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คณะวิศวกรรมศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
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PLANTWIDE CONTROL STRUCTURE DESIGN OF TERT-AMYL METHYL ETHER (TAME) PROCESS

Miss Thihima Tapaneeyapong

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By Miss Thitima Tapaneeyapong
Field of Study Chemical Engineering
Thesis Advisor Assistant Professor Montree Wongsri, D.Sc.

Accepted by the Faculty of Engineering, Chulalongkorn University in Partial Fulfillment of the Requirements for the Master's Degree

…………………………………….Dean of the Faculty of Engineering
(Associate Professor Boonsom Lerdhirunwong, Dr.Ing.)

THESIS COMMITTEE

……………………………………Chairman
(Assistant Professor Amornchai Arpornwichanop, D.Eng.)

……………………………………Thesis Advisor
(Assistant Professor Montree Wongsri, D.Sc.)

…………………………………… Examiner
(Chutimon Satirapipathkul, D.Eng.)

……………………………………External Examiner
(Chaiyapop Siraworakun, D.Eng.)

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วิทยานิพนธ์นี้รายงานการออกแบบโครงสร้างการควบคุมทั้งโรงงานสำหรับกระบวนการเทอร์เอมิลเมทิลอีเทอร์โดยใช้วิธีการออกแบบของวงศ์ศรี วิธีการออกแบบประกอบด้วย 8 ขั้นตอน ซึ่งเน้นการออกแบบระดับทั้งโรงงาน ได้แก่ การกำกับโรงงานให้ได้ดุลมวล การจัดการกับสิ่งรบกวนเพื่อการควบคุมคุณภาพ และการควบคุมให้กระแสขาเข้าของกระบวนการคงที่ เทอร์เอมิลเมทิลอีเทอร์ถูกใช้เป็นสารออกซิเจนเนตในน้ำมันเชื้อเพลิง ใช้สำหรับช่วยเพิ่มปริมาณของค่าออกเทนในน้ำมันเชื้อเพลิงให้สูงขึ้น ส่งผลให้ลดการปล่อยอากาศเสียให้น้อยลงเมื่อนำน้ำมันเชื้อเพลิงไปใช้งาน โดยเทอร์เอมิลเมทิลอีเทอร์เกิดจากการทำปฏิกิริยากันระหว่างไอโซเอมิลีนและเมทานอล ปฏิกิริยาที่เกิดขึ้นเป็นปฏิกิริยาผันกลับได้ กระบวนการผลิตประกอบด้วยถังปฏิกรณ์, หอกลั่นปฏิกิริยา และหอกลั่นแยกสาร 2 หอ นอกจากนั้นยังมีสายรีไซเคิล 2 สาย และสายป้อนสารตั้งต้นอีก 2 สาย สายป้อนกับสายรีไซเคิลของเมทานอลถูกควบคุม และเป็นอัตราส่วนกับสายไอโซเอมิลลีน สารแต่ละตัวถูกควบคุมตามตำแหน่งของตัวบ่งบอกปริมาณของสารนั้นๆ โครงสร้างการควบคุมทั้งโรงงานที่ออกแบบได้มีสมรรถนะเทียบได้กับการออกแบบของ Luyben

ภาควิชา วิศวกรรมเคมี ลายมือชื่อนิสิต

สาขาวิชา วิศวกรรมเคมี ลายมือชื่อ อ.ที่ปรึกษาวิทยานิพนธ์หลัก

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THITIMA TAPANEEYAPONG: PLANTWIDE CONTROL STRUCTURE DESIGN OF TERT-AMYL METHYL ETHER (TAME) PROCESS. ADVISOR: ASST. PROF. MONTREE WONGSRI, Ph.D., 133 pp.

The design of plantwide control structure for tert-amyl methyl ether (TAME) process using Wongsri's design procedure is reported. The design procedure consist of 8 steps which emphasis on plantwide level design: establishing material-balanced plant, disturbance management for quality control, fixing process stream inflows. The TAME is used as a fuel oxygenates to increase the octane number in gasoline. It affects to reduce air pollution. TAME is produced by the catalytic etherification of isoamylenes [2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B)] with methanol. The three main reactions is reversible reaction. The process flowsheet consists of a reactor, a reactive distillation column and two pressure-swing azeotopic distillation columns. In addition, there are two reycle streams and two fresh feed streams. The combined feed of fresh and recycled methanol is regulated and is ratioed to isoamylene flow. Each component is handled at their quantifiers. The designed plantwide control structure performance is comparable to the Luyben's design.

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CHAPTER I

INTRODUCTION

In this chapter presented the importance and reason of research, research objectives, scopes of research, contributions of research, research procedure, research framework, and research plan.

1.1 Importance and Reasons of Research

Nowadays, Plantwide process control has more importance. Because of plantwide process control concerns in the systems and strategies required to control the entire chemical plant. Most industrial processes contain a lot of units operations, several recycle streams and energy integration connected into the process. That makes the complex flowsheet. The recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. That creates a path for disturbance in process. But, the economic can be improved by the recycle streams and energy integration into the process. Therefore, plantwide control are required to operate an entire process achieve the design objective and entire plant safety.

The plantwide control problem is extremely complex and very much open-ended. There are a combination number of possible choices and alternative strategies. And there is no unique correct solution. The general plantwide control problem is how to selection controlled variables, manipulated variables and the measurement. That can be handle disturbances load entering the process and controlling stable process.

tert-Amyl methyl ether (TAME) is used as a fuel oxygenate to increase octane. In the process of TAME consist of many operating units. But, the interests in this process are reactive distillation and reversible chemical reactions in the process. The control of reactive distillation is different from conventional distillation. One important inherent advantage of reactive distillation is the feature of simultaneous production and removal of products. For reversible chemical reactions the removal of the product components drives the reaction toward the product side. Thus, the chemical equilibrium constraint on conversion can be overcome and high conversions can be achieved, even in cases with small chemical equilibrium constrains. Of course, the reactive volatilities among the reactants and products must be such that the products can be fairly easily removed from the region in the column where the reaction is occurring and reactants are not lost from this region.

In this research, it will be studied the new plantwide control structure design procedure of Wongsri (2012). That consists of eight steps of the proposed procedure center around the fundamental principles of plantwide control: energy management, production rate, product quality, operational, environmental and safety constraints, liquid-level and gas pressure inventories, makeup of reactants, component balances, and economic or process optimization.

The goal of this study, focuses on the new plantwide control structure design procedure of Wongsri (2012) applied to *tert*-amyl methyl ether (TAME) process.

1.2 Research Objectives

The objectives of this research are design and evaluate plantwide control structures of TAME production process by using new design procedure of Wongsri (2012).

1.3 Scopes of Research

The scopes of this research can be shown as follows:

1. Steady-state and dynamic simulation of *tert*-amyl methyl ether (TAME) process by using a commercial process simulator.
2. New control structures of *tert*-amyl methyl ether (TAME) process are designed by using Wongsri's procedure (2012).
3. Performance of new control structures for *tert*-amyl methyl ether (TAME) process are evaluated in term of integral absolute error (IAE) and compared with performance control structure given by Al-Arfaj and Luyben (2004).

