main reaction is the production of alkylate which arises from the reaction of 1-butene ($C_4^=$) with isobutane (iC_4):

$$iC_4 + C_4^= \longrightarrow iC_8$$
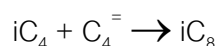
The undesirable reaction also presents at the same time by forming high-molecular-weight component, dodecane (C_{12}):

$$iC_8 + C_4^= \longrightarrow C_{12}$$
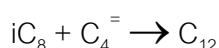
The kinetic expressions and data of the alkylation reactions are those suggested by Mahajanam et al. (2001) which are:

$$R_1 = A_1 \exp^{-E_1/RT} [iC_4] [C_4^=]$$

$$R_2 = A_2 \exp^{-E_2/RT} [C_4^=] [iC_8]$$

All reaction rates are in units of lbmol/ft^3·hr and the parameters are shows in table 4.1

Table 4.1 Alkylation Reaction Kinetic Parameters

Parameter	Reaction 1	Reaction 2
Pre exponential (A_1, A_2)	9.6×10^{13}	2.4×10^{17}
Activation Energy(E_1, E_2) [Btu/lbmol]	2.8×10^4	3.5×10^4
Heat of reaction [Btu/lbmol]	-3.9×10^4	-2.9×10^4

Remark that both reactions are exothermic and irreversible. The activation energy of the second (undesirable) reaction is greater than the main reaction therefore to improve the selectivity; the low temperature reactor and low concentration of 1-butene and iso-octane in the reactor need to be considered. There are two alternatives to suppressed the formation of dodecane (needless), first is to providing a large excess of isobutane, second is to split the fresh BB feed equally among the three reactors to keep the concentration of 1-butene low.

The fresh BB feed contains 50 mol% 1-butene ($C_4^=$), 25 mol% normal-butane (nC_4), 20 mol% isobutane (iC_4) and 5 mol% propane (C_3) is feed and split into the reaction section which composed of three continuous reactors with an equal volume of 500 ft^3. The reactors assumed to be half full of liquid where the reactions take place in the liquid phase. The total vapor products are then put together and feed to the separation section, a depropanizer (DP) column to removed propane (C_3) apart from isobutane (iC_4) compositions. The feed stage is placed at stage 15 out of 17 stages of the DP column. The reflux ratio is high due to the small amount of distillate flow rate to the reflux flow rate. The reflux ratio is then set as 10.50. The DP column operates at pressure of 220 psia and 118 °F in which of the distillate product contain 95 %

composition of C_3 with molar flow rate of 8.2 lbmol/hr and the bottom product contain the major composition of isobutane (iC_4).

The liquid product from the third reactor is heated in the heat exchanger1 (HX1) before entering a 52 stages deisobutanizer (DIB) column which separates isobutane (iC_4), n-butane (nC_4), and alkylate (isooctane iC_8 mainly). The liquid product is feed to the DIB column at stage 8 with the vapor sidestream withdraw from stage 49. The column operates at pressure of 95 psia and 118.6 °F with 0.25 reflux ratio. The additional fresh C_4 is feed at tray 36 where the tray composition is similar to the makeup feed. The distillate from the DIB column contained 89.72 mol% isobutane (iC_4) and 3.73 mol% n-butane (nC_4). The vapor sidestream majorly contained 95 mol% of n-butane with 52.7 lbmol/hr flowrate and the alkylate product of 90% isooctane (iC_8) with 48.36 lbmol/hr is removed at the bottom of the column along with undesirable component, dodecane (C_{12}).

The bottom product of the DP column is used to heat the liquid product entering the DIB column before combing with the overhead product of the DIB column then recycling back and reenter the first reactor with 87.9 mol % isobutane compositions and 2010 lbmol/hr flowrate.
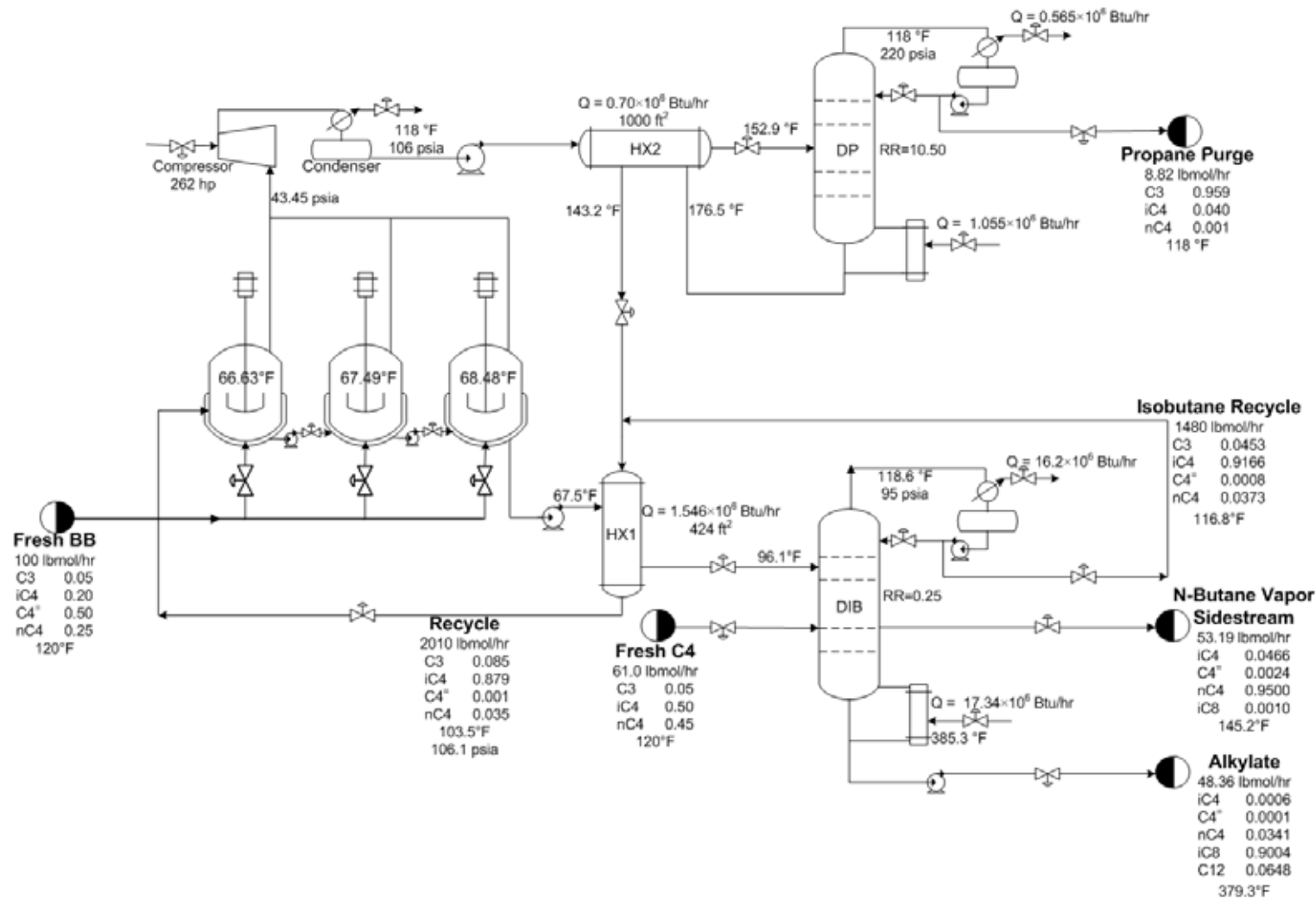
Figure 4.1 Auto-refrigerated Alkylation flowsheet (Luyben,2009)

4.3 Steady State Simulation of an Auto-refrigerated Alkylation Process

The steady state simulation model is performed by using ASPEN HYSYS with information and data collected from Luyben (2009). Appendix A provides the data and conditions for the unit operations which are involved in the process. The Chao-Seader physical property package is used in the ASPEN HYSYS simulations for its low pressure region which is suitable for an alkylation process. The kinetics data for both reactions, main and side reaction, are those suggested by Mahajanam et al. (2001) which are carried out by standard Arrhenius expressions.

4.4 Wongsri (2012) New Control Structures Design Procedure

Step 1: Gather plant information and control objective. List all control variables and available manipulated variables (number of DOF):

I. An independent stream must have a control valve (1 DOF)

II. A heater, cooler, pump, or compressor has one degree of freedom (to adjust heat load or duty or work load)

III. A process to process heat exchanger has one degree of freedom by adding a by-pass line.

IV. A reactor has zero or one degree of freedom depends on its type.

V. A flash separator has two degree of freedom.

VI. A simple distillation column has five degree of freedom.

Note: How to pair manipulated and controlled variables:

I. A control and manipulated variables must have strong causal relationship (high gain)

II. The manipulated variables should not be far from the control variables (zero or minimal dead time)

III. The time constant of the quality loops should be short and the time constant of the inventory loops should be longer.

IV. The manipulated variables should not be saturated for the whole range of the disturbances.

V. The change of the manipulated variables should not or have little effect on others variables (low gains with the remainder of the variables).

Step 2: Energy management via heat exchanger networks.

If potential heat exchanger networks or alternative heat integrated processes (HIPs) exist, list additional control variables and manipulated variables.

Step 3: Establish fixture plant

The principal idea of establishing a fixture plant is to first have entire plant fluid-filled and material-balanced. This idea is similar to creating "hydraulic" control structure proposed by Buckley (1964).

3.1 Keep the raw materials entered and reentered fixed

3.2 Adjust the flow of exit material streams according to their accumulation (products, by-products, and inert)

3.3 Locate the quantifiers for the rest of the components and design the control loops to regulate their inventories in the plant. The material flow in the plant should be fixed. In the case that this cannot be done the change of the material flow must be slow.

Step 4: Handling the disturbances

In this step, we configure the quality control loops by employing the notion of all disturbances management.

4.1 Heat Disturbances

4.1.1 Direct the heat disturbances that are not directly related to quality to the environmental via the next and nearest exit points, usually heaters of coolers, to keep the thermal conditions of process stream constants. The thermal condition of process stream is changed along the process plant, usually by heater or cooler of process to process heat exchanger.

4.1.2 Manage the heat disturbance that related to quality in order to maintain the product constraints

4.2 Material disturbances

The configuration of the control loops depend on the desired material pathways by analyzing the material disturbance tests on changes of composition, total flow, component flow: At reactor, we adjust the reactor inlet temperature in order to keep the reactor outlet composition or the product component flow fixed. For distillation columns, to control top or bottom temperature depend on the material disturbance rejection policy.

Step 5: Find the most disturbed point and design the control loops to alleviate the effects of disturbances.

Step 6: Design the control loops for the rest of the control variables or adding enhanced controls, i.e. cascade, feed forward controls.

Step 7: Optimize economics and improve control performance

Step 8: Validate the designed control structures by rigorous dynamic simulation

CHAPTER V

CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION

5.1 New Control Structures Design

Step 1: Gather plant information and control objective.

In this study, the alkylate product at 90 mol% isooctane (iC_8) with capacity of 22,340 lb/year, is essentially requisites to meet process objectives. The control variables and available manipulated variables (number of Degrees of Freedom) in this auto-refrigerated alkylation process are 19.

Table 5.1 Controlled and available manipulated variables

Controlled Variables (CVs)	Available Manipulated Variables (MVs)
Reactor 3 (R3) Temperature	Vapor Product flowrate
	Compressor work
Reactors (R1, R2, R3) Liquid Level	Liquid product flowrate
Condenser Pressure	Refrigerant drum heat removal
Condenser Liquid Level	Pump duty
DP column Pressure	Condenser heat removal
	Reboiler heat input
	Column feed flowrate
DP column Tray Temperature	Reboiler heat input
	Reflux flowrate
DP column Reflux flowrate	Reflux ratio
	Boil up ratio
	Distillate flowrate

Table 5.1 (Continue) Controlled and available manipulated variables

Controlled Variables (CVs)	Available Manipulated Variables (MVs)
Reflux drum Level (DP column)	Distillate flowrate
	Reflux flowrate
	Vapor boil up flowrate
	Condenser heat removal
	Column feed flowrate
DP column Base Level	Bottom flowrate
	Vapor boil up flowrate
	Column feed flowrate
DIB column Pressure	Condenser heat removal
	Reboiler heat input
	Column feed flowrate
	Fresh C4 feed flowrate
DIB column Tray Temperature	Reboiler heat input
	Reflux flowrate
DIB column Reflux flowrate	Reflux ratio
	Distillate flowrate
	Side stream flowrate
Reflux drum Level (DIB column)	Distillate flowrate
	Reflux flowrate
	Column feed flowrate
DIB column Base Level	Bottom flowrate
	Side stream flowrate
	Vapor boil up flowrate
	Column feed flowrate

Table 5.2 Manipulated variables and control degrees of freedom

Unit	Manipulated variable	Quantity	DOF
Independent streams	Flow rate	4	4
Compressor	Power	1	1
Condenser	Heat removal Liquid effluent	1	2
Pump	Work	1	1
Distillation column Depropanizer (DP)	Distillate flow, Bottom flow, Reflux flow, Reboiler heat removal Condenser heat input	1	5
Side stream distillation column Deisobutanizer (DIB)	Distillate flow, Bottom flow, Reflux flow, Side stream flow, Reboiler heat removal, Condenser heat input	1	6
Total degrees of freedom			19

Step 2: Energy management via heat exchanger networks.

There is no alternative heat integrated processes available in this auto-refrigerated alkylation process since the process is operating at low temperature. Also, the heat exchangers gather in the process have already assigned heat from the bottom flowrate of both columns to used as preheat before entering the columns. Therefore, adding more heat exchanger networks results as increasing operating costs to power the run of the refrigeration system.

Table 5.3 represented the thermal data of hot and cold streams of an auto-refrigerated alkylation process which has been used in pinch analysis. The process includes of two hot streams and two cold streams. Hot streams are streams that need cooling; in this process are bottom stream of the DP column and distillate stream of the DIB column. Whereas cold streams are the streams that need heating, which are reactor product entering the DP and the DIB column.

Table 5.3 Thermal data of an auto-refrigerated alkylation process for pinch analysis

Stream Name	Supply Temperature, T_S (°F)	Target Temperature, T_T (°F)	W (KBtu/°F)
H1: Bottom stream of DP column	176.5	103.5	19.99
H2: Top stream of DIB column	116.8	103.5	61.02
C1: Reactor Product entering DP	118.0	152.9	19.19
C2: Reactor Product entering DIB	67.5	96.1	52.68

The supply and target temperature of the stream is indicating as T_S and T_T. While $W(mC_P)$ of a stream is the magnitude of heat capacity flowrate (KBtu/°F); which is define from the mass flowrate (m) and the specific heat capacity of the stream (Btu/lb °F).

The grid diagram of the heat exchanger network shown in figure 5.1 is employed in the auto-refrigerated alkylation process. The diagram illustrates action of the heat load, Q being used by heat exchanger 1 and 2 (HX1, 2).
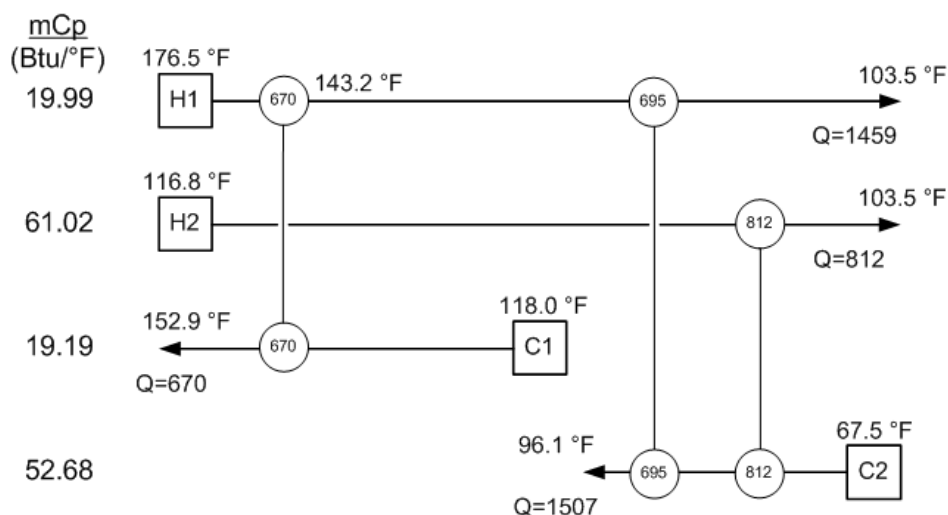
Figure 5.1 Grid diagram of the heat exchanger network

Step 3: Establish fixture plant

The principal idea of establishing a fixture plant is to first have entire plant fluid-filled and material-balanced. This idea is similar to creating "hydraulic" control structure proposed by Buckley (1964).

3.1 Keep the raw materials entered and reentered fixed

The raw materials entered and reentered the alkylation process are keeping fixed to maintain the feed compositions of the throughput and recycle flows in order to prevent the snowball effect. Therefore, the fresh BB is fixed and the makeup fresh C_4 is brought in to the process as the raw materials in order to hold amount of the recycle stream, shown in figure 5.2. The recycle stream reentered the process is drawn from the distillate product of the DIB column and bottom product of the DP column.