1.4 Contributions of Research

The contribution of research can be shown as follows:

1. Steady state and dynamic models of *tert*-amyl methyl ether (TAME) process has been simulated by using commercial simulation software.
2. The new plantwide control structures of *tert*-amyl methyl ether (TAME) process are designed by using Wongsri's procedure (2012).
3. Evaluated the performance of the new design plantwide control structures compare with the performance of control structure of reference case given by Al-Arfaj and Luyben (2004).

1.5 Research Procedure

Procedure plants of this research are:

1. Study the plantwide control theory, the *tert*-amyl methyl ether (TAME) process and concerned information.
2. Simulate steady-state operation and dynamic operation of *tert*-amyl methyl ether (TAME) process by using commercial process simulator.
3. Simulate the reference control structure is obtained from Al-Arfaj and Luyben (2004).
4. Study the Wongsri's plantwide control structures and design procedure (2012).
5. Design new plantwide control structures of *tert*-amyl methyl ether process followed the Wongsri's procedure (2012).
6. Simulate the dynamic operation of *tert*-amyl methyl ether (TAME) process with the new design control structures.
7. Evaluate the dynamic performance of the new control structures based on the external disturbance loads.
8. Analyze and discuss of the design and simulate results.
9. Conclude the research.

1.6 Research Framework

This the thesis consisting of six chapters as follows:

Chapter I: Present importance and reasons, objectives, scopes, contributions and procedure of the research.

Chapter II: present literature review related to plantwide control structures design procedure and the review of previous work on the *tert*-amyl methyl ether (TAME) process design.

Chapter III: purpose the basic of control, plantwide control structures design principle.

Chapter IV: Description of the *tert*-amyl methyl ether (TAME) process and plantwide control structure design procedure of Wongsri.

Chapter V: Description of the designed control structures, which applied to *tert*-amyl methyl ether (TAME) process. Comparison the dynamic responses of the control structure of reference case and new control structures designed by Wongsri's design procedures when the process was disturbed by load and thermal disturbances.

Chapter IV: Present the conclusions of research and recommendations.

CHAPTER II

LITERATURE REVIEWS

Several years ago, plantwide control structure design has been interested and studied widely. In this chapter, to shows a literature review of this research. That presents a review of the previous works on the plantwide control structure design and TAME production process.

2.1 Literature Review of Plantwide Control Structure Design

Terrill and Douglas (1987) have studied HDA process from a steady state point of view and determined that the process can be held very close to its optimum for a variety of expected load disturbances by using the following strategy: (1) Fix the flow of recycle gas through the compressor at its maximum value, (2) Hold a constant heat input flowrate in the stabilizer, (3) Eliminate the reflux entirely in the recycle column, (4) Maintain a constant hydrogen-to-aromatic ratio in the reactor inlet by adjusting hydrogen fresh fed, (5) Hold the recycle toluene flowrate constant by adjusting fuel to the furnace, (6) Hold the temperature of the cooling water leaving the partial condenser constant.

Wongsri (1990) studied a resilient HENs design. He presented a simple but effective systematic synthesis procedure for the design of resilient HEN. His heuristic design procedure is used to design or synthesize HENs with pre-specified resiliency. It used physical and heuristic knowledge in finding resilient HEN structures. The design must not only feature minimum cost, but must also be able cope with fluctuation or changers in operating condition. A resilient HEN synthesis procedure was developed based on the match pattern design and a physical understanding of the disturbances propagation concept. The disturbance load propagation technique was developed from the shift approach and was used in a systematic synthesis method. The design condition was selected to be the minimum heat load condition for easy accounting and interpretation. This is a condition where all process streams are at their minimum heat loads.

Luyben (1994) reported snowball effect. The snowball effect is a small change in load causing a very large change in the recycle flowrate. Luyben suggest that how can the offered control structure prevent snowballing and why the conventional structure cause the snowball effect. Consecutive first-order reactions and second-order reaction was studied in this case. He confirmed that the snowball effect could be removed by switching the conventional structures, fresh feed flowrate control and reactor level control by manipulating reactor effluent flowrate, to reactor effluent flow control and reactor level control by manipulating fresh feed flowrate. The fixed flowrate of reactor effluent in one-recycle processes can prevent the snowballing. In two or more recycle streams processes can be prevented the snowball effect by fixing the flowrate of each recycle.

Luyben (1996) presented one of the central problems in developing a steady-state process flowsheet. There is finding the number of variables that must be specified to completely define the process. This number is called the design degrees of freedom. The number of design optimization variables can be calculated by subtracting all variables that are set by specifications on production rate, product qualities, safety constraints, and environmental limitations. For complex industrial processes, there are many hundreds of variables and equations, and it is difficult to make sure that the correct variables and equations have been defined. The design of a control structure requires that the control degrees of freedom be known. It is very easy to calculate the number of variables that can be controlled because it is equal to the number of manipulated variables. These variables are different than the design optimization variables. Several progressively more complex recycle process case studies are used to show these results. The practical significance is that we do not need a model and we can avoid the error procedure of accounting for all variables and equations.

Luyben, Tyreus and Luyben (1997) presented a general heuristic design procedure. The nine step of the proposed procedure center around the fundamental principles of plantwide control: energy management, production rate, product quality, operational, environmental and safety constraints, liquid level and gas-pressure inventories, makeup of reactants, component balances and economic or process optimization. This procedure was illustrated with three industrial examples: the vinyl acetate monomer process, Eastman process and HDA process. The procedure produced a workable plantwide control strategy for a given process design.

Skogestad et al. (2000) reviewed on the plantwide control with emphasis on the five tasks, selection of controlled variables, manipulated variables, measurements, control configuration, and controller type. There are two main parts of those tasks. First part is a top-down consideration which degrees of freedom are available to meet. The top-down analysis consists of the first and the second task, the selection of controlled variables, and the selection of manipulated variables. The three last tasks, the selection of measurements, control configuration, and controller type, are used for stabilizing the process, called a bottom-up design. For the first task, the steady-state economics is very useful. There is much-needed link between steady-state optimization and process control. The actual bottom-up design of the control system is done after the control problem has been defined.

Skogestad et al. (2004) improved the procedure presented in 2000. The procedure was expanded from five steps to eight steps. The change in procedure is an emphasis on degree of freedom analysis, selection of controlled variables, control system complexity, inventory control, and loss in performance by bottom-up design. The procedure is still divided in two main parts. The first four steps are top-down analysis including of operational objectives and consideration of degrees of freedom. And the last four steps are bottom-up design of the control system for stabilizing control layer. The fifth and the sixth step are the analysis of control layer using a linear multivariable dynamic model. The steady-state model is not important. The third and the seventh step are the analysis of optimization layer using a nonlinear steady-state model. Dynamics are normally not needed except bath processes and cases with frequent grade changes. This procedure is the analysis based on the mathematical method. However, the mathematical procedure is complex.

Konda, et al. (2005) presented the novel plantwide control (PWC) methodologies are becoming increasingly important as chemical processes are becoming more and more integrated with recycles for reason of safety, environmental considerations, and economics. They proposed an integrated framework of simulation and heuristics. By adopting this framework, simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The proposed framework is then successfully applied to an industrially relevant case study: the hydrodealkylation of toluene (HDA) process. An analysis of results shows that the proposed framework build synergies between the powers of both the simulation and the heuristics, thereby resulting in a practical plantwide control structure methodology that leads to a viable control system.

Konda et al. (2006) used simulation-based heuristic approach for designing plantwide control structure. This work is proposed for obtaining both of economic and operational benefits. The approach consists of two stages. The first stage, Alternatives are systematically originated and ranked based on economics. Then, A few top-ranked alternatives are forwarded to the second stage for analysis on their dynamics to define the best process that is economical as well as easy to operate. In addition, he presented the important steps for designing plantwide control through control degrees of freedom. The control degrees of freedom are measured in cases of highly integrated processes. The proposed is for giving a maximum number of flows that be able to manipulate simultaneously in a process, and some (or all) of them can be utilized based on process requirement. The procedure is clearly simpler than the conventional approach.

Detjareansri (2009) presented plantwide control structures design using Wongsri (2009), eight-step procedure. The control structures are illustrated for an alkylation process. And the dynamic performances of the process are then held two types of disturbance, material and energy. The performances are evaluated and compared to Luyben’s base case. The result showed that the performances of process using Wongsri (2009) are good, which presented by IAE numbers and total number of process energy consuming.

Luyben, W.L. (2011) proposed some general design principles in a concise form that should aid the engineer in completing the daunting task of developing an effective flowsheet and control structure. A rich variety of cases studies are presented that illustrate in an in-depth and quantitative way the application of these general principles. Effective development of a chemical process requires the simultaneous consideration of both steady-state economic and dynamic controllability aspects of the process. Ten complex processes that contain a variety of features commonly occurring in many important industrial plants were presented. Conventional proportional-integral (PI) plantwide control structures are developed and tested for their ability to maintain product quality during typically large disturbances. For this work, he intended to cut through this maze of information and present the essential principles of design and control in a brief, readable form that can be easily comprehended by students and engineers in the chemical, petroleum, and biochemical industries.

Arrayasinlapathorn (2011) propose plantwide control structures design of methyl acetate process which designed by control structure design procedures of Wongsri 2012. The wongsri procedure consists of 8-step that can be used to design the effective control structure of any processes. There are easy steps and the operator can follow easily. For the designed control structures of the methyl acetate process which was designed by Wongsri’s procedure can be handled the disturbances (total feed, feed temperature and composition change).

2.2 Literature Review of TAME Production Process

Subawalla and Fair (1999) discussed the design guidelines for solid catalyzed reactive distillation systems. They presented the iterative procedures to estimate reactive column catalyst mass, reactive zone height, theoretical stages, reflux ratio, packed height, and column diameter. These guidelines provided good initial estimates and serve as a starting point for detailed design. They summarized the key conclusions from their modeling and experimental studies as following. (1) They recommend the use of a prereactor upstream of a reactive column for systems that the reaction rates decline abruptly only when compositions and temperatures approach equilibrium. (2) For most systems the operating pressure is driven by temperatures and reaction rates. However, there is an upper pressure limit beyond which rates actually decrease because of reactant depletion due to relative volatility and/or azeotropic effects, and a decrease in departure from chemical equilibrium. (3)

Reactive columns require one reactant in large excess when large relative volatility differences exist between reactants. (4) Stringent purity specifications on either the distillate or bottoms product can alter the reactive zone location when either the height of the stripping or rectification section is increased. (5) The feed location is adjusted to minimize product decomposition when a prereacted product-containing stream is fed to a reactive column. (6) Selecting an appropriate amount of catalyst is an important aspect of reactive column design. Inadequate catalyst volume reduces residence time and gives poor conversion. For equilibrium-limited systems, excess catalyst, particularly when it is inappropriately located, may result in product decomposition. A good initial estimate for catalyst mass is obtained by simulating a sequence of ideal plug-flow reactors and separators in series. (7) Short-cut methods (e.g., Fenske Underwood method) give reasonable estimates for the number of nonreactive stripping and rectification stages. (8) Since the packing catalyst density limits the amount of catalyst per unit volume, when residence time limitations occur (inadequate catalyst mass), either the column diameter or reactive zone height has to be increased to accommodate the additional catalyst mass. (9) Since the reflux ratio impacts both reaction and separation efficiency, conventional short-cut methods for determining minimum reflux cannot be easily extended to reactive columns. (10) They recommend that the rate-based (nonequilibrium) approach be used for simulation and design for reactive columns, particularly when thermophysical and transport property data and reliable column hydraulic models are available.

Al-Arfaj, M.A. and Luyben, W.L. (2004) studied the plantwide design and control of the *tert*-amyl methyl ether (TAME) process with reactive distillation. They synthesized to design a complete the flowsheet by using a pressure-swing azeotropic separation methanol recovery. When the reactive distillation column was designed and handled properly, the rest of the process should be easy to manage. A very important is the applicability of an effective control structure on different reactive distillation systems of the same class. The system they studied was the etherification of TAME process. Previously, they studied the ETBE process, which is also an etherification process. Although they differ somewhat in the physical and chemical properties but, they are similar that they both have two reactants. After carefully testing the high-conversion TAME process, they concluded that it should be considered a “pseudo-neat” process because both reactants must be used in the correct proportions to maintain high conversion and the purity of TAME. Using this analogy, they developed a control structure for the TAME reactive distillation based on the control structure that was used with the ETBE “neat” reactive distillation. The other units of the flowsheet were controlled to achieve the objective of each unit. The overall mass balance and the methanol inventory were taken into consideration to avoid reactant buildup or depletion. Combining all these considerations resulted in a plantwide control structure that is very effective. In conclusion, it is found that effective control structures could be used interchangeably with minor changes on different reactive distillation systems of the same class.

Luyben, W.L. (2005) presents a quantitative steady-state and dynamic comparison of the pressure-swing process and an extractive-distillation process for methanol recovery section in *tert*-amyl methyl ether (TAME) process. Water is the extractive agent. The plantwide dynamic controllability performances of the two systems are essentially equivalent. The design and control of two alternative separation sections in the reactive distillation process to produce TAME have been studied. Both processes are capable of producing high-purity TAME. The process that uses extractive distillation is much more attractive in terms of steady-state economics. Capital investment and energy costs are very significantly lower. The two processes have essentially the same satisfactory dynamic controllability. Their plantwide control structures have similarities and differences.

Luyben, W. L. and Cheng-ching yu (2008) presented an extensive treatment of both steady-state design and dynamic control of reactive distillation systems by using rigorous nonlinear models. Both generic ideal chemical systems and actual chemical systems are studied. Economic comparisons between conventional multiunit processes and reactive distillation are presented. Reactive distillation columns in isolation and in plantwide systems are considered. There are many parameters that affect the design of a reactive distillation column. Some of these effects are counterintuitive because they are different than in conventional distillation. This is one of the reasons reactive distillation is such a fascinating subject.