3.2 Adjust the flow of exit material streams according to their accumulation.

The flow of exit material stream referred to the product stream, the vent stream and the purge stream of the process. In this study, the propane (C_3) purge is conduct out of the process through the distillate of the DP column with limited flowrate and 95 mol % propane compositions. The vapor that contains 95mol % normal butane (nC_4) compositions and the alkylate product with 90 mol % isooctane (iC_8) is carried out by the side stream and the bottom of the DIB column respectively, as shown in figure 5.3 (a) and (b).
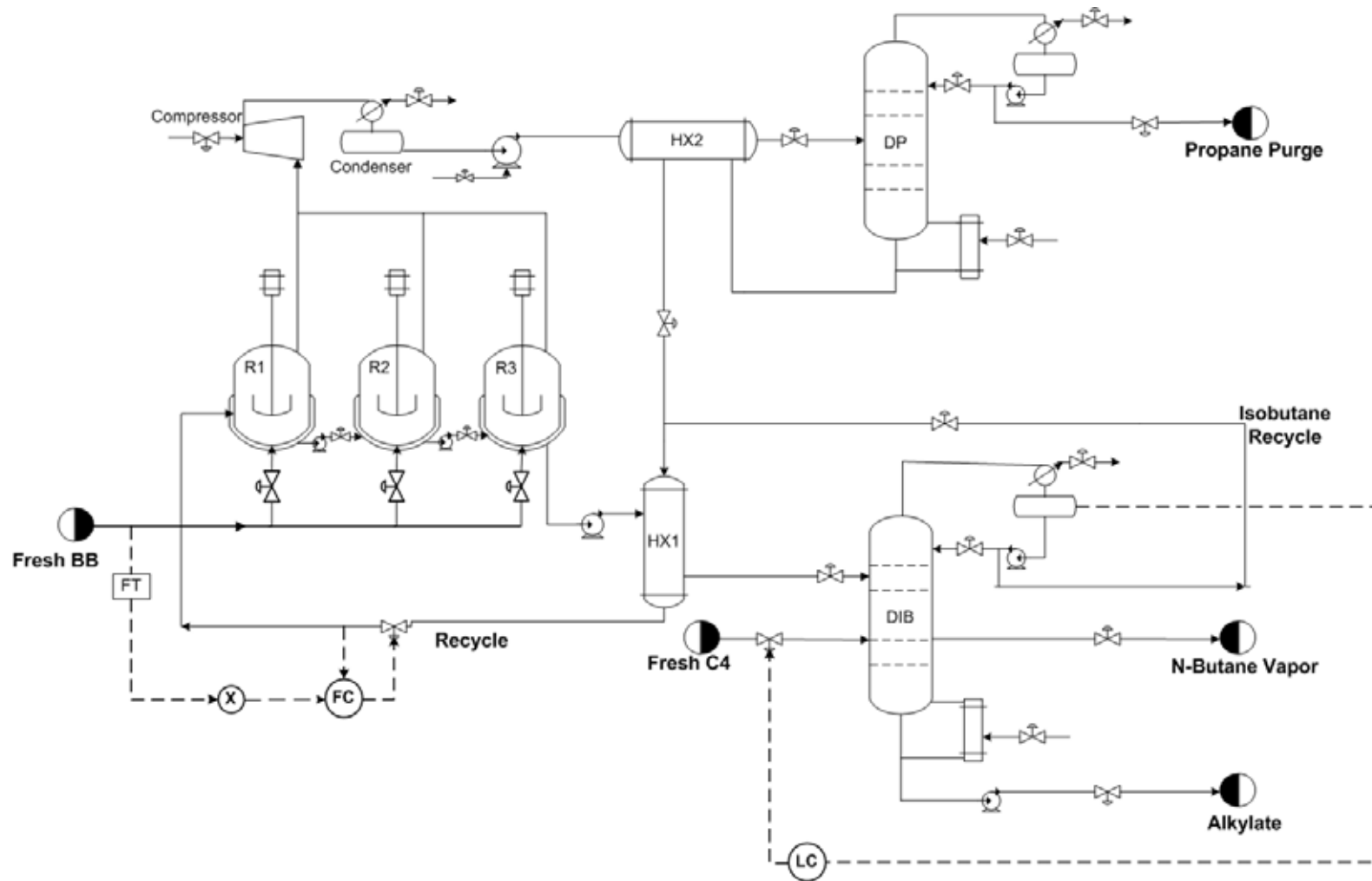
Figure 5.2 Control structure of fixing the raw materials entered and reentered the process
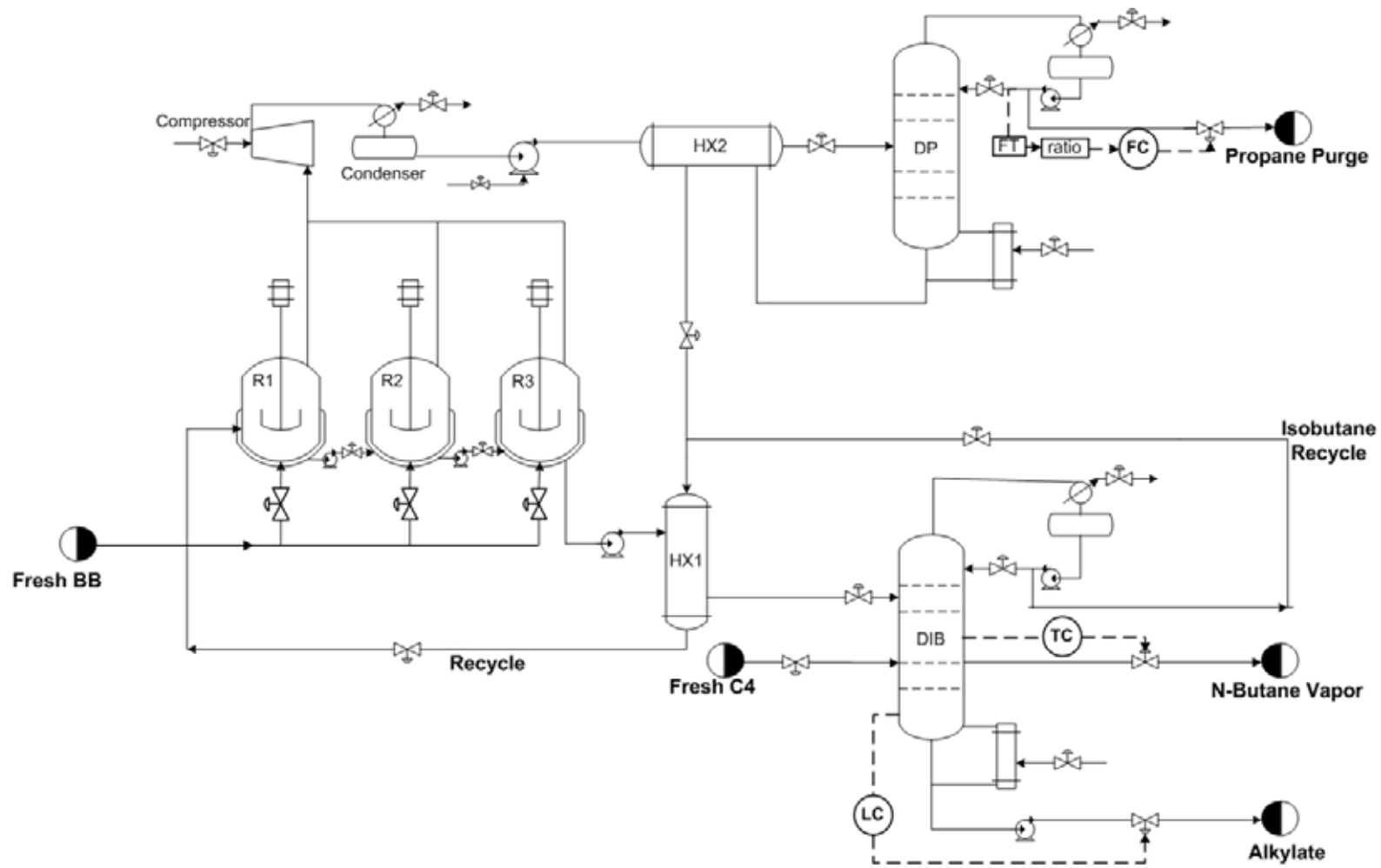
Figure 5.3(a) The exit material streams adjusted according to their accumulation (option1).
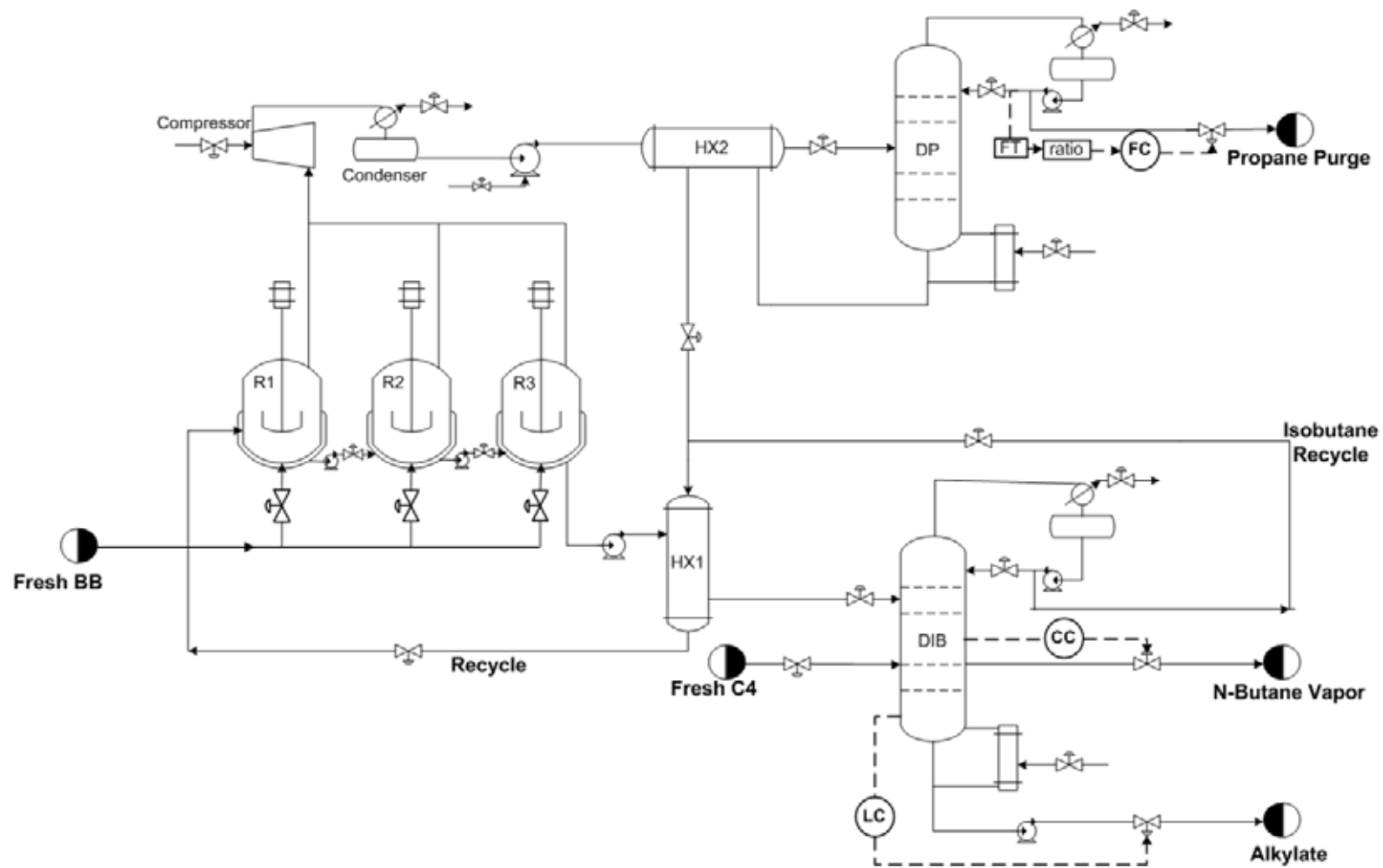
Figure 5.3(b) The exit material streams adjusted according to their accumulation (option2).

3.3 Locate the quantifiers for the rest of the components and design the control loops to regulate their inventories in the plant. The material flow in the plant should be fixed. In the case that this cannot be done the change of the material flow must be slow.

The quantifier of the components can be implies as a quantity or amount of the specified component such that pressure is vapor quantifier, level is liquid quantifier and so forth. In this study, the level controllers are adjoined to three reactors and to the bottom of the DP and DIB column to maintain the liquid production level and the amount of liquid in the base of the columns. The pressure controllers are installed to observe the amount of vapor in refrigerant cooler (condenser) and the column's condenser.

Table 5.4 shows the components involved in the alkylation process and located the quantifiers and inventories of those components. The flowsheet in Figure 5.4 shows the design control loops for the components inventories and located the components quantifiers apart from exit material streams as mentioned in step 3.2.

Table 5.4 The located quantifiers of the components.

Components	Quantifiers
propane (C_3)	DP Condenser
isobutane (iC_4)	DP Reboiler, DIB Condenser
1-butene ($C_4^=$)	No quantifier
normal butane (nC_4)	Directed to DIB side stream
isooctane (iC_8)	DIB Reboiler
dodecane (C_{12})	DIB Reboiler

Figure 5.5 (a) and (b) shows the control structures obtain directly from following the step 3.1 through 3.3.
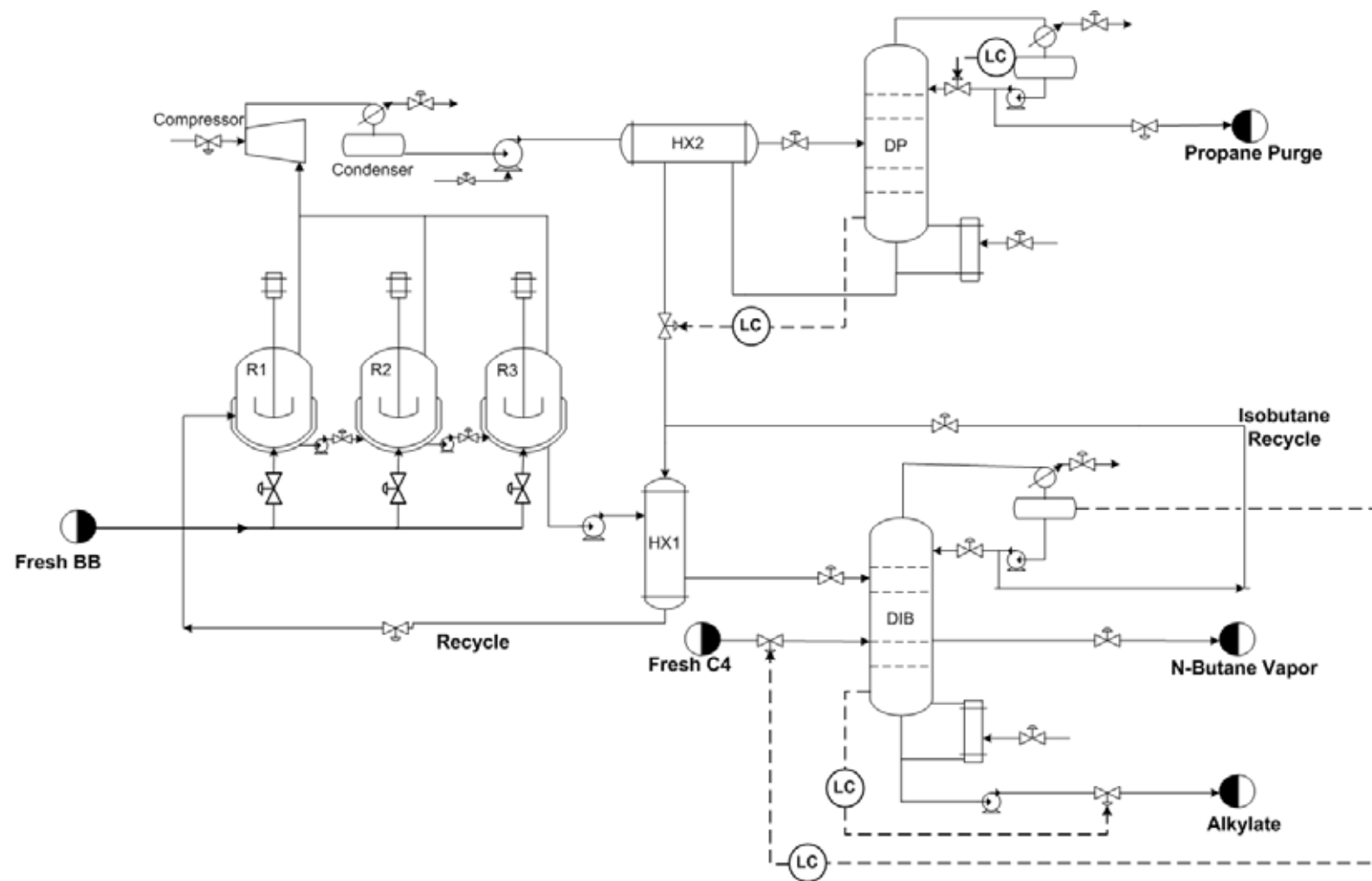
Figure 5.4 The design control loops for the components inventories and located the components quantifiers
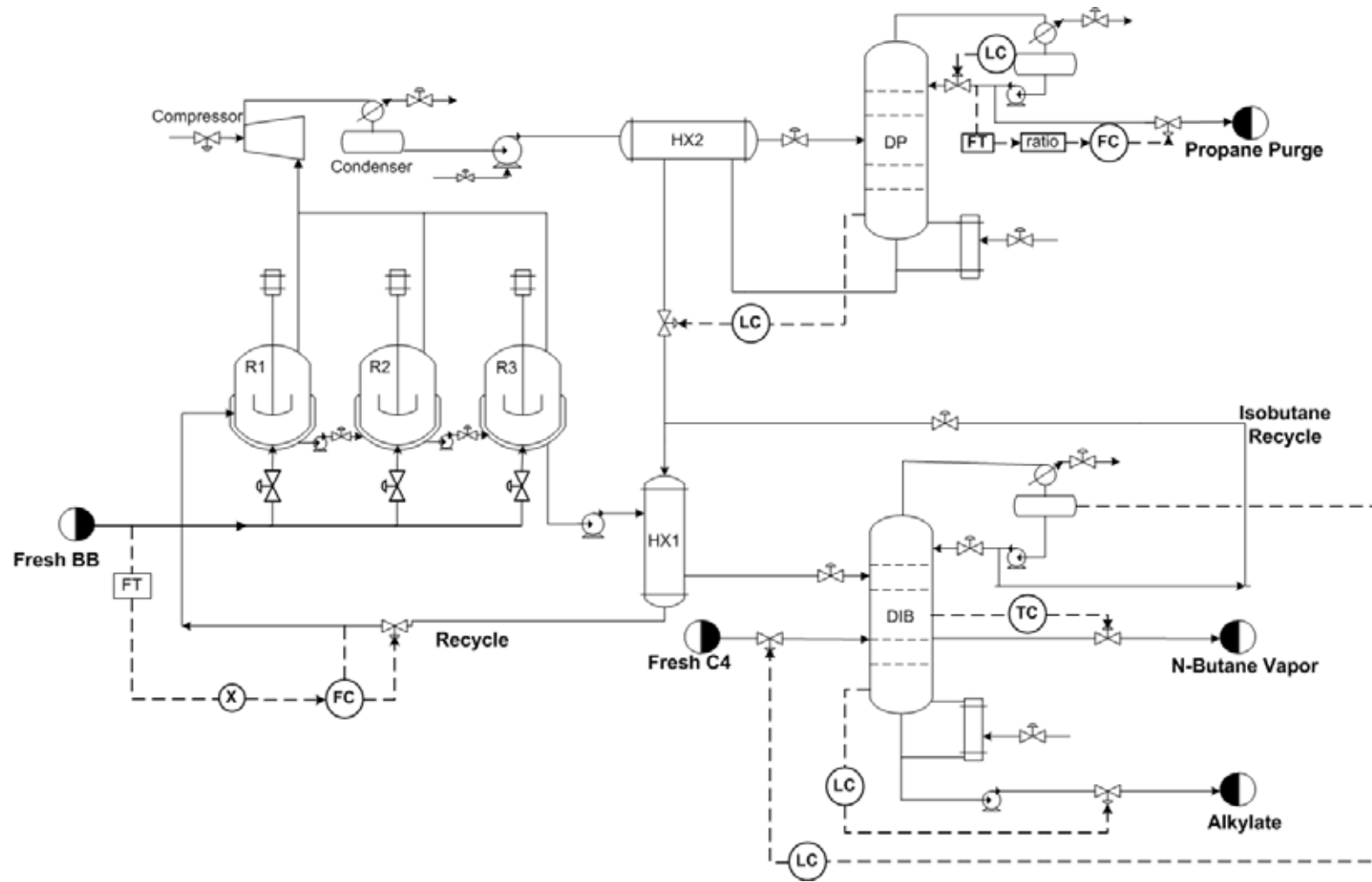
Figure 5.5 (a) The fixture plant control structure (option1).
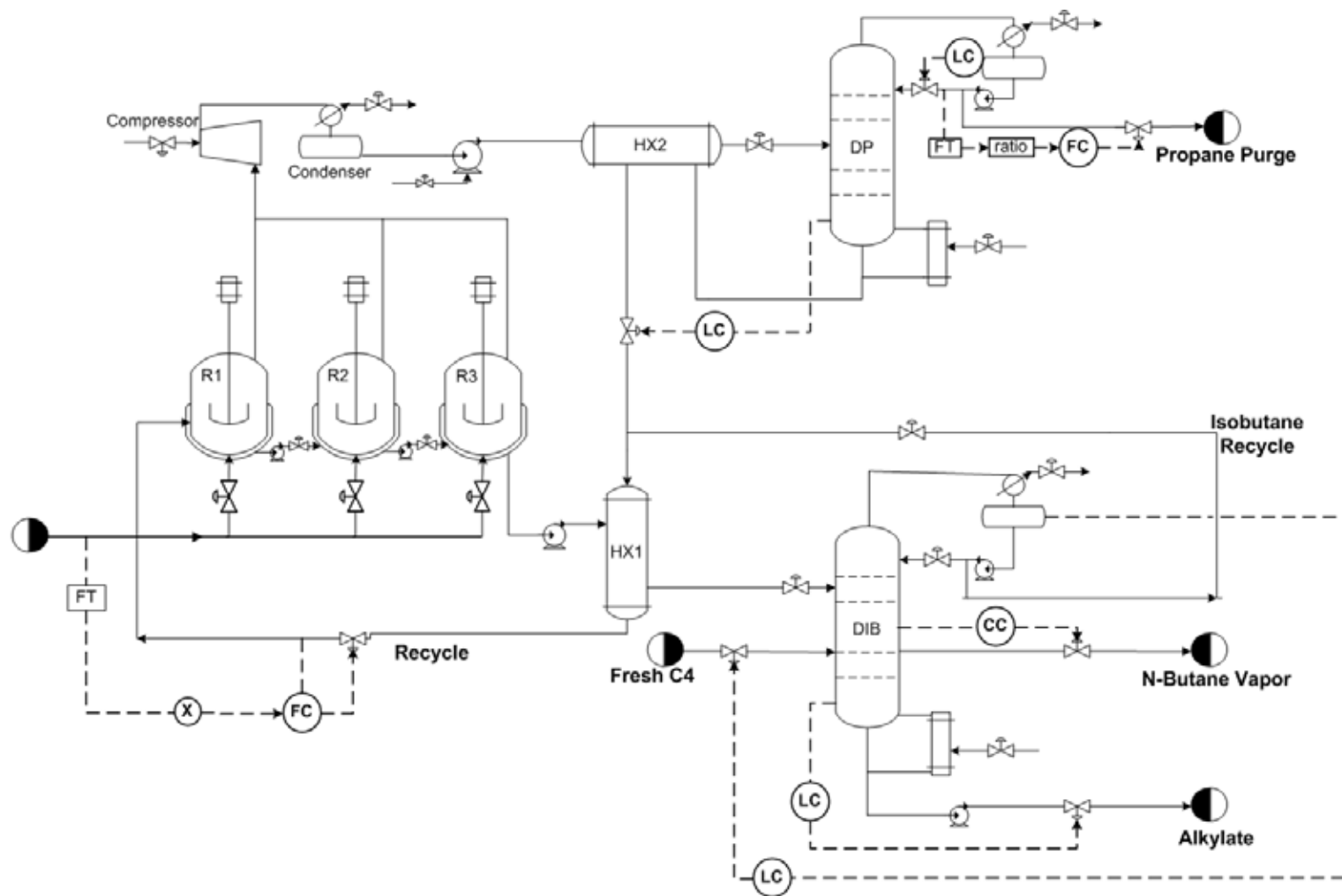
Figure 5.5 (b) The fixture plant control structure (option2).

Step 4: Handling the disturbances

In this step, we configure the quality control loops by employing the notion of all disturbances management.

4.1 Heat Disturbances

4.1.1 Direct the heat disturbances that are not directly related to quality to the environmental via the next and nearest exit points to keep the thermal conditions of process stream constants.

In this step, the heat disturbances that have been entered to the process needed to be removed via available unit operations which involved with heat transfer. The heat exit points include compressor work, condenser duty, reboiler and total condenser energy stream of distillation columns. Note that the disturbances in this step should not affect to quality. Figure 5.6 shows the heat disturbances available exit points.

In this study, the disturbed heat arise in reaction section can be directed to the refrigerant (condenser) heat removal. In case that the heat disturbed has not been completely removed, the bypass control of process-to-process heat exchangers technique is applied. The bypass valve is then installed to the side which temperature is needed to be control or the opposite side. Figure 5.7 shows an alternatives control structures make used of bypassing the hot streams of heat exchager1 and 2 (HX1 and HX2).
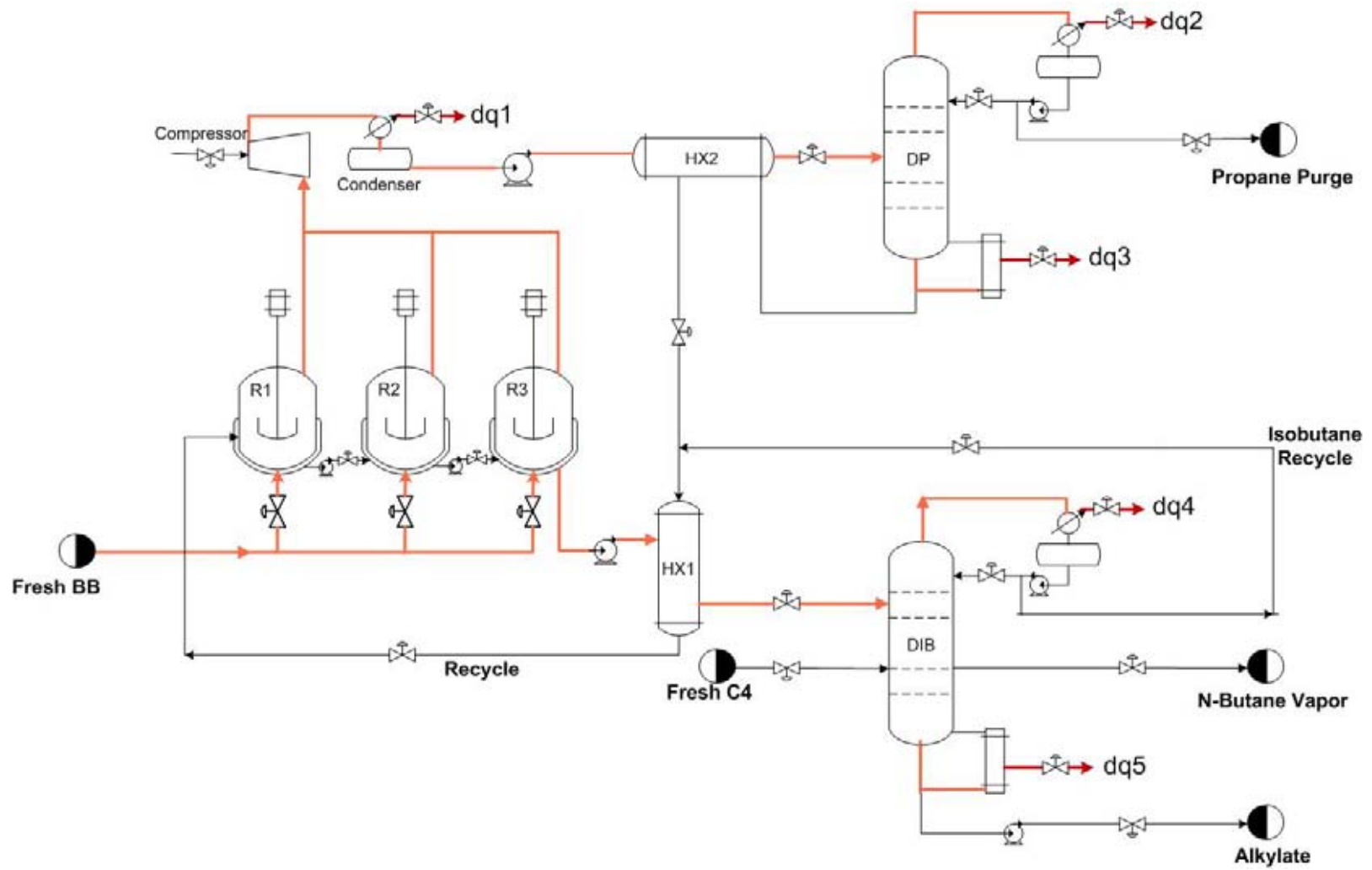
Figure 5.6 The heat disturbances pathways
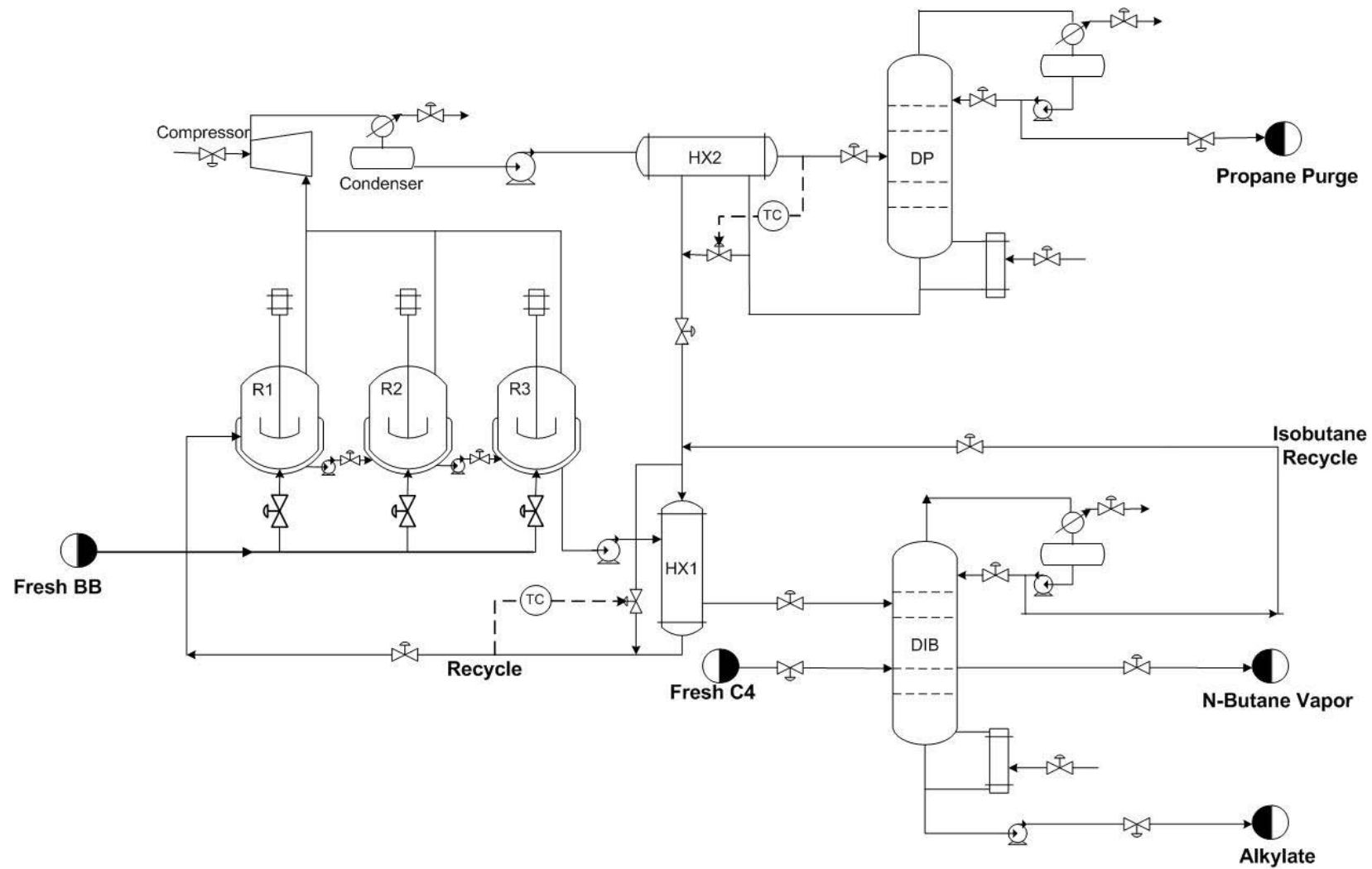
Figure 5.7 Flowsheet of control scheme that directed heat which is not related to the quality (By passing hot streams)

4.1.2 Manage the heat disturbance that related to quality in order to maintain the product constraints.

If the feed composition and the column pressure are constant, temperature can be used as an indirect measurement of compositions. When the bottom product compositions need to be controlled, the temperature sensor should be located in the lower half of the column. However when the distillate or overhead product compositions need to be controlled, the temperature sensor need to be located in the upper half.

Since the reactors operate at low temperature which required refrigeration. The refrigeration is done by removing the liquid that has been boiled up using a compressor. Therefore, the heat disturbance in the reaction section is managed via their vapor product by manipulating the compressor work. The DP bottom product (iC_4) impurity is manipulated by the DP column reboiler heat input as a single-end temperature control. In the second column, DIB, the dual –end control is employed to control the purity of the side stream vapor (nC_4) by manipulating the reflux flowrate and the side stream flowrate. Also, the purity of the bottom product (iC_8) is managed by the DIB column reboiler heat input, as shown in figure 5.8.

Figure 5.8 Flowsheet of control scheme that manage the heat disturbances related to the quality.

4.2 Material disturbances

The configuration of the control loops depend on the desired material pathways by analyzing the material disturbance tests on changes of composition, total flow, component flow.

The alkylate product quality (iC_8) can be affected primarily by two components, 1-butene ($C_4^=$) and isobutane (iC_4). Any excess of $C_4^=$ in the reaction section can leads to the undesirable reaction which produce dodecane (C_{12}). Therefore the temperatures of the reactors are set to be low to improve the selectivity.

The material pathways point out the control structures of each material due to their direction in the process. Isobutane (iC_4) and 1-butene ($C_4^=$) are primarily components that effected the alkylate product quality, mainly isooctane (iC_8). Any excesses of $C_4^=$ in the reaction section resulted in production of an undesirable components, dodecane (C_{12}). Therefore, $C_4^=$ is verify to be used up in three reactors, or else recycled back to the process via the bottom of the depropanizer (DP) and the distillate of the deisobutanizer (DIB) column. The iC_8 and C_{12} are generated from the reactions are taken out of the process by the side stream and the bottom product of the DIB column. The leftover are then recycled back to the reactors. The C_3 entered the process through the fresh BB and fresh C4 stream and leaved at the distillate of the DP column, otherwise it is recycled back to reenter the process by the bottom product of the DB column and the distillate product of the DIB column. The iC_4 and nC_4 are introduced to the process by fresh BB and fresh C4 stream. The iC_4 travelled by reactor vapor and liquid product, then through the bottom of the DP column. Though, the iC_4 and nC_4 in liquid product phase from the reactors are travelled to the distillate flow of the DIB column before recycling back to the first reactor.

All control structures established from step 4.2 are shown as following figure 5.9 to 5.14.
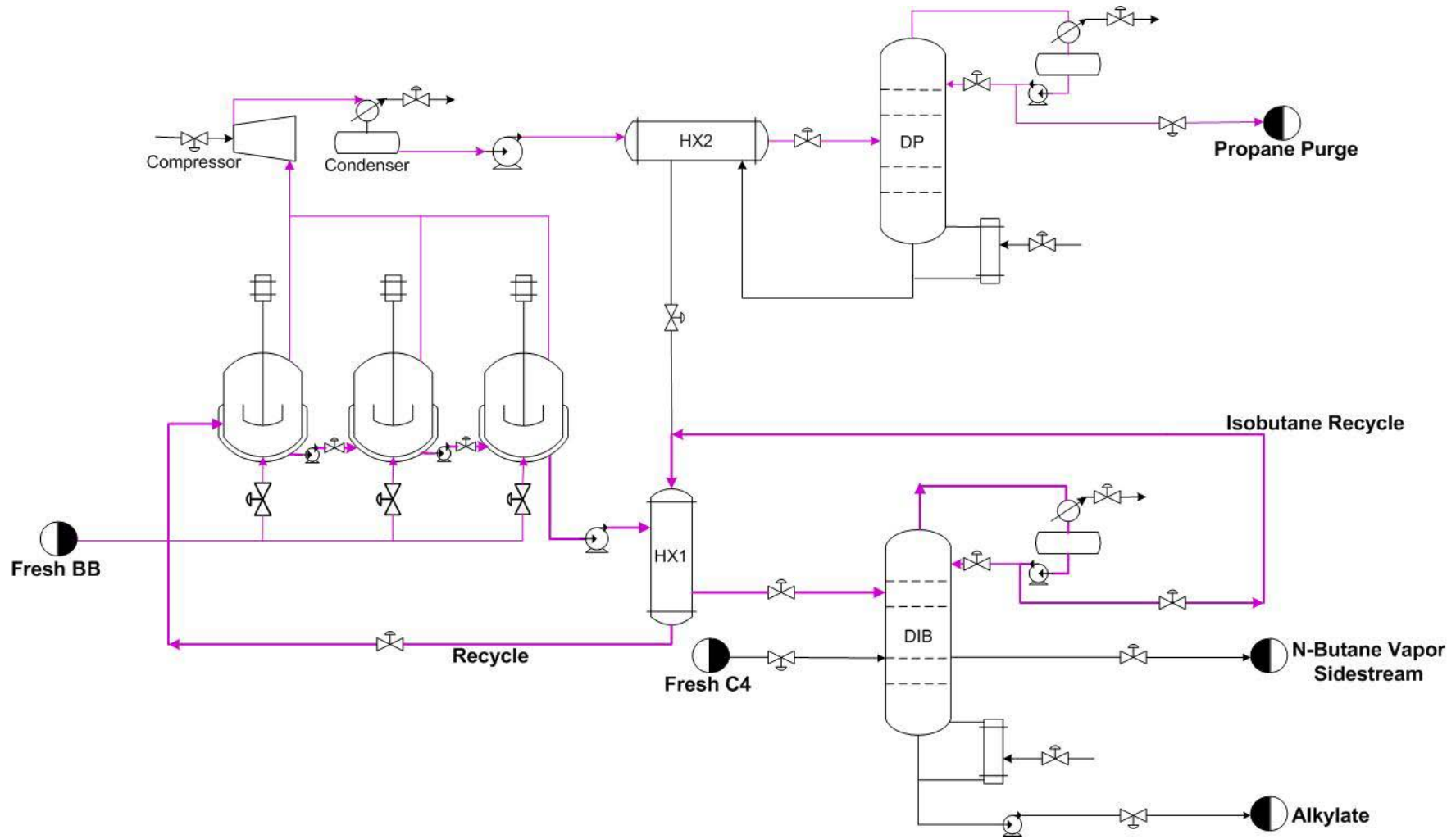
Figure 5.9 propane (C_3) pathways
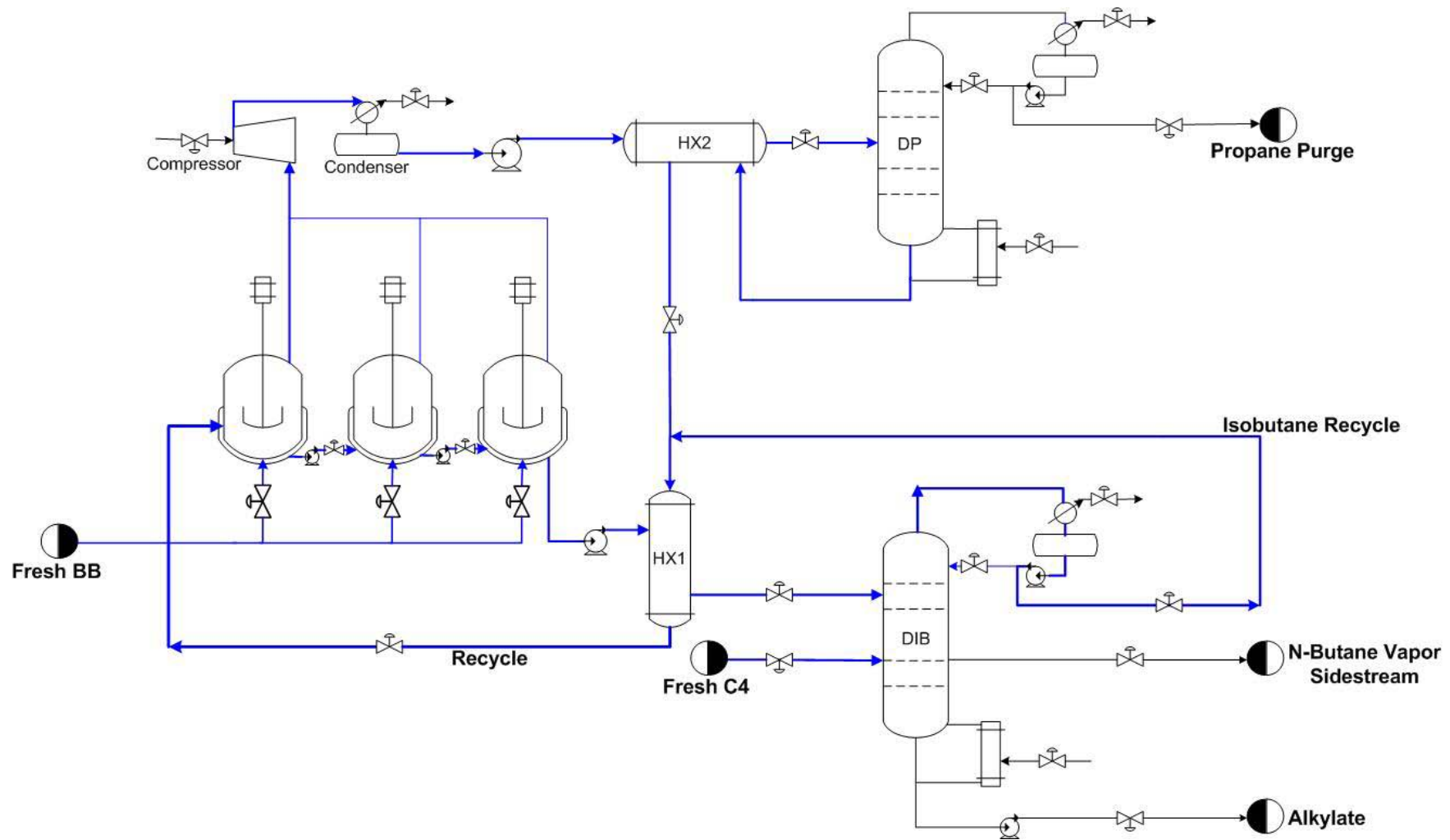
Figure 5.10 isobuane (iC$_4$) pathways
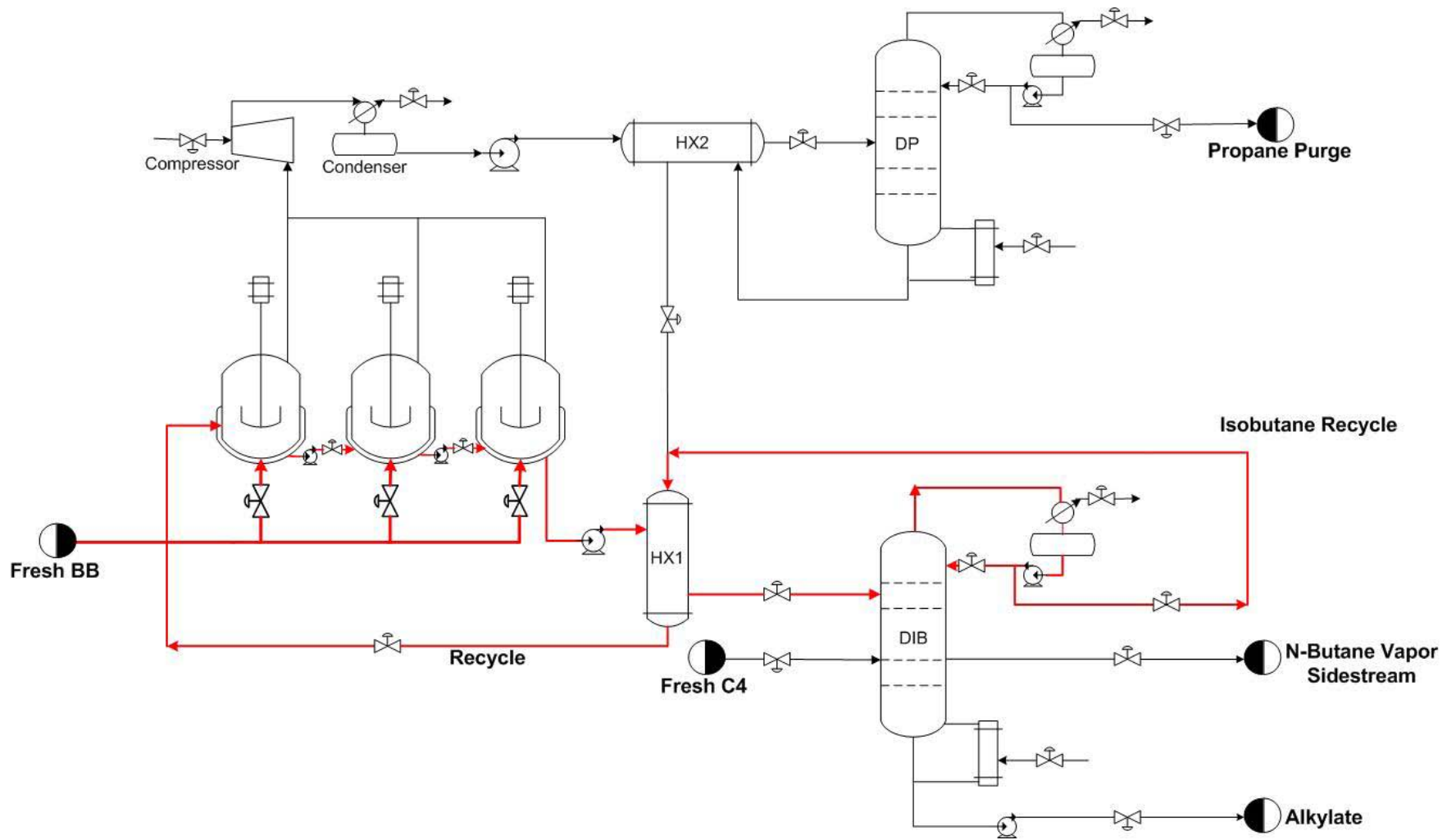
Figure 5.11 1-butene ($C_4^=$) pathways
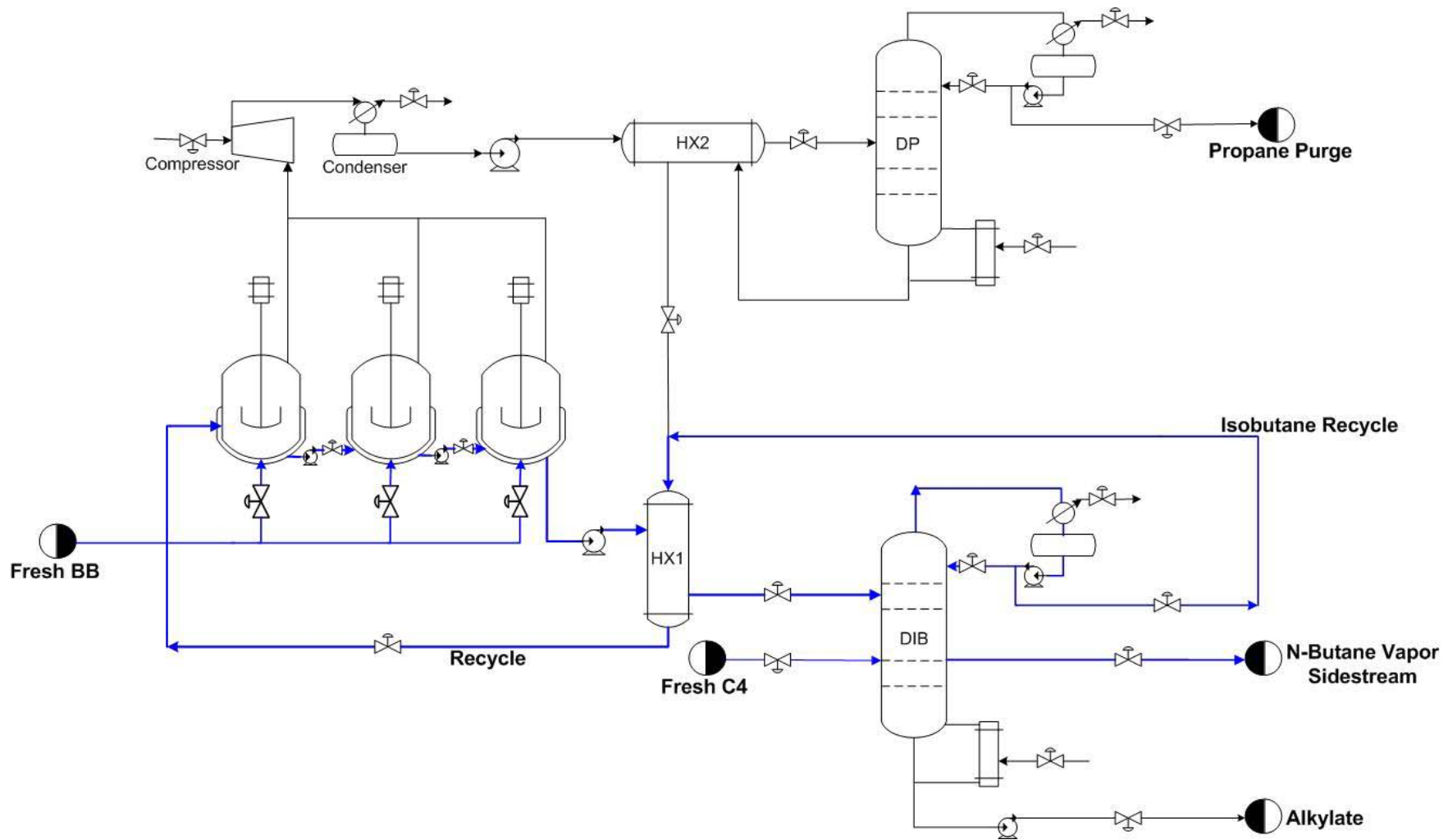
Figure 5.12 normal butane (nC_4) pathways
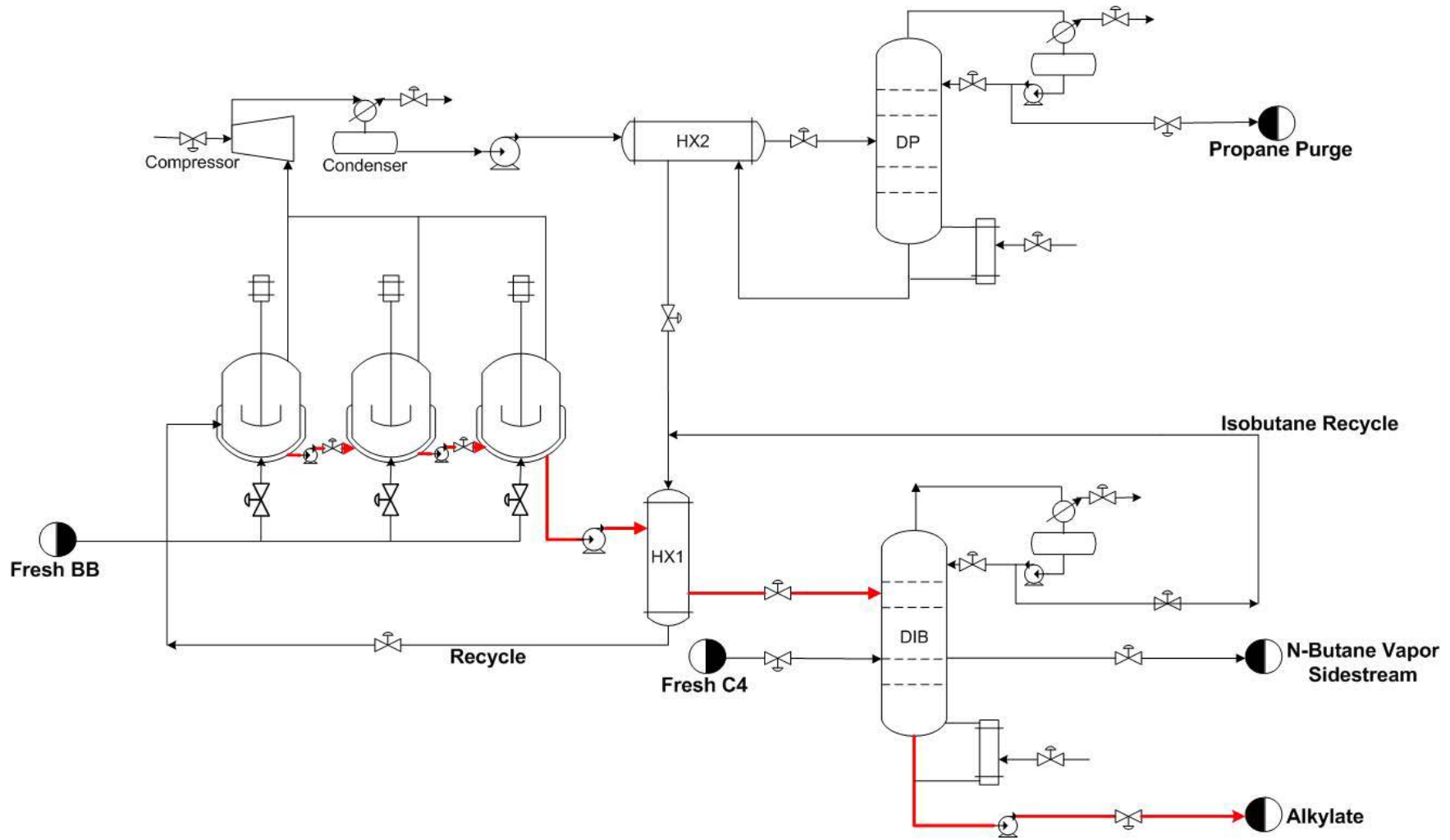
Figure 5.13 isooctane (iC$_8$) pathways
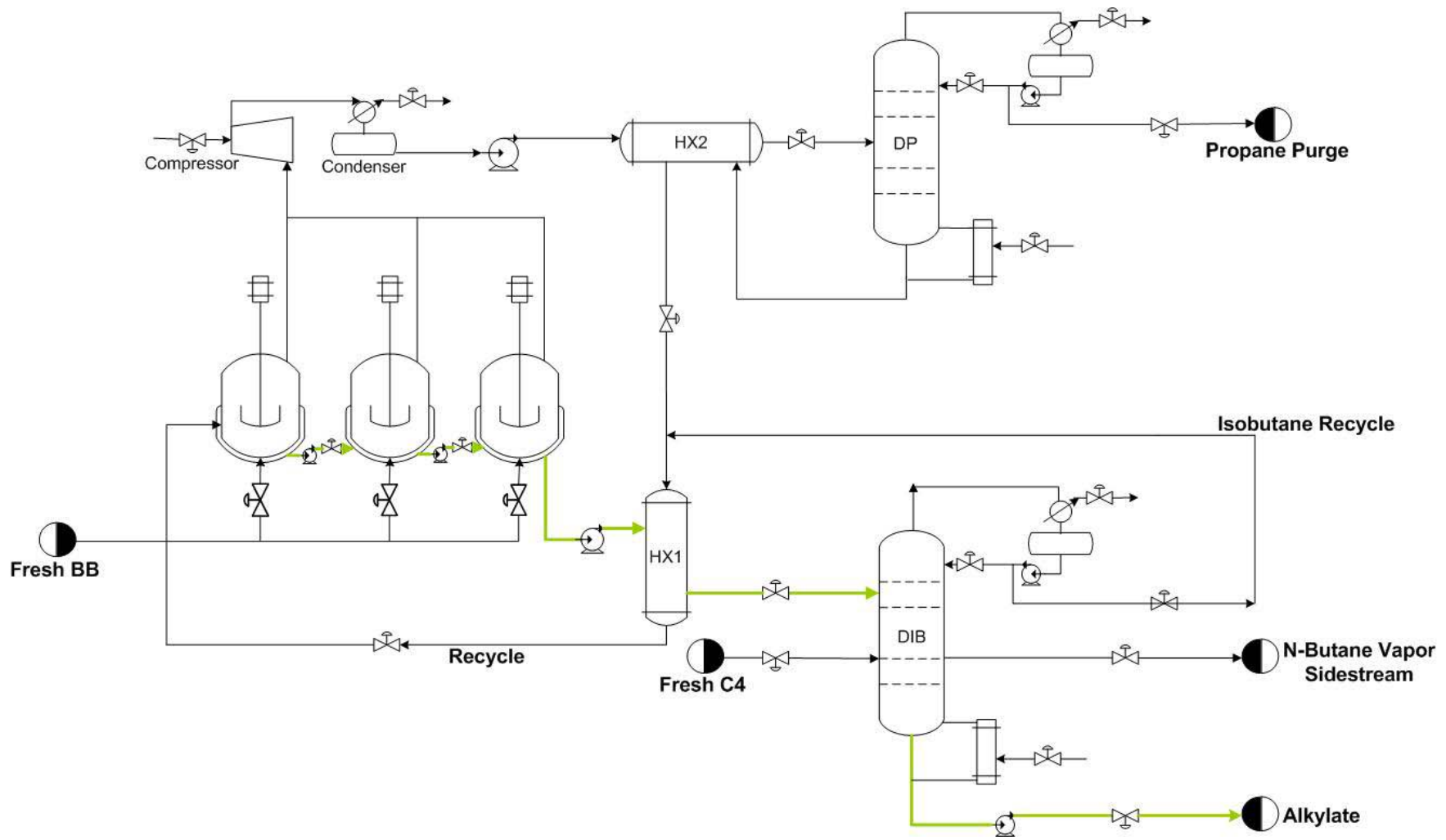
Figure 5.14 dodecane (C_{12}) pathways