CHAPTER III

PLANTWIDE CONTROL STRUCTURES DESIGN PRINCIPLE

3.1 Basics of Plantwide Control

Most of chemical plant has a lot of unit operations connected both in series and parallel that consist of reaction sections, separation sections and heat exchanger network. Therefore, Plantwide control syructure process involves the system and strategies required to control entire plant consisting of many interconnected unit operations. The plantwide control structure is complex because of several recycle stream and energy integration. This chapter will offer about theories related to control elements in the process.

3.1.1 Integrated Process

Three basic features of integrated chemical process lie at the root of our need to consider the entire plant's control system

1) The effect of material recycles.
2) The effect of energy integrations.
3) The need to account for chemical component inventories.

3.1.1.1 Material Recycle

Material is recycled for six basic and important reasons as follows:

1) Increase Conversion: If chemical processes involve reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent must contain both reactants and products. Separation and recycle of reactants are necessary to make process be economically viable.

2) Improve Economics: Generally systems, it is simply cheaper to use a reactor with incomplete conversion and recycle reactants than it is to use of one reactor or multiple reactors in series reaches the desired conversion. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

3) Improve Yields: In reaction systems such as A → B → C, where B is the desired product. Therefore the concentration of B should be kept as low as possible in the reactor and a large recycle of A is required for minimizing the per-pass conversion of A to avoid the formation of the undesirable product C.

4) Provide Thermal Sink: In adiabatic reactors with highly exothermic reaction, it is often necessary to feed excess a reactant or one product to the reactor to prevent large amount of temperature increase. High temperature can create several desired events: it can lead to thermal runaways, catalyst deactivation, undesirable side reactions, mechanical failure of equipment, etc. So the heat of reaction is absorbed by the sensible heat required to raise the temperature of the excess material in the stream flowing through the reactor.

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

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

3.1.1.2 Energy Integration

The reason for the use of energy integration is to improve the thermodynamics efficiency of the process. This translates to reduce utility cost. For energy-intensive processes, the savings can be quite significant.

3.1.1.3 Chemical Component Inventories

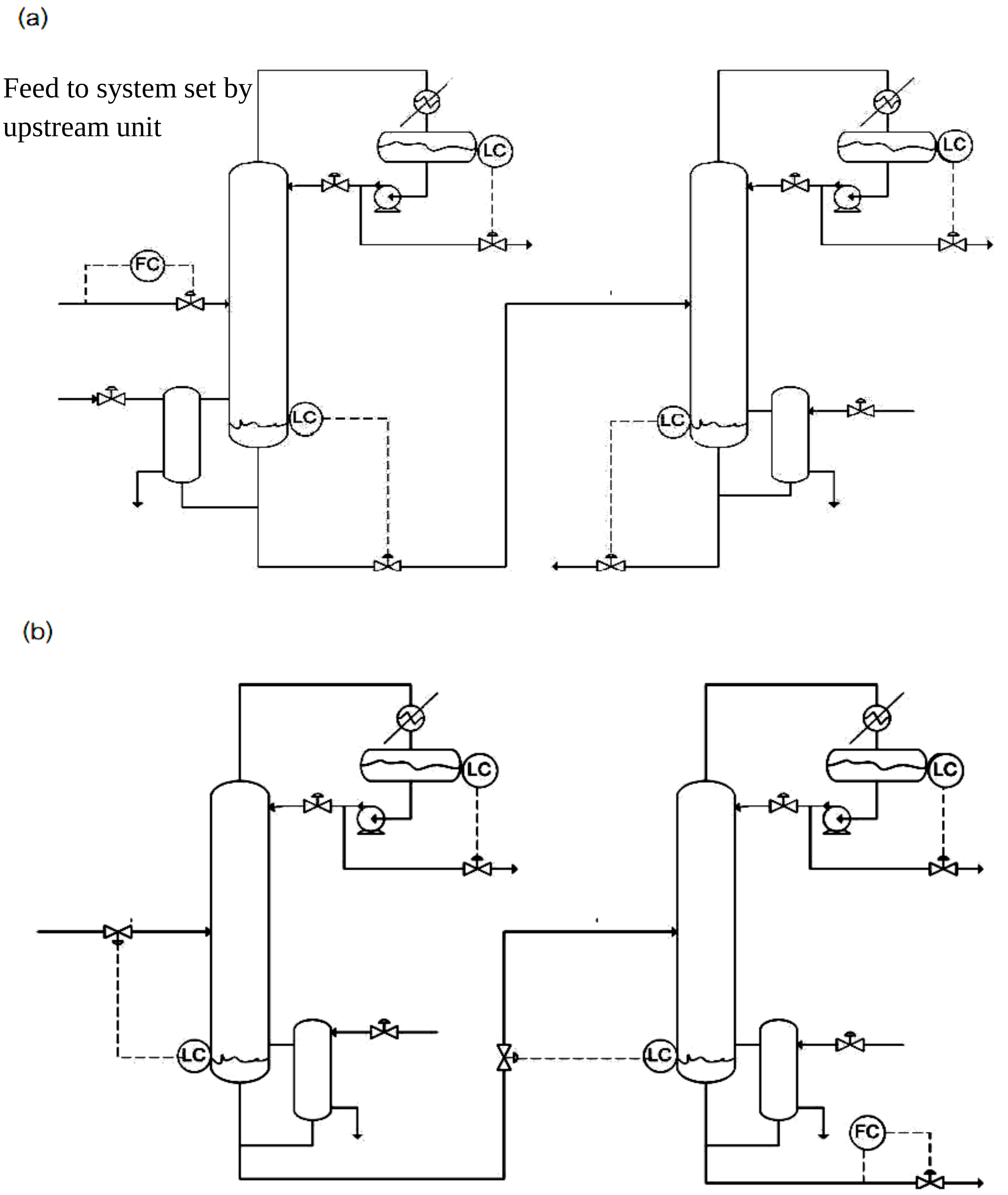
In chemical process can be characterized into three types: reactants, products, and inert. A material balance for all components must be satisfied, but problems usually encounter when we consider reactants (because of recycle) and account for their inventories within the entire process. We want to minimize reactants leaving from the process as impurity or purge because of their value, so we must ensure that every mole of reactant fed to the process is consumed by the reactions, this represents a yield penalty. From the viewpoint of individual units, chemical component balancing is not a problem because exit streams form the units automatically adjust their flows and compositions. However, when we connect units together with recycle streams, the entire system behaves almost like a pure integrator in terms of the reactants. If additional reactant is fed into the system without changing reactor conditions to consume the reactant, this component will build up gradually within the plant because it has no place to leave the system.

3.1.2 The Plantwide Control Problem

3.1.2.1 Units in Series Problem

If units in entire process are arranged in a series configuration and there is no material and energy recycles, the plantwide control problem is greatly simplified and the issues discussed in the previous section are not had to pay a lot of attention. We can simply configure the control scheme on each individual unit to handle load disturbances.

If production rate is set at the front end of the process, the load disturbances to each unit will come from its upstream neighbor only. If the production rate depends on demand and is set at the terminus, changes in throughput will propagate back through the process. So any individual unit will see load disturbances coming from both its upstream and its downstream neighbors. Figure 3.1 shows these two possible configurations, production rate is set at the front end and terminus of the process.



Feed to system set by upstream unit

Bottoms product from system set by downstream unit

Figure 3.1 Units in series (a) Level control in direction of flow (b) Level control in direction opposite flow

3.1.2.2 Effects of Recycle

Two basic effects of recycle:

(1) Time constants in recycle systems, recycle has an impact on the dynamics of the process. The overall time constant can be much different than the sum of the time constants of individual units.

(2) Recycle leads to the “snowball” effect. This has manifestations, one steady state and one dynamic. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates. These disturbances can lead to even larger dynamic changes in flow, which propagate around the recycle loop.

3.1.2.3 Snowball Effect

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

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

3.1.2.4 Reaction/Separation Section Interaction

Different control structures produce different behavior in handling disturbances. To understand the interaction between reaction and separation section, the two control structures of the same process are considered as shown in figures 3.2 and 3.3.

In the first shown in figure 3.2, only the separation section must absorb almost all of changes. To increase production rate of product which is in the bottom stream of distillation column by 20 percent, the overall reaction rate must increase by 20 percent. Because of both reactor temperature and reactor holdup fixed constant, only the composition in the reactor must increase 20 percent. This is a significant change in the composition of the feed stream to the distillation column. The load on the separation section changes significantly producing large variations in recycle flowrates.

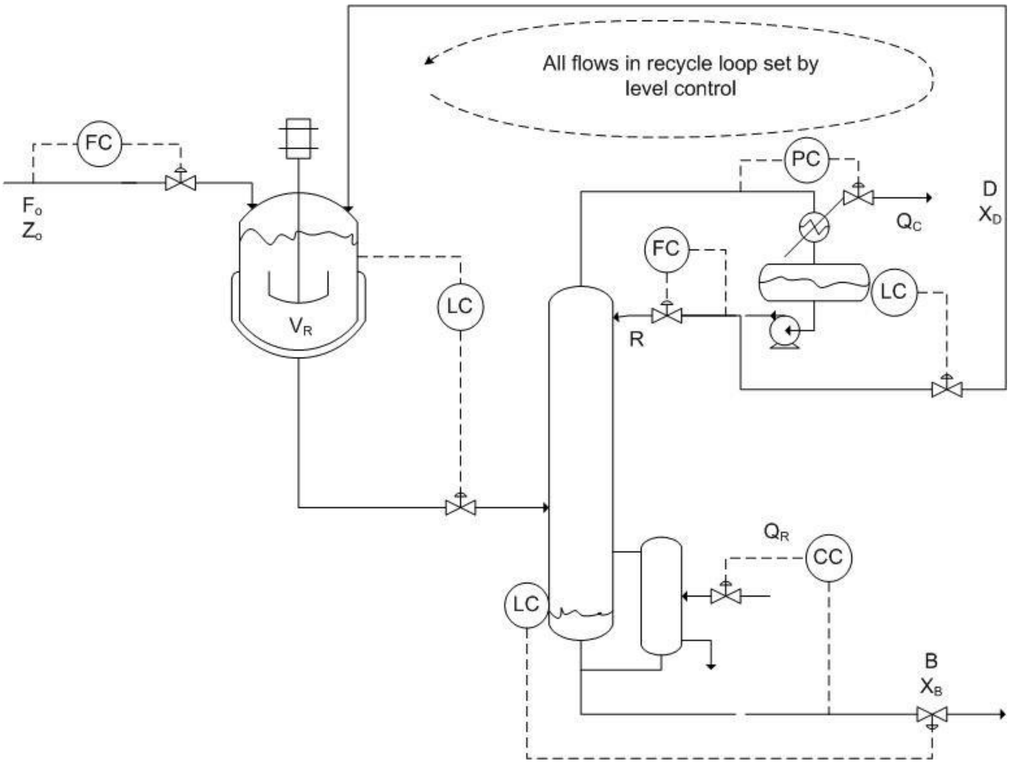


Figure 3.2 Conventional Control Structure with Fixed Reactor Holdup

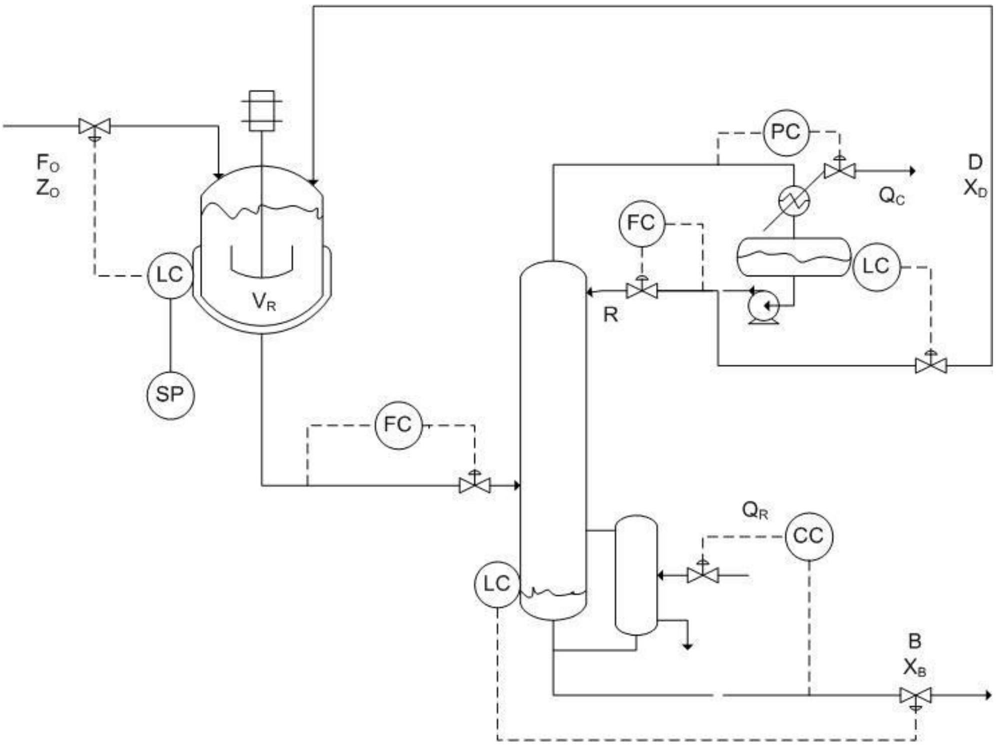


Figure 3.3 Control Structure with Variable Reactor Holdup

In the second structure shown in figure 3.3, both reactor holdup and reactor composition can change, so the separation section sees a smaller load disturbance. The effects of the disturbance can be distributed between the reaction and separation sections result a smaller change in recycle flow.