Step 5: Find the most disturbed point and design the control loops to alleviate the effects of disturbances

In this study, $C_4^=$ composition composition, fresh BB feed flowrate and temperature changed has been tested at steady state conditions to the reaction and separation section. First, the $C_4^=$ composition of the fresh BB stream is increased from 50 to 55 mol% while the iC_4 composition is reduced from 20 to 15 mol%. Also, the opposite case where the iC_4 composition is increased from 20 to 25 mol% while the $C_4^=$ reduced from 50 to 45 mol% as shown in table 5.5. Second, the fresh BB feed flowrate is varied by 20% from its original values as shown in table 5.6. Last, the temperature of the fresh BB feed is varied 20 degree Fahrenheit (°F) to observe the effects of the changed to each unit operation, shown in table 5.7.

In addition, the fresh C_4 which entered the DIB column as a makeup feed is varied by changing its iC_4 composition, feed flowrate and temperature to study their effects on the DIB column as shown by table 5.8 to 5.10.

Table 5.5 Change in the fresh BB composition of butene ($C_4^=$)

Change	butene ($C_4^=$)	isobutane(iC_4)
increased	0.55	0.25
steady state	0.50	0.20
decresed	0.45	0.15

Table 5.6 Change in the fresh BB feed flow

Change	Fresh BB flow [lbmol/hr]
20%	120
Steady state (0%)	100
-20%	80

Table 5.7 Change in the fresh BB feed temperature

Change	Temperature [°F]
20 °F	140
Steady state (SS)	120
-20 °F	100

Table 5.8 Change in the fresh C_4 composition of isobutane (iC_4)

Change	isobutane (iC_4)	propane(C_3)
increased	0.55	0.00
Steady state	0.50	0.05
decresed	0.45	0.10

Table 5.9 Change in the fresh C_4 feed flow

Change	Fresh BB flow [lbmol/hr]
20%	73.2
Steady state (0%)	61.0
-20%	48.8

Table 5.10 Change in the fresh C_4 feed temperature

Change	Temperature [°F]
20 °F	140
Steady state (SS)	120
-20 °F	100

1. Effects on the Reaction Section

The studies of the effects of $C_4^=$ and iC_4 compositions changed on the reaction section (as shown by figure 5.15) shows that as the $C_4^=$ composition in the fresh BB feed increased, the conversion percentages of the main reaction which is the production of iC8 decreased. Where the changed of the fresh BB feed flowrate have small effects on the reaction section (shown in figure 5.15b). As the flowrate of the fresh BB feed increased, the iC_8 product increased referred to the rate law. As a result the conversion

percentages slightly increased. Another studies show that feed temperatures changed have insignificant effect on the reaction conversion. Since the compositions of $C_4^=$ has significant impacts on the conversion of the main reaction, therefore the $C_4^=$ composition in the fresh BB and recycle stream must be strictly control in the process.
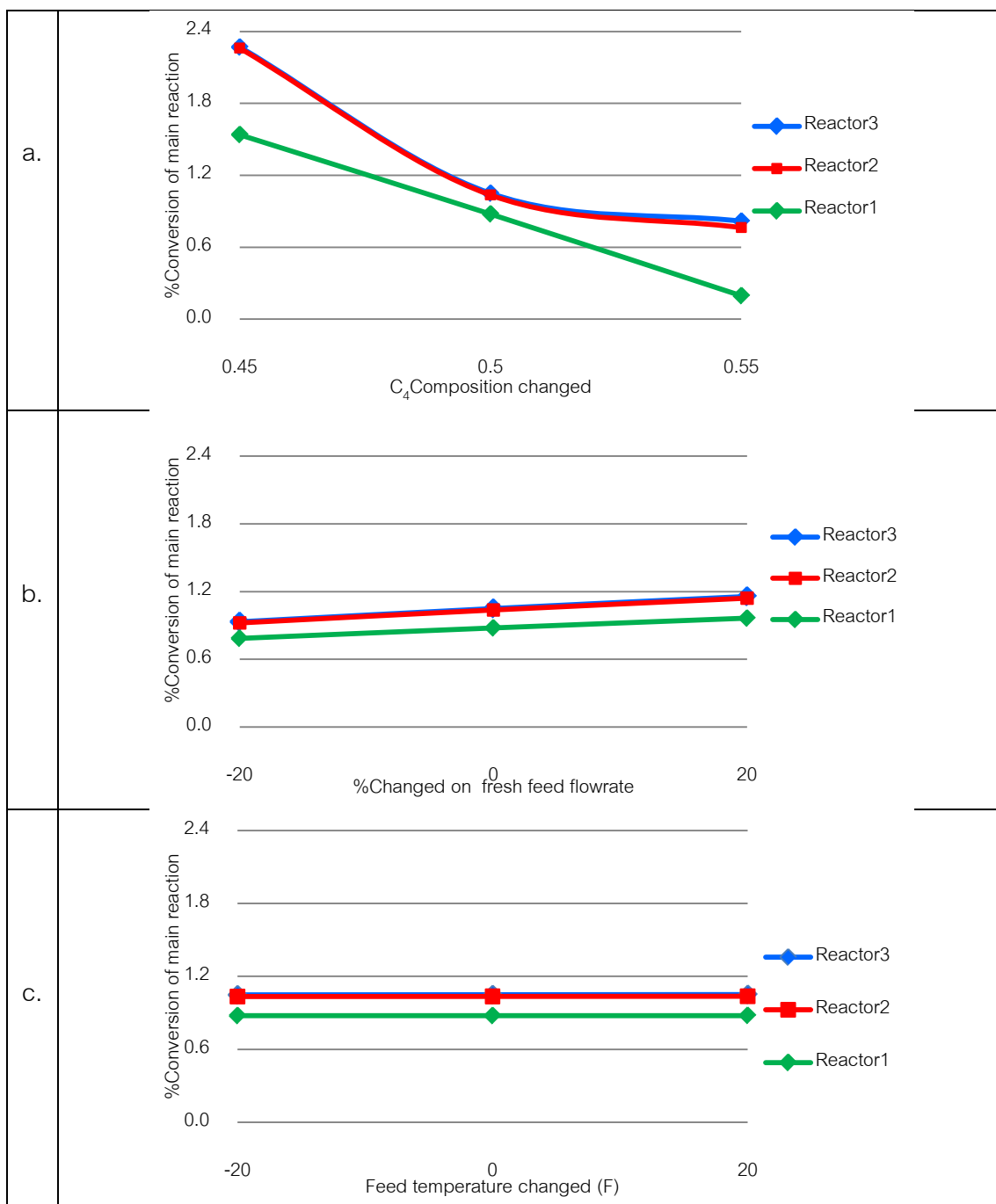
Figure 5.15 Percentage of the main reaction conversion in the reaction section when a.) $C_4^=$ composition, b.) Fresh C_4 feed flowrate and c.) Temperature changed.

2. Effects on the Separation Section

The distillation column with fixed reflux ratio and reboiler heat input is employed to study the effect on temperature profiles when $C_4^=$ compositions, fresh BB flowrate and feed temperature changed. The temperature control is used as the composition control because the direct compositions analyzers are expensive and unreliable so the criteria for selection of the best temperature control tray using the temperature profiles need to be considered.

2.1 Depropanizer Column (DP)

The temperature profiles of the DP column are shown in figure 5.16, where the steepest slope is found around tray 5 to 8. Hence tray 6 is selected to be use as the temperature control by manipulating the reboiler heat input in order to maintain the distillate product composition. The distillate flowrate is controlled by adjusting the flowrate according to reflux rate, which can be simplified as reflux ratio controller.

The temperature profile in figure 5.16a, show that the decreased in $C_4^=$ compositions results as decreasing in temperature profile. Figure 5.16b; show that the temperature profiles decreased when increasing or decreasing the fresh BB feed flowrate. Also the similar trends result in both cases when increasing or decreasing the feed's temperature, show as figure 5.16c.

The reason that the temperatures profiles remain their shape is because the condenser heat removal is manipulated to make up the heat in case that the reboiler heat input is fixed. The changes in the condenser heat removals are always contrary to the change of the fresh BB feed flowrate. Say that when the feed is increased, the condenser heat removal decreased.
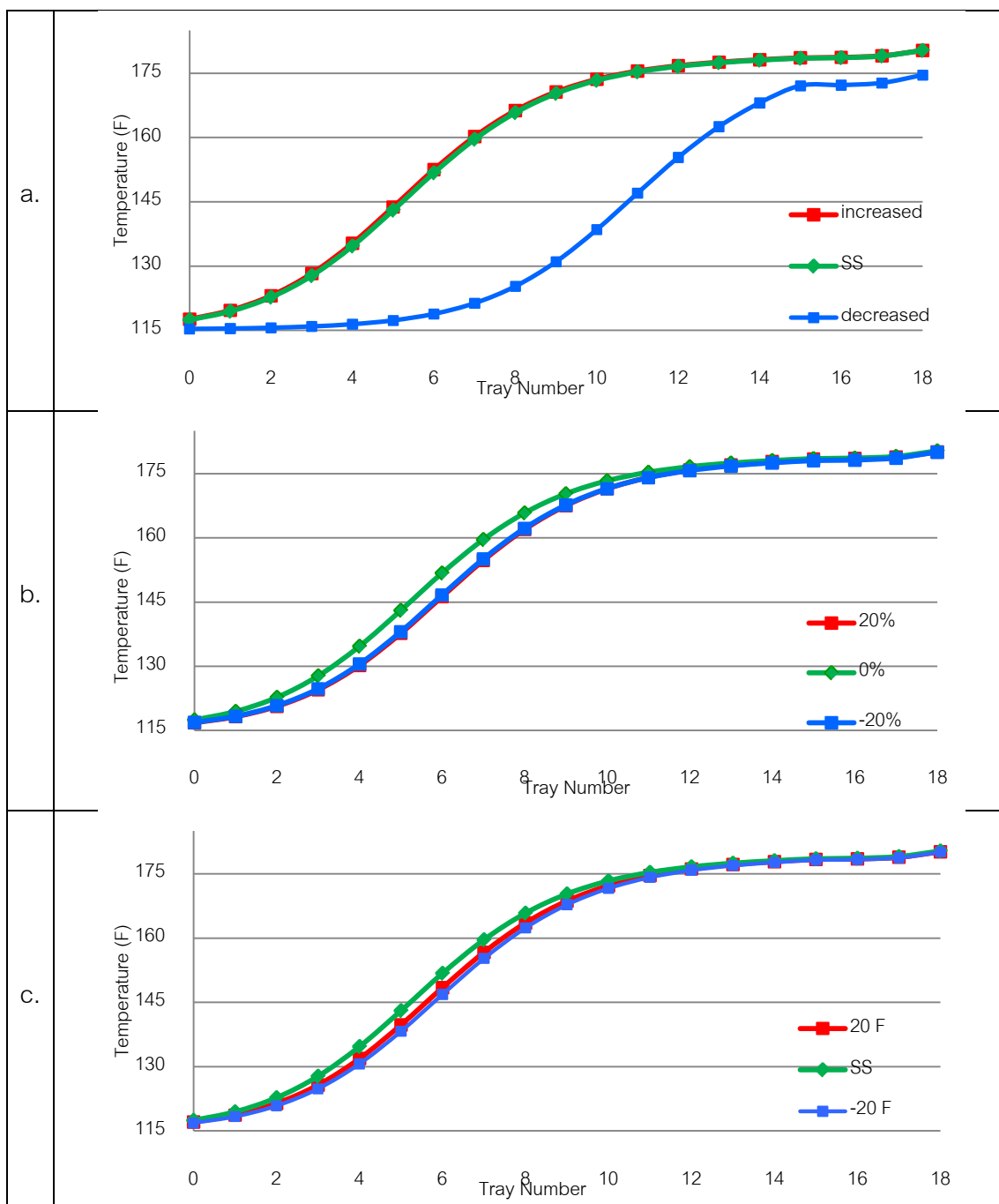
Figure 5.16 temperature profiles of the DP column when a.) $C_4^=$ composition,

b.) Fresh BB feed flowrate and c.) Temperature changed.

2.2 Deisobutanizer Column (DIB)

The effect of the $C_4^=$ compositions, the fresh BB feed flowrate and the feed temperature changed to the DIB column has been studies. Figure 5.17a, shows the slightly rises in temperature profiles as the $C_4^=$ decreased. By decreasing the fresh BB

flowrate, the temperature profile slightly decreased as shown in figure 5.17b. The feed temperature effects on the temperature profiles of the DIB column is shown in figure 5.17c, which are similar for both increasing and decreasing the feed temperature.
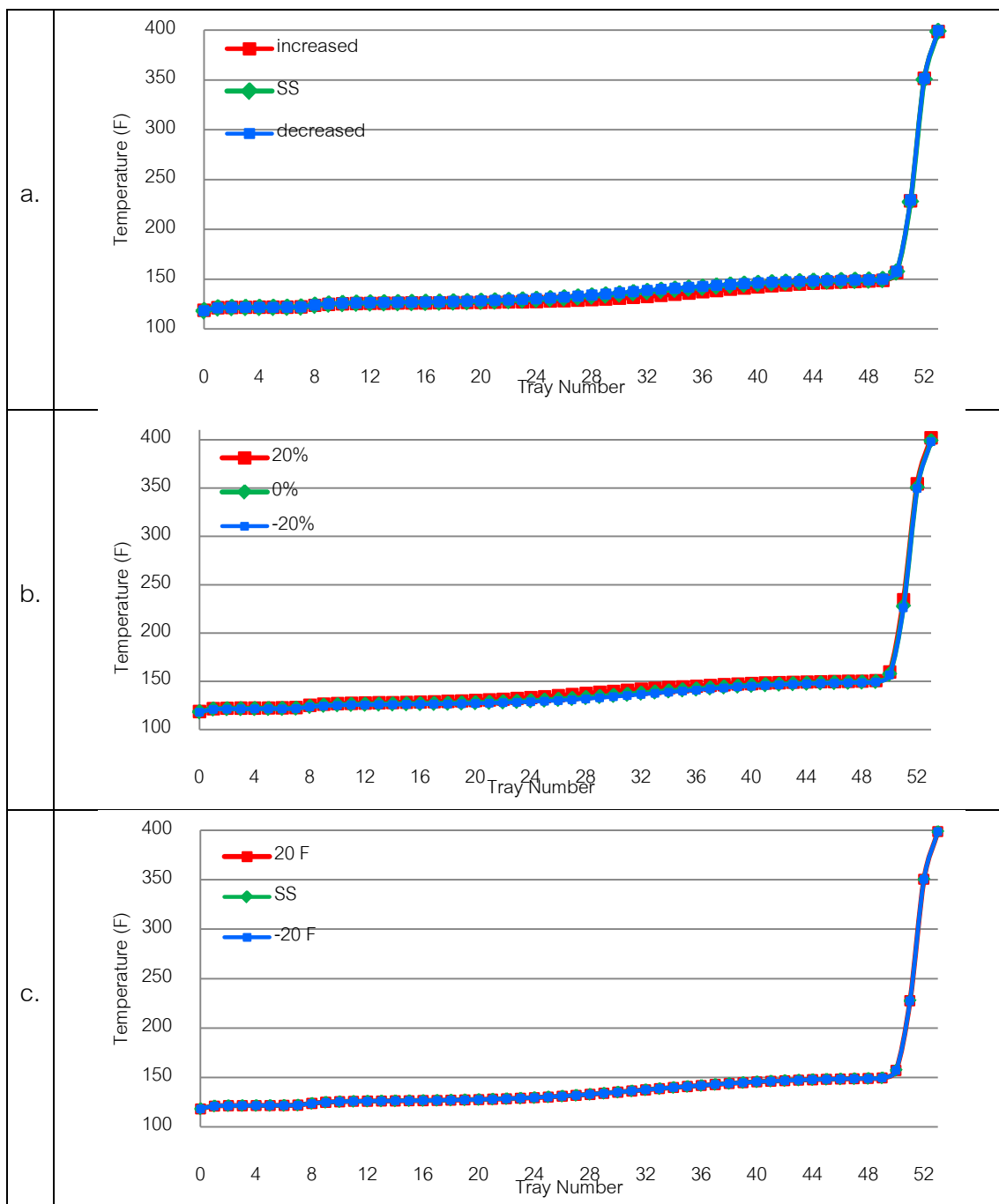
Figure 5.17 temperature profile of the DIB column when a.) $C_4^=$ composition, b.) Fresh BB feed flowrate and c.) Temperature changed.

Furthermore the effect of iC_4 compositions, flowrate and temperature changed of the makeup fresh C_4 feed to the DIB column inlet has been studies. Figure 5.18 gives out the similar temperatures profiles for three variation cases, therefore the fresh C_4 feed has a slight impact on the DIB column.
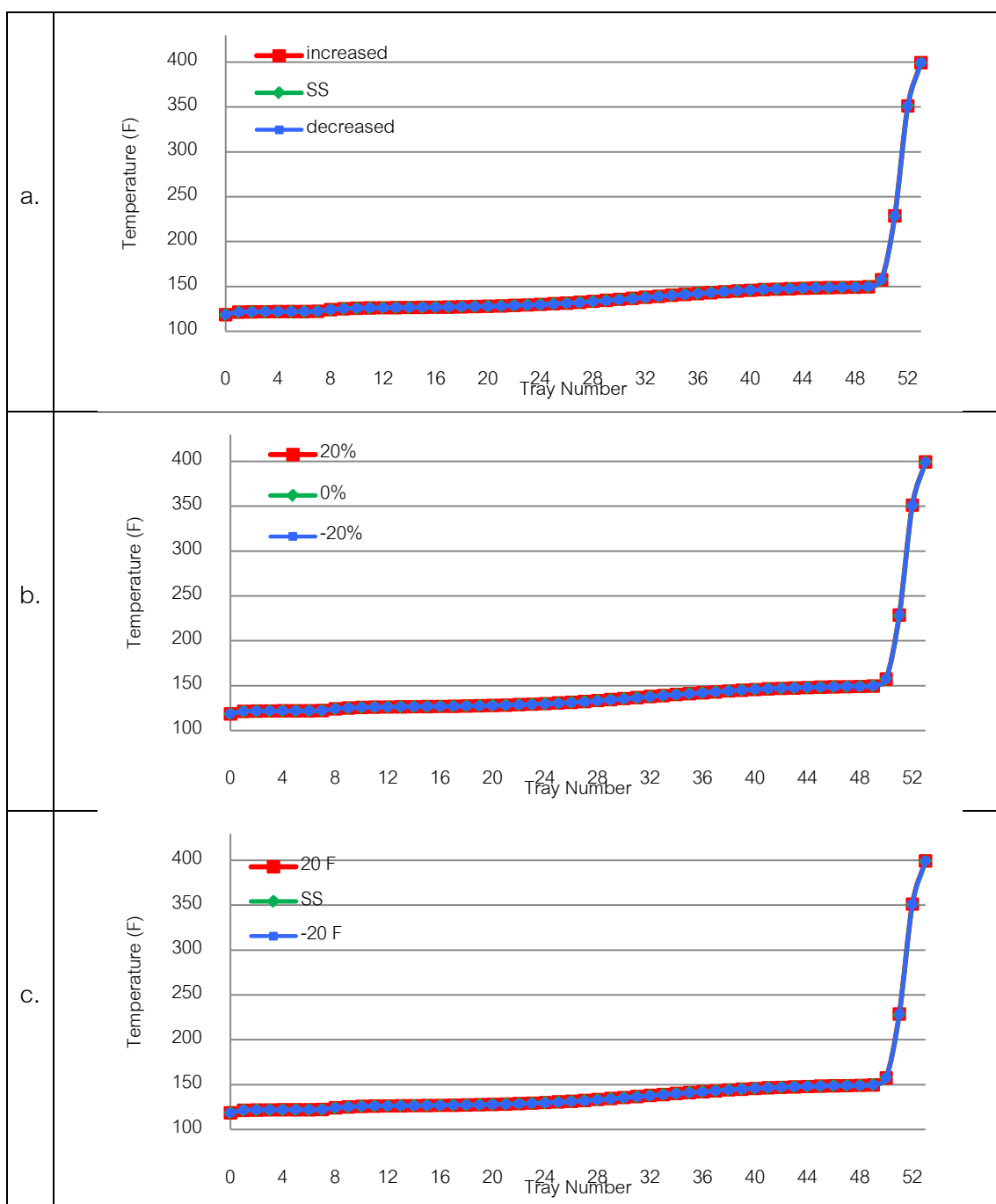
Figure 5.18 temperature profile of the DIB column when a.) iC_4 composition, b.) Fresh C_4 feed flowrate and c.) Temperature changed.

Step 6: Design the control loops for the rest of the control variables or adding enhanced controls, i.e. cascade, feed forward controls.

The inventory variables such as reactors liquid level, the refrigerant drum (condenser) liquid level and pressure are controlled by added up in this step. Moreover, the enhanced controls loops are employed in several positions that need to maintain the inventories or to observe the desired product composition. For instance, the ratio controllers are employed for the inlet flow control loops such as fresh BB feed. Fresh BB feed is flow controlled and split equally into three reactors by measuring the total BB flowrate and sends the signal to manipulate the valve of the first reactor. Then the multiplier is applied with 0.3333 constant and sending the output signals to manipulate the flow controllers which entering reactor 2 and 3. Also the recycle flow is controlled by the recycle-to-fresh BB ratio.

Another enhanced controlled arise in controlling structure of the DP column which has a high number of reflux ratio. Since, the distillate flow of the DP column has very small flow compared to the reflux flow; therefore the reflux flow is used to controlled liquid level in the reflux drum. The temperature measurement is employed to control the quality of the distillate composition (C_3). The single–end temperature control structure is applied with an appropriate tray chosen from previous step. The tray temperature is then controlled with reboiler heat input. The distillate flow is controlled by measuring the signal from the multiplier, which receiving the signal from both reflux flow and distillate composition, as shown by figure 5.19.
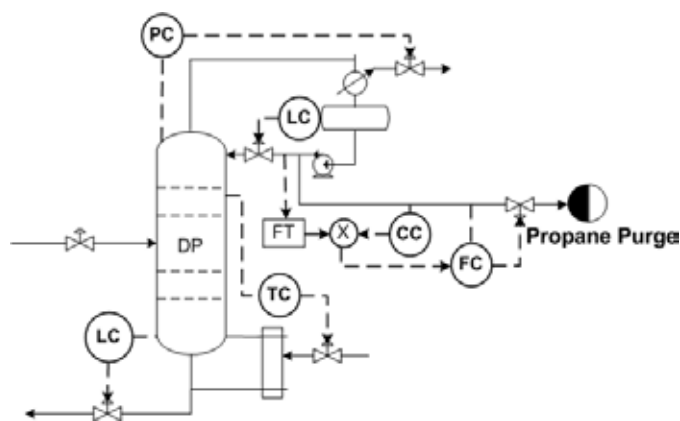
Figure 5.19 Depropanizer column control loops
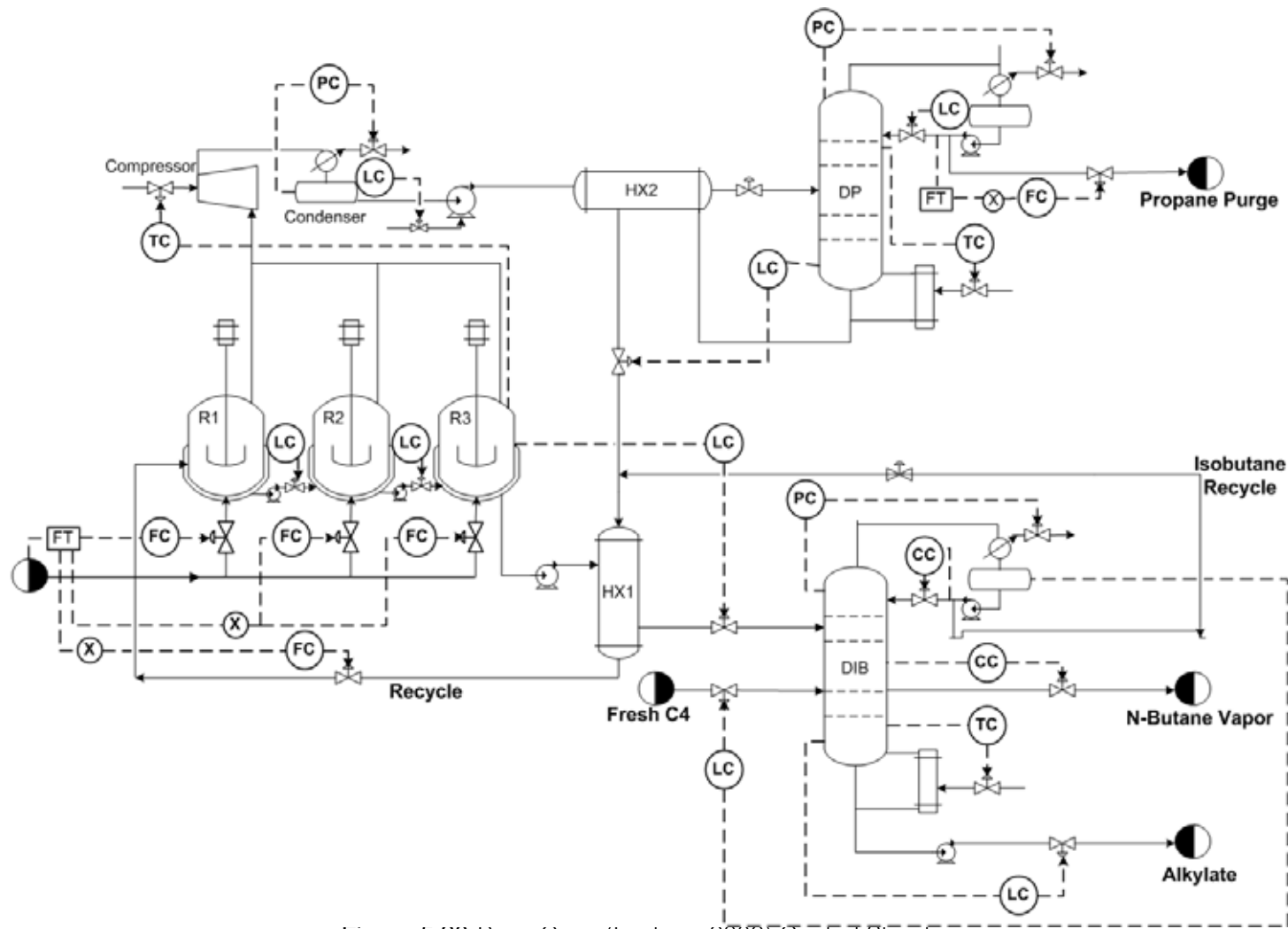
Figure 5.20 Base Case (Luyben, 2009) Control Structure

Table 5.11 Control structure lists of base case

Equipment	Control	Controlled variable	Manipulated variable	Type	Action
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse
BB 1	FC	Flow rate	BB1 flow rate	PI	Reverse
BB 2	FC	Flow rate	BB2 flow rate	PI	Reverse
BB 3	FC	Flow rate	BB3 flow rate	PI	Reverse
Reactor1 (R1)	LC	Liquid level	Liquid out flow	P	Direct
Reactor2 (R2)	LC	Liquid level	Liquid out flow	P	Direct
Reactor3 (R3)	LC	Liquid level	Liquid out flow	P	Direct
	TC	Reactor temperature	Compressor work	PID	Direct
Condenser	PC	Condenser pressure	Condenser duty	PI	Direct
	LC	Liquid level	Duty flowrate	P	Direct
Depropanizer	PC	Condenser pressure	Condenser duty	P	Direct
Column (DP)	TC	Temperature of tray 6	Reboiler duty	PID	Reverse
	FC	Reflux ratio	Distillate flowrate	PI	Reverse
	LC	Reflux drum level	Refux flowrate	P	Direct
	LC	Reboiler level	Bottom flowrate	P	Direct
Deisobutanizer)	PC	Top stage pressure	Condenser duty	P	Direct
Column (DIB	TC	Temperature of tray 52	Reboiler duty	PID	Reverse
	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct
	CC	Side stream (nC_4) purities	Side stream flowrate	PI	Direct
	LC	Reflux drum level	Fresh C_4 flowrate	P	Reverse
	LC	Reboiler level	Bottom flowrate	P	Direct

Figure 5.21 Control Structure 1 (CS1)

Table 5.12 Control structure lists of case 1 (CS 1)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse
BB 1	FC	Flow rate	Feed flow rate	PI	Reverse
BB 2	FC	Flow rate	Feed flow rate	PI	Reverse
BB 3	FC	Flow rate	Feed flow rate	PI	Reverse
Reactor1 (R1)	LC	Liquid level	Liquid out flow	P	Direct
Reactor2 (R2)	LC	Liquid level	Liquid out flow	P	Direct
Reactor3 (R3)	LC	Liquid level	Liquid out flow	P	Direct
	TC	Reactor temperature	Compressor work	PID	Direct
Condenser	PC	Condenser pressure	Condenser duty	PI	Reverse
	LC	Liquid level	Duty flowrate	P	Direct
Depropanizer	PC	Condenser pressure	Condenser duty	P	Direct
Column (DP)	TC	Temperature of tray 6	Reboiler duty	PID	Reverse
	FC	Distillate to reflux flowrate	Distillate flowrate	PI	Reverse
	CC	Propane (C_3) Composition	Distillate to reflux flowrate set point	PID	Direct
	LC	Reflux drum level	Refux flowrate	P	Direct
	LC	Reboiler level	Bottom flowrate	P	Direct
Deisobutanizer	PC	Condenser pressure	Condenser duty	P	Direct
Column (DIB)	TC	Temperature of tray 52	Reboiler duty	PID	Reverse
	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct
	TC	Temperature of tray 49	Side stream flowrate	PID	Direct
	LC	Reflux drum level	Fresh C_4 flowrate	P	Reverse
	LC	Reboiler level	Bottom flowrate	P	Direct
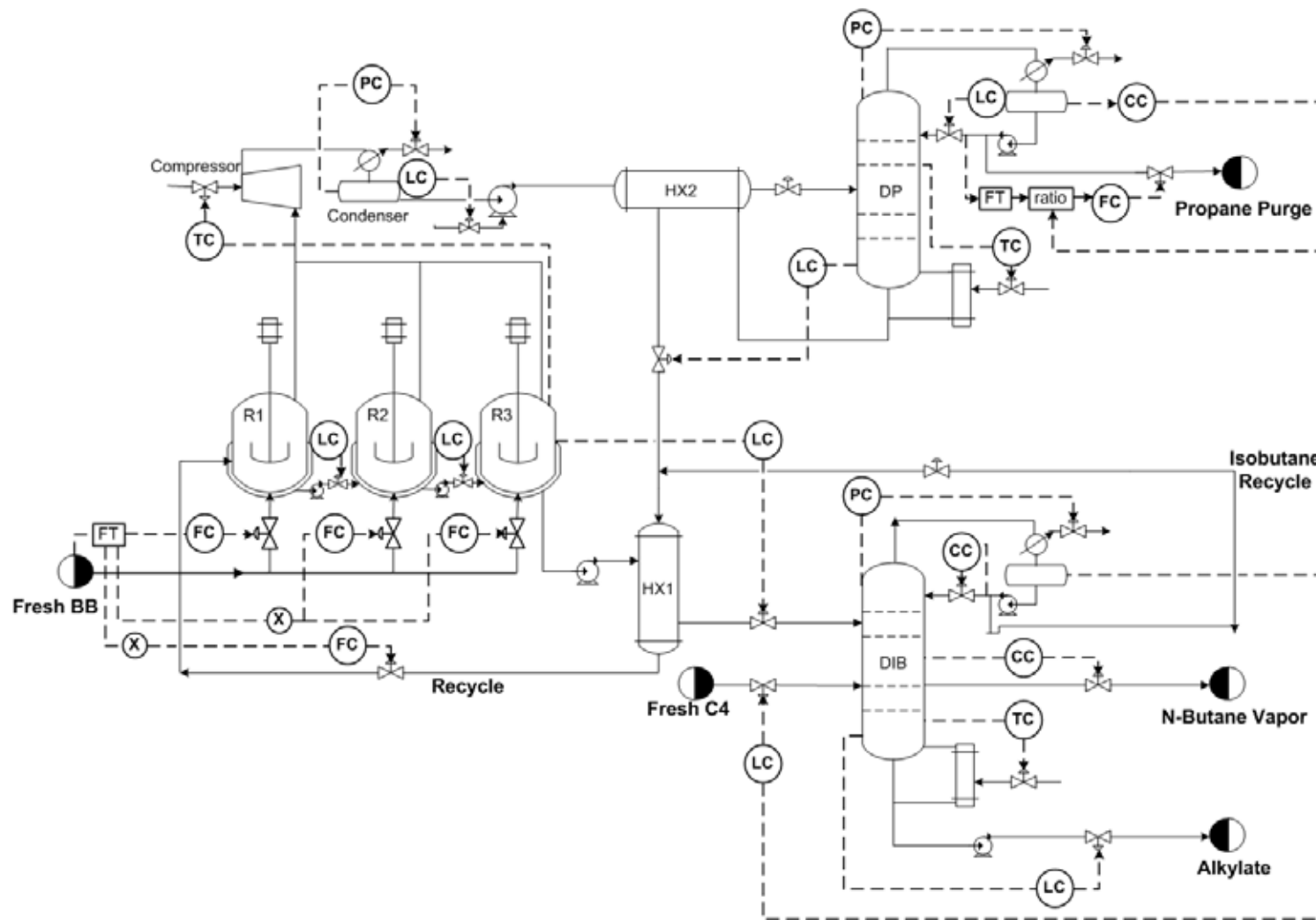
Figure 5.22 Control Structure 2 (CS2)

Table 5.13 Control structure lists of case 2 (CS 2)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse
BB 1	FC	Flow rate	Feed flow rate	PI	Reverse
BB 2	FC	Flow rate	Feed flow rate	PI	Reverse
BB 3	FC	Flow rate	Feed flow rate	PI	Reverse
Reactor1 (R1)	LC	Liquid level	Liquid out flow	P	Direct
Reactor2 (R2)	LC	Liquid level	Liquid out flow	P	Direct
Reactor3 (R3)	LC	Liquid level	Liquid out flow	P	Direct
	TC	Reactor temperature	Compressor work	PID	Direct
Condenser	PC	Condenser pressure	Condenser duty	PI	Reverse
	LC	Liquid level	Duty flowrate	P	Direct
Depropanizer	PC	Condenser pressure	Condenser duty	P	Direct
Column (DP)	TC	Temperature of tray 6	Reboiler duty	PID	Reverse
	FC	Reflux ratio	Distillate flowrate	PI	Reverse
	CC	Propane (C_3) Composition	Distillate to reflux flowrate set point	PID	Direct
	LC	Reflux drum level	Reflux flowrate	P	Direct
	LC	Reboiler level	Bottom flowrate	P	Direct
Deisobutanizer	PC	Condenser pressure	Condenser duty	P	Direct
Column (DIB)	TC	Temperature of tray 52	Reboiler duty	PID	Reverse
	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct
	CC	Side stream (nC_4) purities	Side stream flowrate	PI	Direct
	LC	Reflux drum level	Fresh C_4 flowrate	P	Reverse
	LC	Reboiler level	Bottom flowrate	P	Direct

Step 7: Optimize economics and improve control performance

To control the performance of the process, the proportional integral derivative (PID) controllers are employed to control all quality loops, which are temperature of reactor 3, tray temperature of the depropanizer (DP) and deisobutanizer (DIB) column, the side stream tray temperature, the nC_4 side stream composition and the propane (C_3) composition. The relay-feedback testing is used to design a controller. The ultimate gain (K_u) and ultimate frequency (P_u) from Tyreus-Luyben tuning methods is exerted.