3.1.3 Plantwide Control Design Procedures

Control analysis and control system design for chemical and petroleum processes have traditionally followed the “unit operations approach”. First, all of the control loops were established individually for each unit or piece of equipment in the plant. Then the pieces were combined together into an entire plant. This meant that any conflicts among the control loops somehow had to be reconciled. The implicit assumption of this approach was that the sum of the individual parts could effectively comprise the whole of the plant’s control system. Over the last few decades, process control researchers and practitioners have developed effective control schemes for many of the traditional chemical unit operations. For processes that these unit operations are arranged in series, each downstream unit simply sees disturbances from its upstream neighbor.

Most industrial processes contain a complex flowsheet with several recycle streams, energy integration, and many different unit operation. Essentially, the plantwide control problem is how to development the control loops needed to operate an entire process and achieve its design objective. Recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. They also interconnect separate unit operations and create a pate for disturbance propagation. The presence of recycle streams profoundly alters that is not localized to an isolated part of the process.

In the past, plants with recycle streams contained many surge tanks to buffer disturbance, to minimize interaction, and to isolate units in the sequence of material flow. This allowed each unit to be controlled individually. Prior to the 1970s, low energy costs meant little economic incentive for energy integration. However, there is growing pressure to reduce capital environmental concerns. This has prompted design engineers to start eliminating many surge tanks, increasing recycle streams, and introducing heat integration for both existing and new plants.

Hence economic force within the chemical industry is compelling improved capital productivity. Requirement for on-aim product quality control grow increasing. More energy integration occurs. Improved product yields are achieved via lower reactant per-pass conversion and higher material recycle rates through the process. The product quality, energy integration, and higher yields are all economically attractive in the steady state flowsheet by they present significant challenges to smooth dynamic plant operation. So an effective control system regulating the entire plants operation and a process designed with good dynamic performance play critical parts in achieving the business objectives of reducing operating and capital costs.

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 off 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.

3.1.3.1 Basic Concepts of Plantwide Control

Buckley Basics: Page Buckley (1964) was the first to suggest the idea of separating the plantwide control problem into two parts: material balance control and product quality control. The first part looked at the flow of material through system. A logical arrangement of level and pressure control loops is established, using the flowrates of the liquid and gas streams. Then the second part is choosing appropriate manipulated variables for the product quality control loops. The time constants of product quality control loops are estimated. Most level controllers should be proportional only (P) to achieve flow smoothing.

Douglas doctrines: Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Douglas points out the costs of raw materials and the value of the products. This leads to 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 is needs to avoid losses of reactants and products. The second rests on the principle that yield is worth more than energy.

Downs drill: Jim Downs (1992) has insightfully pointed out the importance of looking as the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. We must ensure that all components (reactants, products, and inert) have a way to leave or be consumed within the process. Most of the reactants fed into the process must be chewed up in the reaction because we want to minimize raw material costs and maintaining high purity products. And the stoichiometry must be satisfied down to the last molecule. Chemical plants often act as pure integrators in terms of reactants due to the fact that we prevent reactants from leaving the process through composition controls.

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

1. All recycle loops should be flow controlled to prevent the snowball effect.
2. A fresh reactant feed stream cannot be flow controlled unless there is essentially complete one-pass conversion of one of the reactants.
3. If final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). If the feed is saturated liquid, changes in feed flowrate or feed composition have less of dynamic effect on distillate composition than they do on bottoms composition.

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

Shinskey schemes: Greg Shinskey (1988) has proposed a number of “advances control” structures that permit improvements in dynamic performance.

Tyreus tuning: The P-only controller is used for liquid levels and sets 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 PI controllers, the relay- feedback test is a simple and fast way to obtain the ultimate gain (Ku) and ultimate period (Pu). Either the Ziegler-Nichlos settings or the Tyerus-Luyben (1992) settings can be used:

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

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

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

3.1.3.2 Steps of Plantwide Process Control Design Procedure.

Luyben et al., (1997) presented a nine basic steps heuristic design procedure for a workable plantwide control strategy. Each of steps is as follows:

Step 1: Establish control objectives.

Step 2: Determine control degrees of freedom

Step 3: Establish energy management system

Step 4: Set production rate

Step 5: Control product 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 Component Balances.

Step 8: Control Individual Unit Operations

Step 9: Optimize Economics or Improve Dynamic Controllability

3.2 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 Fig. 3.4a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig. 3.4b.

Figure 3.4 Control of P/P heat exchangers**;** (a) use of bypass; (b) use of auxiliary utility exchanger

3.2.1 Bypass Control

When the bypass method is employed for unit operation control, several choices about the bypass location and the control point are considered. Fig. 3.5 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.

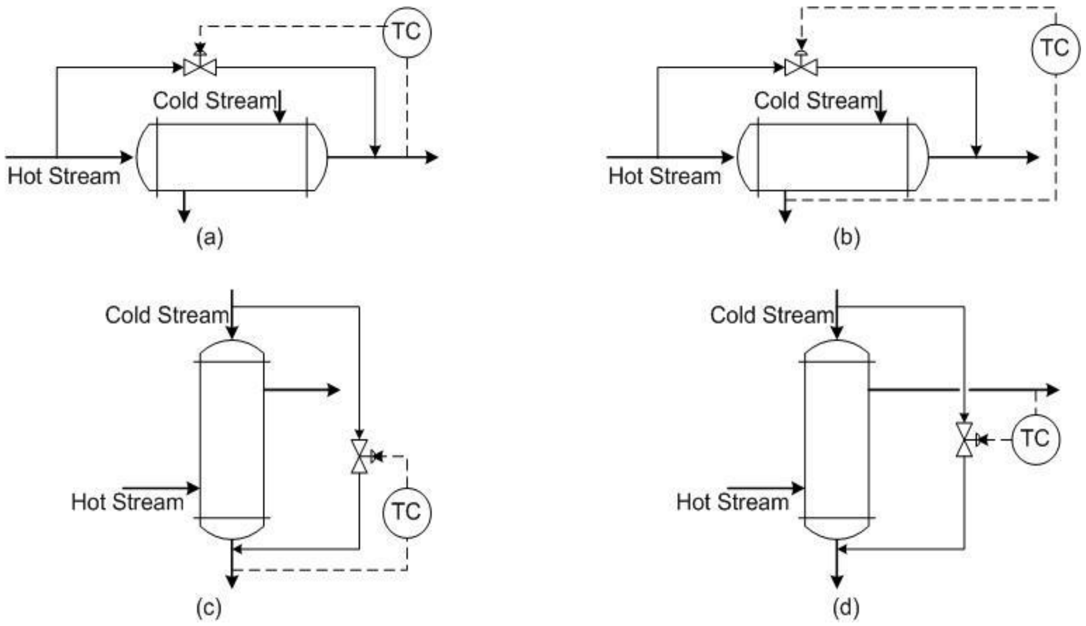


Figure 3.5 Bypass controls of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

3.2.2 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 stand point. Though, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control stand point. 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 thermosiphonreboiler. 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 thermosiphonreboiler, which serves as an auxiliary reboiler. The column tray temperature controller would manipulate the stream to the thermosiphonreboiler.

3.3 Heat Exchanger and Plantwide Energy Management

Another important issue in process design is energy conservation. Common ways to improve the conservation is to install feed-effluent heat exchangers (FEHEs) around rectors and distillation columns where one streams is heated, another must be cooled. 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. So the energy integration is required to reduce the utility cost in addition to improve thermodynamic efficiency of the process.

3.3.1 Heat Exchanger Dynamics

Heat exchangers have fast dynamics compared with other unit operations in a process. The time constant to measured large exchangers could be in second up to a few minutes. 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.

3.3.2 Heat Pathway

In the process, the energy required for heating certain streams can be 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 into three different paths as illustrate in Fig. 3.6. The first pathway shows the heat expend to the environment generated by exothermic reaction and by degradation of mechanical work. This pathway is from inside the process to outside. It is also possible to convert some of the heat to work as it is removed from high temperature in the process. A second pathway carries heat from utilities into the process. Mechanical work is extracted from the heat as it flows from a high supply temperature to the lower temperature of the environment. This pathway goes through the process and is needed to satisfy the thermodynamic work requirements of separation. Work is also extracted from the heat stream to overcome process inefficiencies with stream mixing and heat transfer.

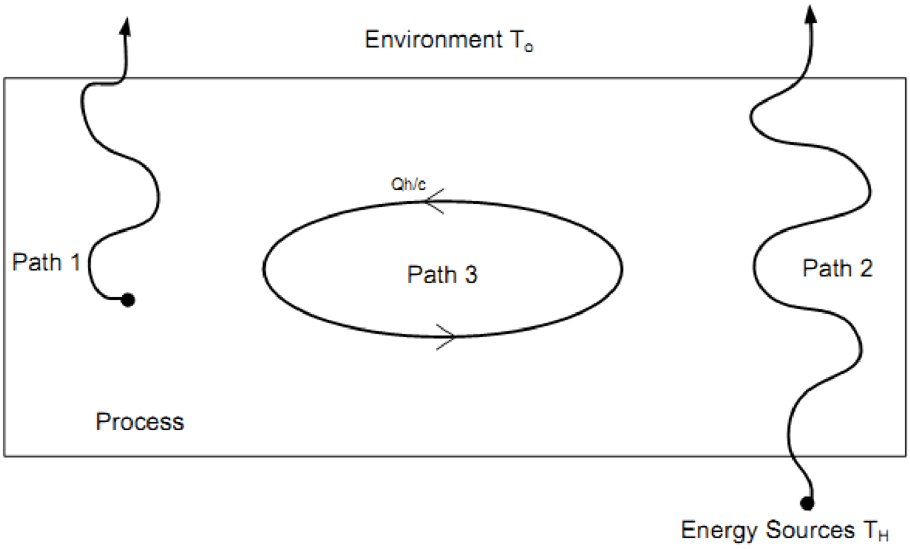


Figure 3.6 Heat Pathways

The third pathway is an internal process pathway. Here, heat circulates 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.

3.3.3 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.

3.4 Basics of Reactive Distillation

Reactive distillation is attractive in those systems where certain chemical and phase equilibrium conditions exist. In this section we describe the ideal classical situation, which will serve to outline the basics of reactive distillation. Consider the system in which the chemical reaction involves two reactants (A and B) producing two products (C and D). The reaction takes place in the liquid phase and is reversible.

$$A + B \leftrightarrow C + D$$

For reactive distillation to work, we should be able to remove the products from the reactants by distillation. This implies that the products should be lighter and/or heavier than the reactants. In terms of the relative volatilities of the four components, an ideal case is when one product is the lightest and the other product is the heaviest, with the reactants being the intermediate boiling components.

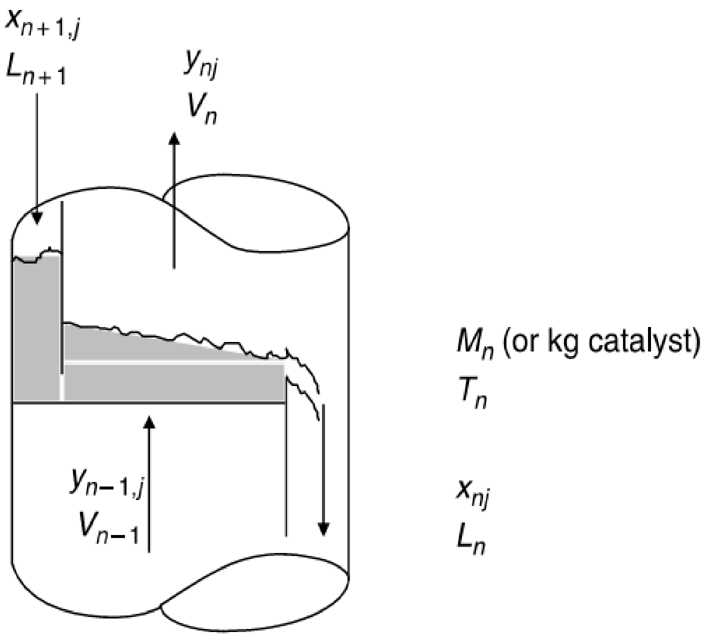
$$\alpha C > \alpha A > \alpha B > \alpha D$$

In this situation the lighter reactant A is fed into the lower section of the column but not at the very bottom. The heavier reactant B is fed into the upper section of the column but not at the very top. The middle of the column is the reactive section and contains N_{RX} trays. Figure 3.7 shows a single reactive tray on which the net reaction rate of the reversible reaction depends on the forward and backward specific reaction rates (k_F and k_B) and the liquid holdup (or amount of catalyst) on the tray (M_n). The vapor flowrates through the reaction section change from tray to tray because of the heat of the reaction.

As component A flows up the column, it reacts with descending B. Very light product C is quickly removed in the vapor phase from the reaction zone and flows up the column. Likewise, very heavy product D is quickly removed in the liquid phase and flows down the column.

The section of the column above where the fresh feed of B is introduced (the rectifying section with N_R trays) separates light product C from all of the heavier components, so a distillate is produced that is fairly pure product C. The section of the column below where the fresh feed of A is introduced (the stripping section with N_S trays) separates heavy product D from all of the lighter components, so a bottom is produced that is fairly pure product D. The reflux flowrate and the reboiler heat input can be manipulated to maintain these product purities.