The proportional integral (PI) controllers are usually used in the pressure loops. And all the liquid level loops in the process used the proportional (P) controllers. The gains of the P controllers are equal to 2 except for the DP reflux drum level as a result of using the reflux flow to control level.

Step 8: Validate the designed control structures by rigorous dynamic simulation

The new control structures (CS 1 and CS 2) design using Wongsri design procedure are test with fresh BB feed flow, feed temperature and $C_4^=$ composition changed. The responses of the entire process are shown as a graph plotted versus operates time (15 hours). The solid lines are for an increased in the disturbances and the dashed lines are for a decreased in the disturbances. The responses of each structure are shown as;

a) Fresh BB feed flowrate   unit: (lbmol/hr)

b) Fresh C4 feed flowrate   unit: (lbmol/hr)

c) Recycle flowrate   unit: (lbmol/hr)

d) Reactor 3 temperature   unit: (°F)

e) Alkylate flowrate   unit: (lbmol/hr)

f) (iC_8) Alkylate composition

g) Side stream flowrate   unit: (lbmol/hr)

h) (nC_4) Side stream composition

i) Propane purge flowrate   unit: (lbmol/hr)

j) (C_3) Propane purge composition

1. Fresh BB feed flow change

The fresh BB feed is varied by changing the set point value of the fresh feed controller by 5% from normal value of 100 lbmol/hr to 95 lbmol/hr and 105 lbmol/hr. The changed start after a period of 1 hour at the normal value, as shows in table 15, responses of variables disturbed by fresh BB feed flow changed. The temperature of reactor 3 can handled the disturbances after operating times of 5 hours for all control structures. The alkylate product composition and flowrate at the deisobutanizer (DIB) column are controlled after 7.5 hours after operating times for basecase control structure, but only 5 hours sre used for the control structure 1 and 2 (CS 1 and CS 2). While the side stream (nC_4) composition could not reached the set point after operating for 15 hours. But after operating for 20 hour it will reach the new set point. Result from using the temperature measurement instead of the composition measurement.

The propane purge flow is smoothly controlled after an operated time of 10 hours. Whither, the propane (C_3) composition is strictly controlled for control structure 1 and 2, as a result of the cascade control.

Table 5.14 Dynamic responses with fresh BB feed changed.
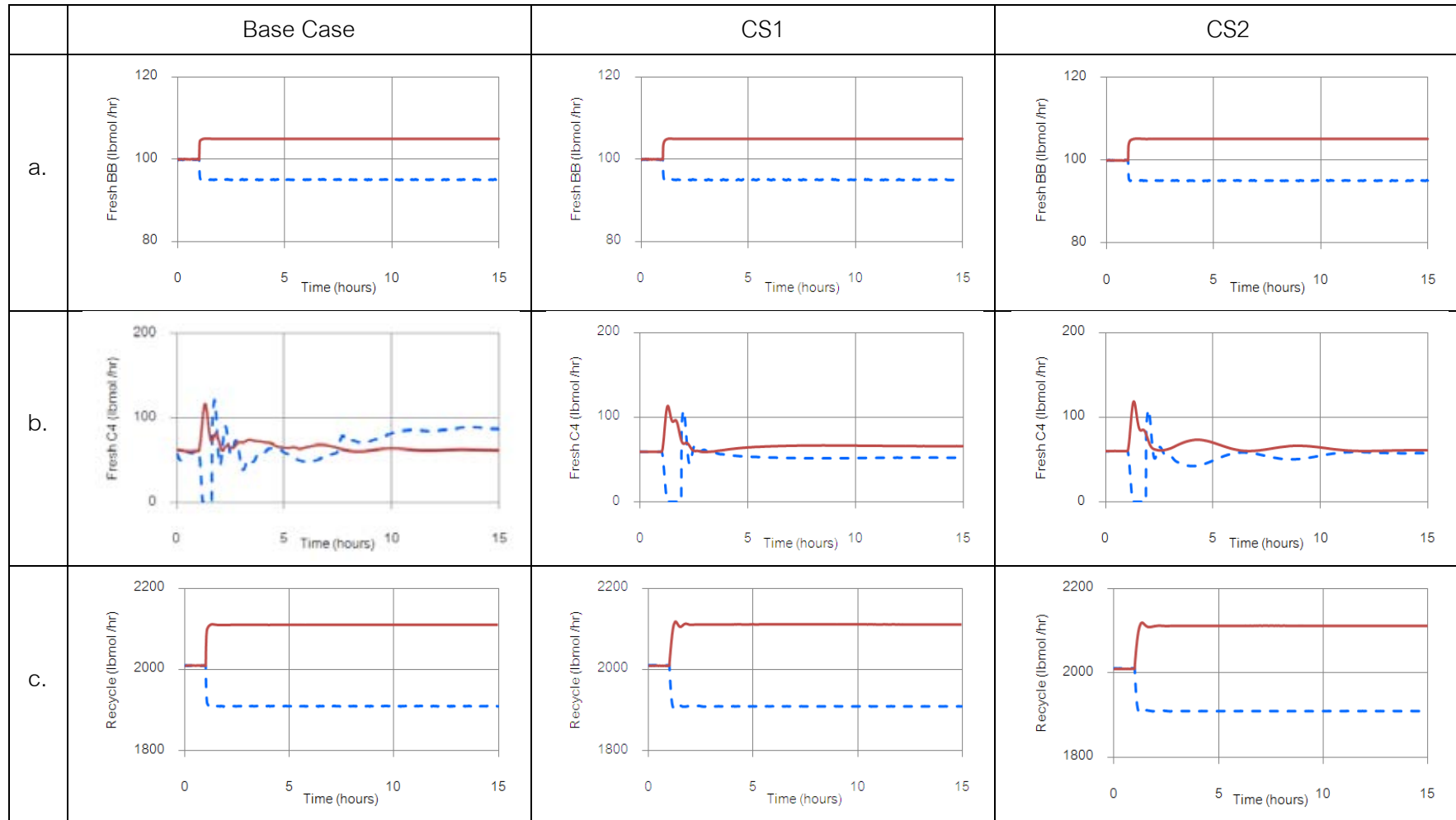
	Base Case	CS1	CS2
a.			
b.			
c.			

Table 5.14 (Continue) Dynamic responses with fresh BB feed changed.

	Base Case	CS1	CS2
d.			
e.			
f.			

Table 5.14 (Continue) Dynamic responses with fresh BB feed changed.

	Base Case	CS1	CS2
g.			
h.			
i.			

Table 5.14 (Continue) Dynamic responses with fresh BB feed changed.

	Base Case	CS1	CS2
j.			
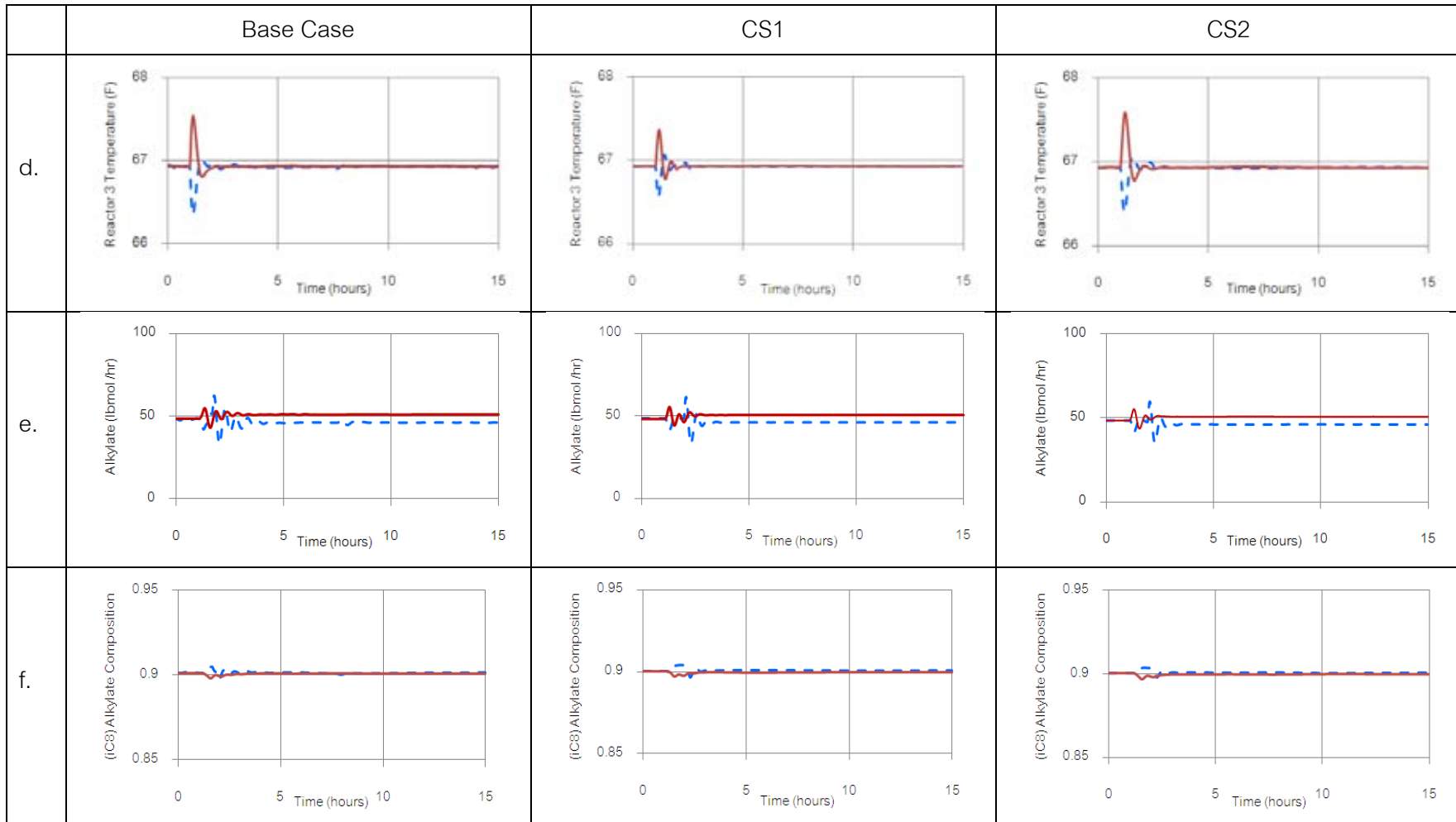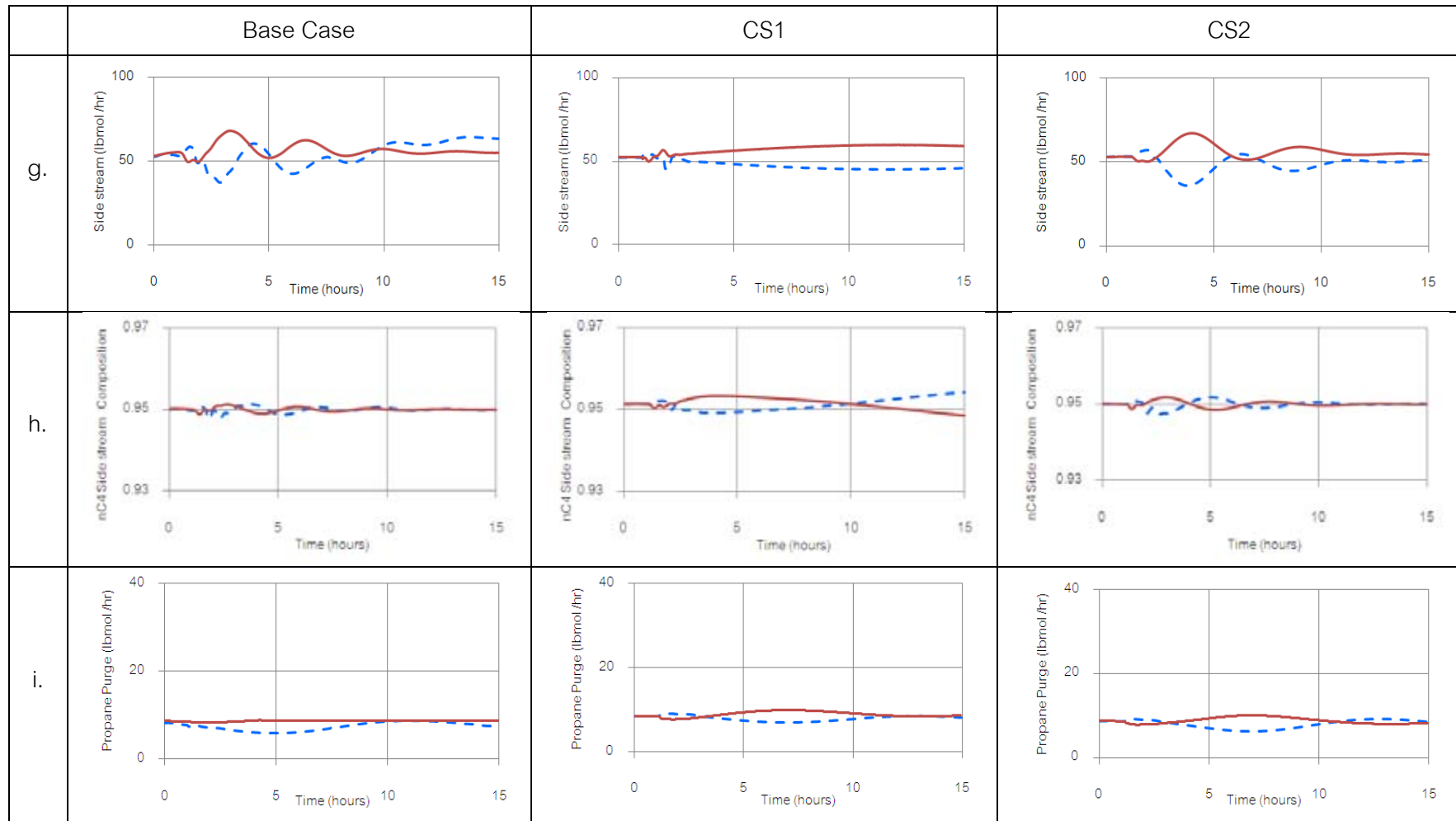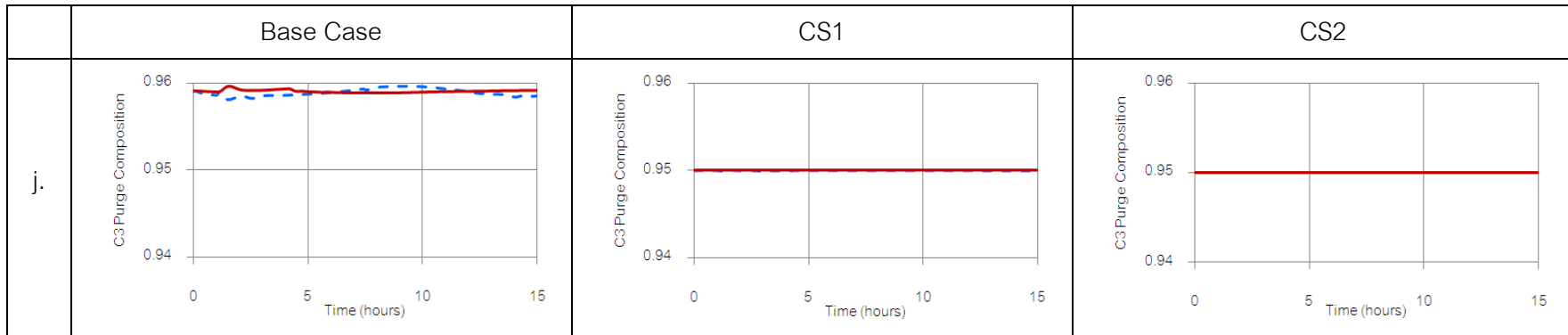
2. $C_4^=$ composition changed

The 1-butene ($C_4^=$) composition is changed from 50 to 55 mol% while the iC_4 composition is reduced from 20 to 15 mol%. Also, the opposite case where the iC_4 composition is increased from 20 to 25 mol% while the $C_4^=$ reduced from 50 to 45 mol% are disturbed to measured the process responds.

The makeup fresh C_4 feed are fluctuated in first 5 hours to maintain the recycle stream quantity before reaching its new setting point. The alkylate product purity (iC_8), side stream purity (nC_4) and the propane (C_3) purge purity of CS2 are smoothest of them all. Note that a changing in the side stream (nC_4) composition occurred from using the temperature controller to imply the composition. Where the propane (C_3) composition of control structure 1 and 2 are strictly uniform which is result from the cascade control of the composition and distillate flow.

Table 5.15 Dynamic responses with $C_4^=$ composition changed.
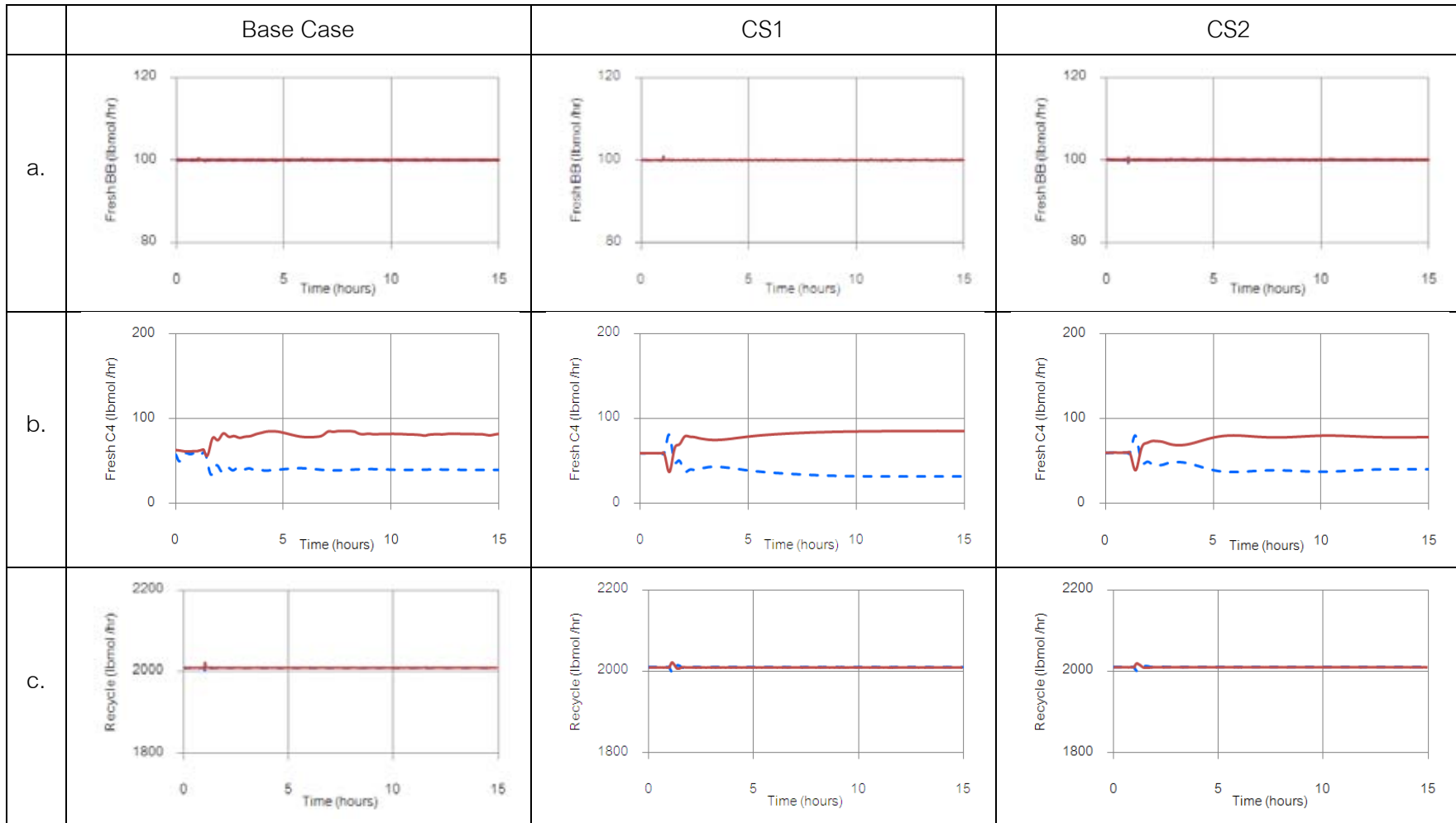
	Base Case	CS1	CS2
a.			
b.			
c.			

Table 5.15 (Continue) Dynamic responses with $C_4^=$ composition changed.

	Base Case	CS1	CS2
d.			
e.			
f.			

Table 5.15 (Continue) Dynamic responses with $C_4^=$ composition changed.
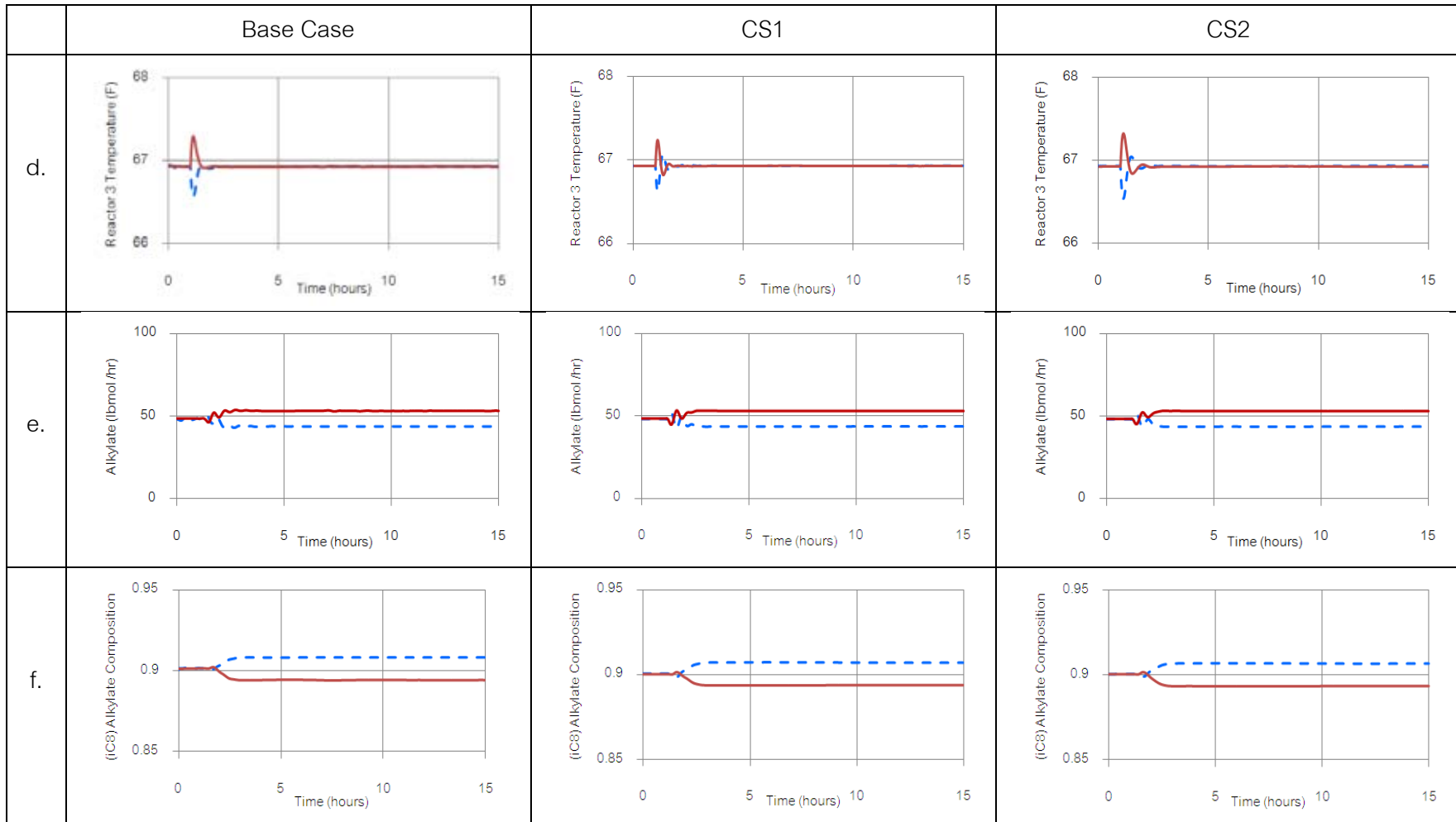
	Base Case	CS1	CS2
g.			
h.			
i.			
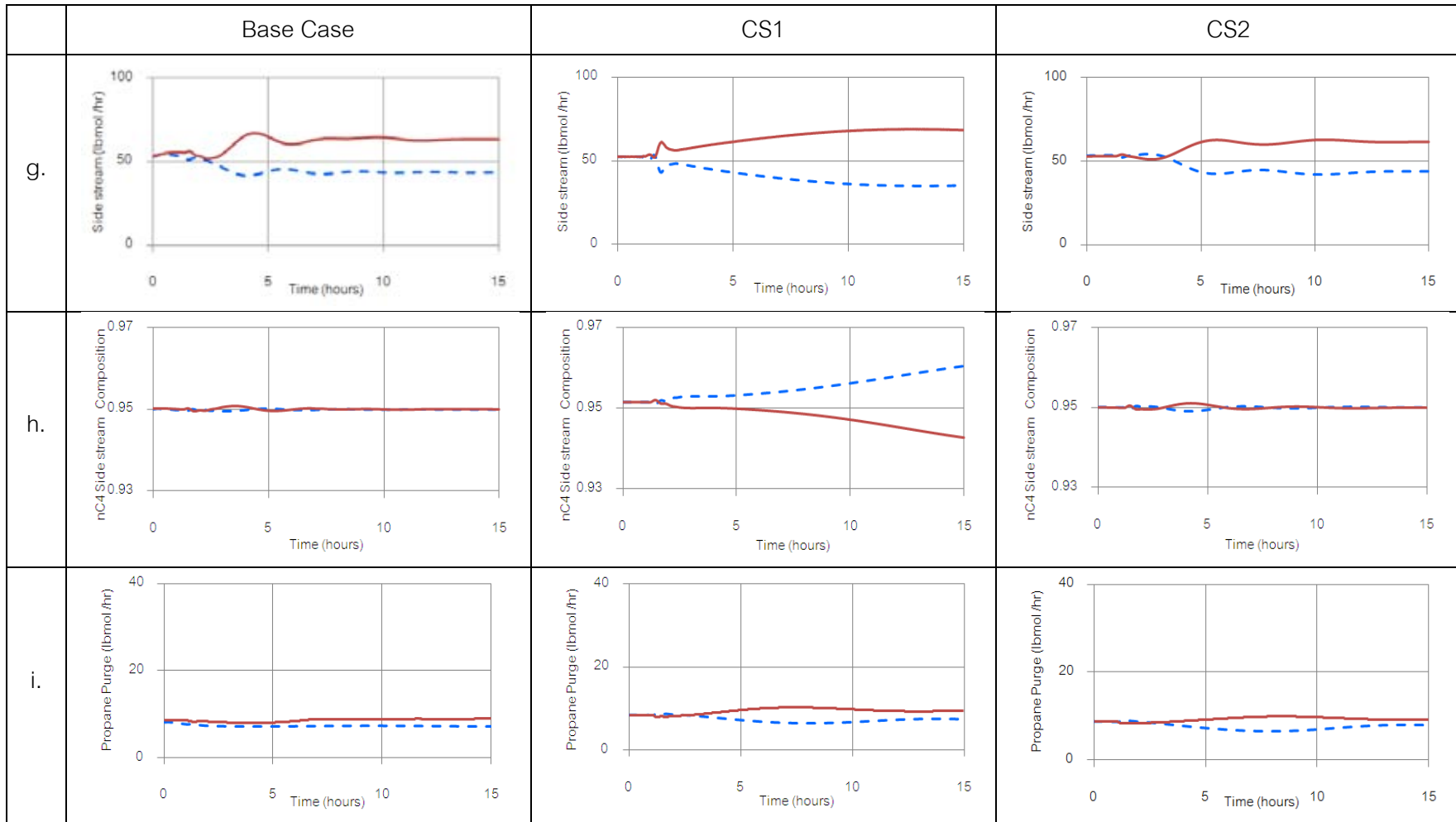
Table 5.15 (Continue) Dynamic responses with $C_4^=$ composition.

	Base Case	CS1	CS2
j.			

3. Feed temperature changed

Feed temperature is varied by 5 degree Fahrenheit from 120 °F to 115 °F and 125 °F. The side stream flow of the base case control structure reached its setting point after 10 hours of operating times. While the side streams flow of the other two control structures can reach their settling point right after 5 hours of operating times.

Table 5.16 Dynamic responses with feed temperature changed.
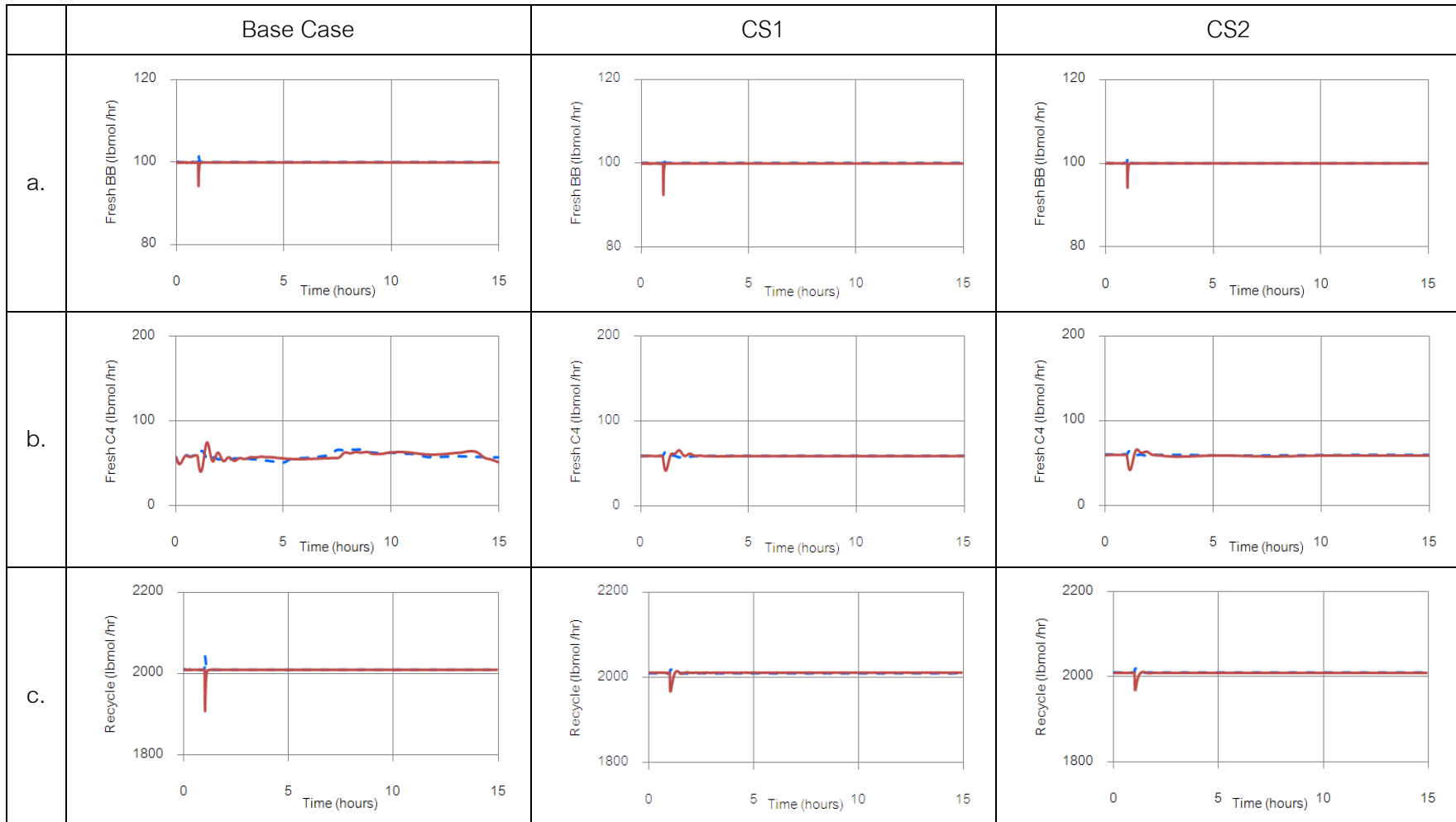
	Base Case	CS1	CS2
a.			
b.			
c.			

Table 5.16 (Continue) Dynamic responses with feed temperature changed.

	Base Case	CS1	CS2
d.			
e.			
f.			

Table 5.16 (Continue) Dynamic responses with feed temperature changed.

	Base Case	CS1	CS2
g.			
h.			
i.			

Table 5.16 (Continue) Dynamic responses with feed temperature changed.

	Base Case	CS1	CS2
j.			
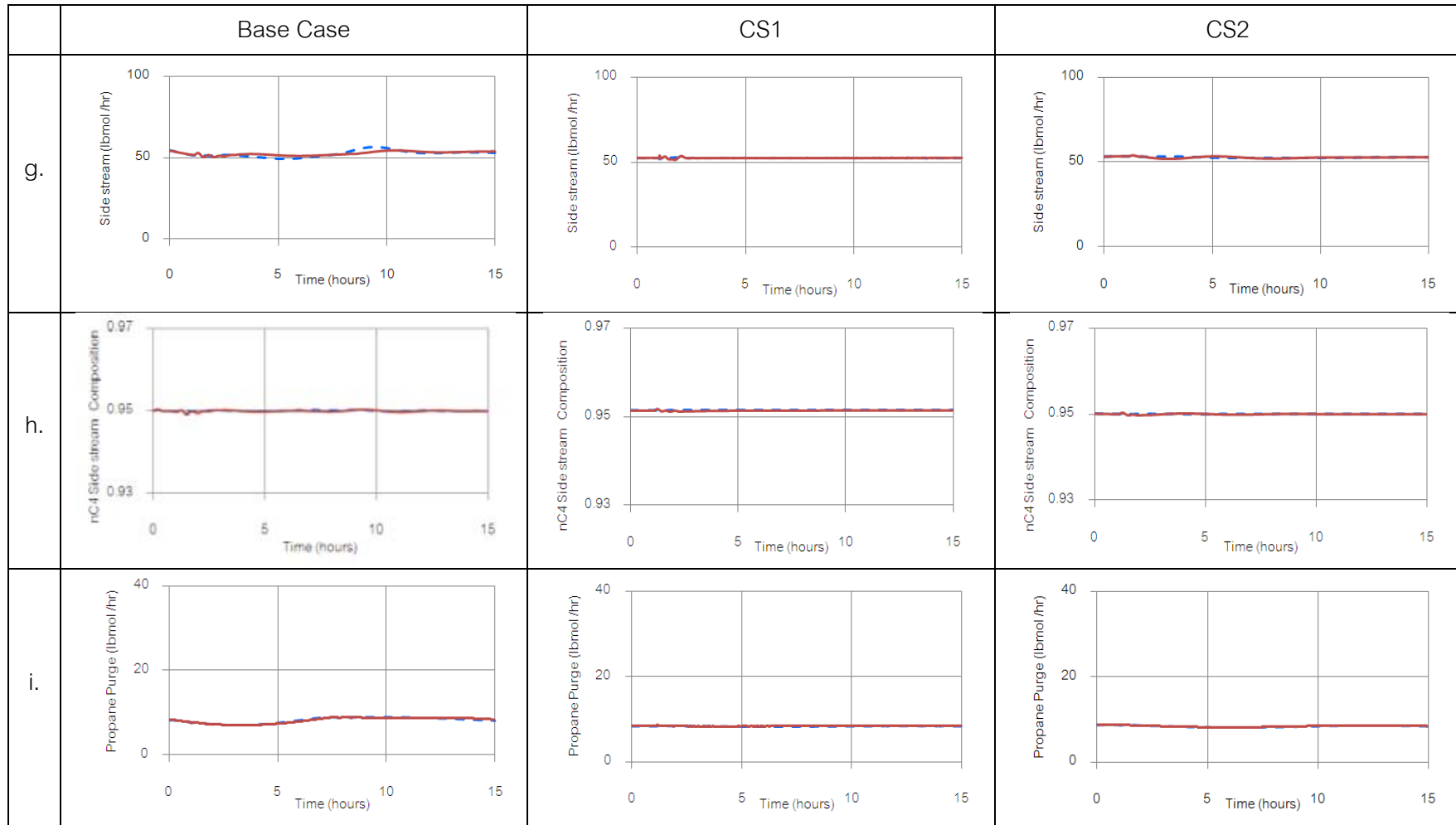
Furthermore, the temperature controller on tray 49 of the DIB column of control structure 1 (CS 1) has been studied. Table 5.17 shows that the temperature of the side stream began to reach its setting point after 30 hours of operating times. The (nC_4) composition of the side stream cannot be controlled when the feed composition is changed due to the limitation of the temperature on the boiling point of each composition, as shown in table 5.18 where a) Represent the dynamic responses when feed flow changed; b) represent the dynamic responses when feed composition (nC_4) changed and c) represent the dynamic responses when feed temperature changed.

Table 5.17 Dynamic responses of the DIB column tray 49 temperature

	Base Case	CS1	CS2
a			
b			
b			
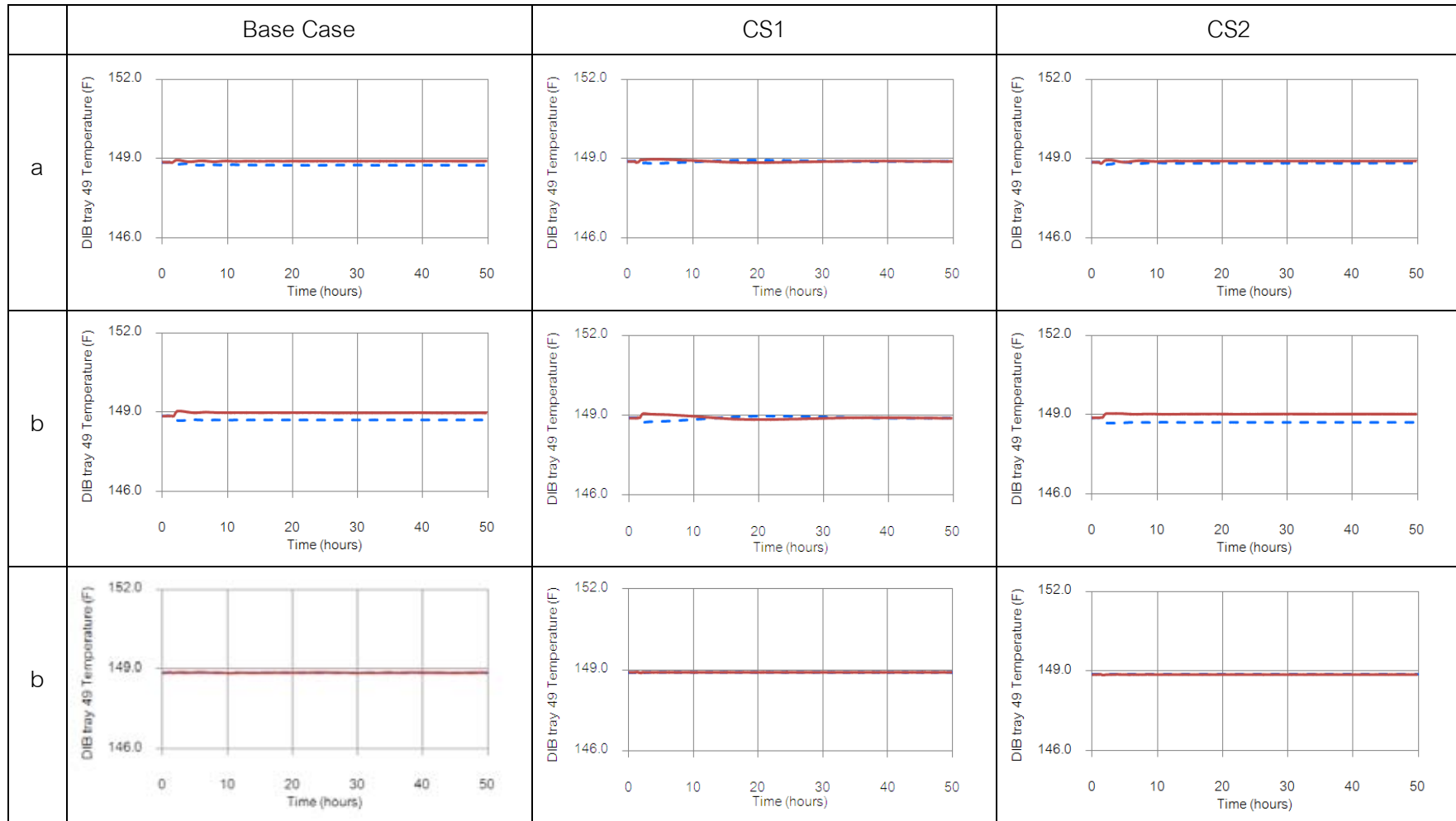
Table 5.18 Dynamic responses of the side stream (nC_4) composition of the control structure 1 (CS 1)
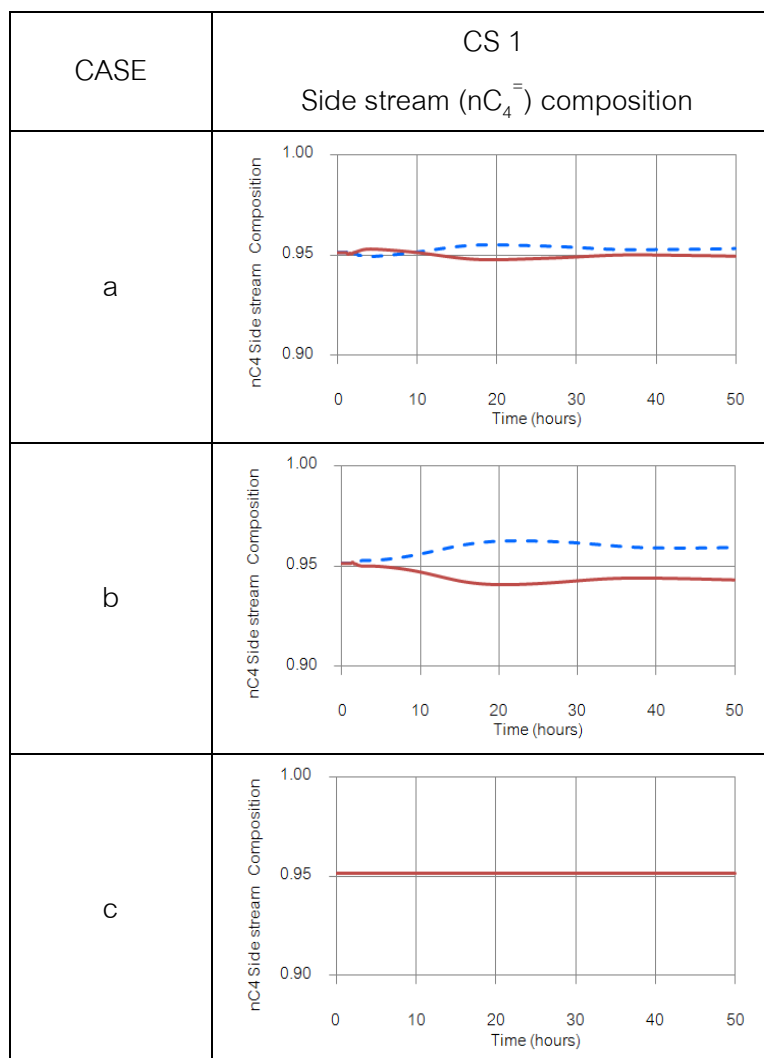
CASE	CS 1 Side stream ($nC_4^=$) composition
a	
b	
c	

a) Represent the dynamic responses when feed flow changed; b) represent the dynamic responses when feed composition (nC_4) changed and c) represent the dynamic responses when feed temperature changed

5.2 IAE analysis

The Integral absolute error (IAE) is used as a control structure performance measurement when various types of disturbances are tested. The value is sum by the error above and below the set point, with all treated as positive, over the period time. The IAE analysis of temperature and pressure loop is consider as a safety loop while composition is considered as a quality loop. In order to have smooth and stable operation, the safety loop is significantly important. Therefore, the finest control structure is chosen from the smallest IAE value. Table 5.19 to 5.21 shows the IAE value of each control structures which has been disturbed by several type of disturbances. From the data given can be summarized that the control structure 2 (CS 2) has the smallest IAE value.

Table 5.19 IAE of safety control loop with fresh feed changed.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.078703	0.018332	0.316496	0.413531
CS1	0.201285	0.011172	0.067699	0.280157
CS2	0.215340	0.012157	0.035308	0.262805

Table 5.20 IAE of safety control loop with feed $C_4^=$ composition changed.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.074800	0.007000	0.491080	0.572880
CS1	0.136041	0.007000	0.283593	0.426634
CS2	0.154086	0.006912	0.180324	0.341322

Table 5.21 IAE of safety control loop with feed temperature changed.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.089628	0.020060	0.378415	0.488103
CS1	0.024431	0.003620	0.058424	0.086475
CS2	0.041746	0.002618	0.015500	0.059864

5.3 Utilities cost

The process utilities include cooling water, heated water, compressed air, refrigerants and electricity. The prices of each utility are given as followed:

- Cooling water $0.354 per GJ
- Low pressure stream $6.08 per GJ
- Electricity $16.8 per GJ (to convert to $/kWh multiplied with 0.0036)

Note that all cost are in unit of million $ per year. Table 23 to 25 shows the utilities cost of each control structure when facing various type of disturbances.

Table 5.20 Utilities cost with fresh feed changed.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	m$/year	GJ	m$/year	kWh	m$/year	
Base case	181993.6	0.0644	171449.1	1.0424	6417.51	0.1078	1.2147
CS1	171917.1	0.0609	166487.5	1.0122	6168.70	0.1036	1.1767
CS2	171279.2	0.0606	166499.3	1.0123	6174.66	0.1037	1.1767

Table 5.21 Utilities cost with feed $C_4^=$ composition changed.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	m$/year	GJ	m$/year	kWh	m$/year	
Base case	194888.3	0.0690	169382.1	1.0298	6405.70	0.1076	1.2064
CS1	178111.3	0.0631	166567.1	1.0127	6087.61	0.1023	1.1781
CS2	173966.6	0.0616	166573.0	1.0128	6092.40	0.1024	1.1767

Table 5.22 Utilities cost with feed temperature changed.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	m$/year	GJ	m$/year	kWh	m$/year	
Base case	198382.7	0.0702	168861.9	1.0267	6442.76	0.1082	1.2051
CS1	171599.7	0.0607	166548.3	1.0126	6065.26	0.1019	1.1753
CS2	171262.2	0.0606	166513.3	1.0124	6071.51	0.1020	1.1750

From the utilities cost table results that for the fresh feed, feed $C_4^=$ composition, and feed temperature changed, the smallest utilities cost belongs to case CS2 followed by case CS1 and base case. As a result, base case has the highest utilities cost when facing all types of disturbances, though, case CS 2 has the smallest utilities cost.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The new plantwide control structures design procedure of Wongsri has been applied to design the control structures for an auto-refrigerated alkylation process. The 8 steps procedure is straightforward and can be catch up easily even for those who is not in the control field. The performance of each structure is evaluated by the IAE value to find the most handle and controllable control structure interrupts by the disturbances. The control structure 2 (CS2) proven to be the finest structure by the IAE and cost of utilities. The designed control of the auto-refrigerated alkylation process should be further established since the control structure 1 which employed the temperature measurement to infer the compositions could not be able to handle various types of disturbances. For that reason, the composition controller is much stiffer.

6.2 Recommendation

The recommendation for further study can be done by focusing on the control structures of the high reflux ratio column. Also, bypassing the heat exchangers in the process, evaluate the IAE and the utilities cost compared to the normal control structure. Bypassing the heat exchanger should leads to minimizing the heat exchanger and by pass control valve size.

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APPENDICES

APPENDIX A

PROCESS STREAMS AND EQUIPMENTS DATA

Table A.1 Streams Data

Stream	Fresh BB	BB1	BB2	BB3	Total Recycle	Total 1
Flow (lbmol/hr)	100.00	33.33	33.33	33.33	2010.0	2043.33
Temperature (°F)	120.00	120.00	120.00	120.00	103.50	64.20
Pressure (psia)	84.41	84.41	84.41	84.41	106.30	43.42
Mole fraction						
C_3	0.0500	0.0500	0.0500	0.0500	0.0850	0.0844
iC4	0.2000	0.2000	0.2000	0.2000	0.8788	0.8677
C4=	0.5000	0.5000	0.5000	0.5000	0.0008	0.0090
nC4	0.2500	0.2500	0.2500	0.2500	0.0354	0.0389
iC8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table A.1 (Continued) Streams Data

Stream	Vapor 1	Liquid 1	Total 2	Vapor 2	Liquid 2	Total 3
Flow (lbmol/hr)	395.80	1631.00	1664.00	69.92	1578	1611
Temperature (°F)	64.90	64.90	65.06	65.85	65.85	66.09
Pressure (psia)	43.42	43.42	43.36	43.36	43.36	43.36
Mole fraction						
C_3	0.1570	0.0677	0.0673	0.1513	0.0643	0.0640
iC4	0.8143	0.8797	0.8660	0.8158	0.8675	0.8537
C4=	0.0008	0.0010	0.0110	0.0008	0.0010	0.0113
nC4	0.0279	0.0419	0.0461	0.0319	0.0472	0.0514
iC8	0.0001	0.0094	0.0093	0.0002	0.0190	0.0186
C12	0.0000	0.0003	0.0003	0.0000	0.0010	0.0010

Table A.1 (Continued) Streams Data

Stream	Vapor 3	Liquid 3	Total Vapor	Compressor Outlet	Refrigerant Drum (Condenser) Outlet
Flow (lbmol/hr)	69.11	1525.00	534.80	534.80	534.80
Temperature (°F)	66.93	66.93	65.24	133.10	116.50
Pressure (psia)	43.36	43.36	43.25	114.70	106.0
Mole fraction					
C_3	0.1457	0.0610	0.1548	0.1548	0.1548
iC4	0.8170	0.8548	0.8148	0.8148	0.8148
C4=	0.0007	0.0009	0.0008	0.0008	0.0008
nC4	0.0362	0.0527	0.0295	0.0295	0.0295
iC8	0.0003	0.0286	0.0001	0.0001	0.0001
C12	0.0000	0.0020	0.0000	0.0000	0.0000

Table A.2 (Continued) Streams Data

Stream	DP Inlet	Propane Purge	DP Bottom	HX2 Outlet	Fresh C4	DIB Inlet
Flow (lbmol/hr)	534.70	8.16	526.40	526.40	58.90	1525.00
Temperature (°F)	152.70	118.0	176.60	143.20	120.00	96.15
Pressure (psia)	231.40	220.00	220.70	214.30	120.00	111.10
Mole fraction						
C_3	0.1548	0.9500	0.1424	0.1424	0.0500	0.0609
iC4	0.8148	0.0499	0.8267	0.8267	0.5000	0.8548
C4=	0.0008	0.0000	0.0008	0.0008	0.0000	0.0009
nC4	0.0295	0.0001	0.0300	0.0300	0.4500	0.0527
iC8	0.0001	0.0000	0.0001	0.0001	0.0000	0.0286
C12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020

Table A.1 (Continued) Streams Data

Stream	iC4 Recycle	Total 4	HX 1 Outlet	nC4 Vapor Side stream	Alkylate
Flow (lbmol/hr)	1483.00	2010.00	2010.00	52.67	48.36
Temperature (°F)	116.90	124.00	103.50	148.90	385.30
Pressure (psia)	95.00	107.50	106.30	93.38	98.66
Mole fraction					
C_3	0.0646	0.0850	0.0850	0.0000	0.0000
iC4	0.8972	0.8788	0.8788	0.0465	0.0006
C4=	0.0009	0.0008	0.0008	0.0026	0.0001
nC4	0.0373	0.0354	0.0354	0.9500	0.0341
iC8	0.0000	0.0000	0.0000	0.0009	0.9006
C12	0.0000	0.0000	0.0000	0.0000	0.0646

Figure A.1 Flowsheetof Process Streams Data
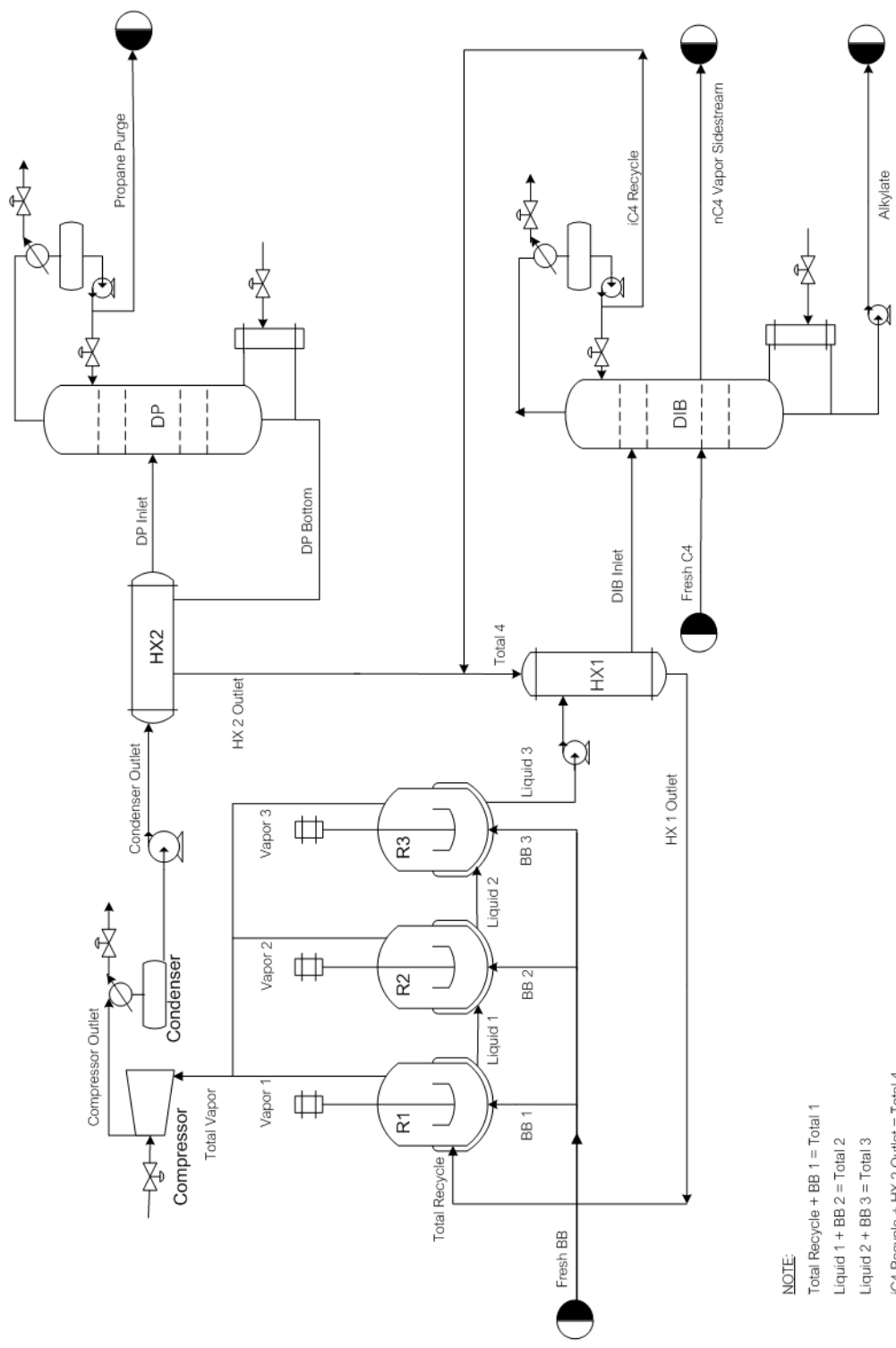
NOTE:

Total Recycle + BB 1 = Total 1

Liquid 1 + BB 2 = Total 2

Liquid 2 + BB 3 = Total 3

iC4 Recycle + HX 2 Outlet = Total 4

Table A.2 Equipments data

Unit Operation	Properties	Size
Reactor (R1)	Volume (ft^3)	500.00
Reactor (R2)	Volume (ft^3)	500.00
Reactor (R3)	Volume (ft^3)	500.00
Refrigerant drum (Condenser)	Volume (ft^3)	69.473
Depropanizer Column		
Tray spacing	Spacing (ft)	1.804
Column diameter	Diameter (ft)	4.921
Reflux drum	Volume (ft^3)	70.629
Sump	Volume (ft^3)	95.942
Deisobutanizer Column		
Tray spacing	Spacing (ft)	1.804
Column diameter	Diameter (ft)	17.123
Reflux drum	Volume (ft^3)	283.209
Sump	Volume (ft^3)	203.377

APPENDIX B

TUNNING PARAMETERS OF EACH CONTROL STRUCTURE

Table B.1 Type of controllers and tuning parameters of Base case

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse	100 lbmol/hr	0-200	0.5	0.3	
BB 1	FC	Flow rate	BB1 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 2	FC	Flow rate	BB2 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 3	FC	Flow rate	BB3 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
Reactor1 (R1)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor2 (R2)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor3 (R3)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
	TC	Reactor temperature	Compressor work	PID	Direct	66.93 °F	0-100	6.03	7.08	1.57
Condenser	PC	Condenser pressure	Condenser duty	PI	Direct	106 psia	79.5-132.5	2	10	
	LC	Liquid percent level	Duty flowrate	P	Direct	50%	0.-100	2		
Depropanizer	TC	Temperature tray 6	Reboiler duty	PID	Reverse	151.8 °F	100-200	0.94	11.2	2.49
Column (DP)	FC	Reflux ratio	Distillate flowrate	PI	Reverse	10.50		0.5	0.3	
	LC	Reflux drum percent level	Refux flowrate	P	Direct	50%	0-100	5		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	220 psi	165-275	2	10	
Deisobutabizer	TC	Temperature tray 52	Reboiler duty	PID	Reverse	295.6 °F	250-350	0.22	7.72	1.72
Column (DIB)	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct	0.0373	0-1	4.54	9.14	2.03
	CC	Side stream (nC_4) purities	Side stream flowrate	PI	Direct	0.95	0-1	2	10	
	LC	Reflux drum percent level	Fresh C_4 flowrate	P	Reverse	50%	0-100	2		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	95 psi	71.25-118.75	2	10	

Table B.2 Type of controllers and tuning parameters of Control Structure 1 (CS 1)

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse	100 lbmol/hr	0-200	0.5	0.3	
BB 1	FC	Flow rate	BB1 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 2	FC	Flow rate	BB2 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 3	FC	Flow rate	BB3 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
Reactor1 (R1)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor2 (R2)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor3 (R3)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
	TC	Reactor temperature	Compressor work	PID	Direct	66.93 °F	0-100	6.03	7.08	1.57
Condenser	PC	Condenser pressure	Condenser duty	PI	Direct	106 psia	79.5-132.5	2	10	
	LC	Liquid percent level	Duty flowrate	P	Direct	50%	0.-100	2		
Depropanizer	TC	Temperature tray 6	Reboiler duty	PID	Reverse	151.8 °F	100-200	0.94	11.2	2.49
Column (DP)	FC	Reflux ratio setpoint	Distillate flowrate	PI	Reverse	10.50	0-17.64	0.5	0.3	
	CC	Composition of C_3	Reflux ratio setpoint	PID	Direct	0.95	0-1	14.2	3.90	0.87
	LC	Reflux drum percent level	Refux flowrate	P	Direct	50%	0-100	5		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	220 psi	165-275	2	10	

Table B.2 (continue) Type of controllers and tuning parameters of Control Structure 1 (CS 1)

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
Deisobutabizer	TC	Temperature tray 52	Reboiler duty	PID	Reverse	295.6 °F	250-350	0.22	7.72	1.72
Column (DIB)	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct	0.0373	0-1	4.54	9.14	2.03
	TC	Temperature tray 49	Side stream	PI	Direct	148.9	100-200	14	66	58.4
	LC	Reflux drum percent	Fresh C_4 flowrate	P	Reverse	50%	0-100	2		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	95 psi	71.25-118.75	2	10	

Table B.3 Type of controllers and tuning parameters of Control Structure 2 (CS 2)

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
Fresh BB feed	FC	Flow rate	Feed flow rate	PI	Reverse	100 lbmol/hr	0-200	0.5	0.3	
BB 1	FC	Flow rate	BB1 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 2	FC	Flow rate	BB2 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
BB 3	FC	Flow rate	BB3 flow rate	PI	Reverse	33.33 lbmol/hr	0-66.66	0.5	0.3	
Reactor1 (R1)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor2 (R2)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
Reactor3 (R3)	LC	Liquid percent level	Liquid out flow	P	Direct	50%	0-100	2		
	TC	Reactor temperature	Compressor work	PID	Direct	66.93 °F	0-100	6.03	7.08	1.57
Condenser	PC	Condenser pressure	Condenser duty	PI	Direct	106 psia	79.5-132.5	2	10	
	LC	Liquid percent level	Duty flowrate	P	Direct	50%	0.-100	2		
Depropanizer	TC	Temperature tray 6	Reboiler duty	PID	Reverse	151.8 °F	100-200	0.94	11.2	2.49
Column (DP)	FC	Reflux ratio setpoint	Distillate flowrate	PI	Reverse	10.50	0-17.64	0.5	0.3	
	CC	Composition of C_3	Reflux ratio setpoint	PID	Direct	0.95	0-1	14.2	3.90	0.87
	LC	Reflux drum percent level	Refux flowrate	P	Direct	50%	0-100	5		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	220 psi	165-275	2	10	

Table B.3 (continue) Type of controllers and tuning parameters of Control Structure 2 (CS 2)

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	τ_i	τ_D
Deisobutabizer	TC	Temperature tray 52	Reboiler duty	PID	Reverse	295.6 °F	250-350	0.22	7.72	1.72
Column (DIB)	CC	Distillate (nC_4) impurities	Reflux flowrate	PID	Direct	0.0373	0-1	4.54	9.14	2.03
	CC	Side stream (nC_4)	Side stream	PI	Direct	0.95	0-1	2	10	
	LC	Reflux drum percent	Fresh C_4 flowrate	P	Reverse	50%	0-100	2		
	LC	Reboiler percent level	Bottom flowrate	P	Direct	50%	0-100	2		
	PC	Top stage pressure	Condenser duty	PI	Direct	95 psi	71.25-118.75	2	10	

VITAE

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