One of the most important design parameters for reactive distillation is column pressure. Pressure effects are much more pronounced in reactive distillation than in conventional distillation. In normal distillation, the column pressure is selected so that the separation is made easier (higher relative volatilities). In most systems this corresponds to low pressure. However, low pressure implies a low reflux-drum temperature and low-temperature coolant. The typical column pressure is set to give a reflux-drum temperature high enough (49°C, 120°F) to be able to use in expensive cooling water in the condenser and not require the use of much more expensive refrigeration.



$$R_n = M_n\left(k_{F(T_n)}x_{nA}x_{nB} - k_{B(T_n)}x_{nC}x_{nD}\right)$$

$$V_n = V_{n-1} + \frac{-\lambda R_n}{\Delta H_V}$$

Figure 3.7 A single reactive tray

In reactive distillation, the temperatures in the column affect both the phase equilibrium and chemical kinetics. A low temperature that gives high relative volatilities may give small specific reaction rates that would require very large liquid holdups (or amounts of catalyst) to achieve the required conversion. In contrast, a high temperature may give a very small chemical equilibrium constant (for exothermic reversible reactions), which makes it more difficult to drive the reaction to produce products. High temperatures may also promote undesirable side reactions. Thus, selecting the optimum pressure in a reactive distillation column is very important.

Reactive distillation is also different from conventional distillation in that there are both product compositions and reaction conversion specifications. The many design degrees of freedom in a reactive distillation column must be adjusted to achieve these specifications while optimizing some objective function such as total annual cost (TAC). These design degrees of freedom include pressure, reactive tray holdup, number of reactive trays, location of reactant feed streams, number of stripping trays, number of rectifying trays, reflux ratio, and reboiler heat input.

Another design aspect of reactive distillation that is different from conventional is tray holdup. Holdup has no effect on the steady-state design of a conventional column. It certainly affects dynamics but not steady-state design. Column diameter is determined from maximum vapor-loading correlations after vapor rates have been determined that achieve the desired separation. Typical design specifications are the concentration of the heavy key component in the distillate and the concentration of the light key component in the bottoms. However, holdup is very important in reactive distillation because reaction rates directly depend on holdup (or the amount of catalyst) on each tray. This means that the holdup must be known before the column can be designed and before the column diameter is known. As a result, the design procedure for reactive distillation is iterative. A tray holdup is assumed and the column is designed to achieve the desired conversion and product purities. The diameter of the column is calculated from maximum vapor-loading correlations. Then the required height of liquid on the reactive trays to give the assumed tray holdup is calculated. Liquid heights greater than 10–15 cm (4–6 in.) are undesirable because of hydraulic pressure-drop limitations. Thus, if the calculated liquid height is too large, a new and smaller tray holdup is assumed and the design calculations repeated. An alternative, which may be more expensive in terms of capital cost, is to make the column diameter larger than that required by vapor loading.

CHAPTER IV

TERT-AMYL METHYL ETHER (TAME) PROCESS

4.1 Introduction *tert*-Amyl Methyl Ether (TAME) Process.

tert-Amyl methyl ether (TAME) is used as an oxygenate to gasoline. It is added for three reasons as follows:

1. To increase octane enhancement.
2. To replace banned tetraethyl lead.
3. To raise the oxygen content in gasoline.

The TAME train uses C5 fraction from a petroleum refinery and methanol as raw materials. TAME is produced by the catalytic etherification of isoamylenes [2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B)] with methanol. The three main reversible reactions in this process are the following:

$$\text{2M1B} + \text{Methanol} \leftrightarrow \text{TAME}$$

$$\text{2M2B} + \text{Methanol} \leftrightarrow \text{TAME}$$

$$\text{2M1B} \leftrightarrow \text{2M2B}$$

4.2 Reaction Kinetics

In this process, the reactions kinetics using simple power-law models are the following:

$$R_1 = A_{f1}e^{-Ef1/RT}x_{2M1B}x_{MeOH} - A_{b1}e^{-Eb1/RT}x_{TAME}$$

$$R_2 = A_{f2}e^{-Ef2/RT}x_{2M2B}x_{MeOH} - A_{b2}e^{-Eb2/RT}x_{TAME}$$

$$R_3 = A_{f3}e^{-Ef3/RT}x_{2M1B} - A_{b3}e^{-Eb3/RT}x_{2M2B}$$

When: A_f = The forward preexponential (kmol s^{-1} kg^{-1})

A_b = The backward preexponential (kmol s^{-1} kg^{-1})

E_f = The forward activation energy (kJ/mol)

E_b = The backward activation energy (kJ/mol)

x = The component liquid mole fraction

T = The temperature (K)

R = The ideal gas constant (J $mol^{-1}K^{-1}$)

The kinetic parameters for three reactions are shown in Table 4.1.

Table 4.1 The kinetic parameters. (Al-Arfaj and Luyben, 2004)

Reaction	A_f (kmol s^{-1} kg^{-1})	E_f (kJ/mol)	A_b (kmol s^{-1} kg^{-1})	E_b (kJ/mol)
Rxn1	1.3263×10^{8}	76.1037	2.3535×10^{11}	110.5409
Rxn2	1.3718×10^{11}	98.2302	1.5414×10^{14}	124.9940
Rxn3	2.7187×10^{10}	96.5226	4.2933×10^{10}	104.1960

4.3 Process Description

The process flowsheet for *tert*-amyl methyl ether is shown in Figure 4.4 which it consists of a prereactor, one reactive distillation column, and two conversional distillation columns. In 1999, the steady-state designs of a prereactor and a reactive-distillation column were proposed by Subawalla and Fair. Then, Al-Arfaj and Luyben (2004) presented the designed complete plant by using a pressure-swing azeotropic distillation for recovery the methanol reactant. The plantwide control structure was developed for three distillation columns with two recycles and two feed streams. The methanol fresh feed is essentially pure. The hydrocarbon feed is a mixed C5 stream that consists of 2M1B, 2M2B, n-pentane, i-pentane, 1-pentene, and cis2-pentene. That comes from an upstream catalytic cracking unit.

The fresh feed of methanol and C5s feed to prereactor. The prereactor is a tubular reactor. It is containing 9544 kg of catalyst and a catalyst bulk density of 900 kg /m^3. The reactor tube is 0.0254 m in diameter and 6 m in length. The number of tube is 3488 tubes.

Effluent of prereactor is fed to reactive distillation column (C1) at 1228 kmol/hr. The column has 36-stage and the reactor effluent is fed on stage 28. The numbering stages from top, stage 1 being the condenser. The excess methanol stream is fed on stage 23 of this column. The reactive stages in the column contain 1100 kg of catalyst/tray and catalyst is presented on stages 7–23 at 235 kmol/hr. The operating pressure is 4 bar. TAME is the highest boiling component. The reflux ratio is 4, that gives 99.2 mol% TAME at bottoms product. The distillate flowrate is 1103 kmol/hr. There is 27.8 mol% methanol that is near azeotrope.

The distillate of Column C1 (D1) is fed to stage 5 of first column pressure-swing. The first of two column pressure-swing (methanol recovery column) has 10-stage. The column operates at 2 bar. The reflux ration is 0.4. The bottom purity is 99.9 mol% methanol, which this stream is recycle back to mix with methanol fresh feed.

The distillate (D_2) stream from the methanol recovery column has a composition of 22.5 mol% methanol. This stream is fed to second column pressure-swing on stage 5 which the column is high pressure column. The separation operates at 10 bar and uses 10 stages for recycled back methanol (33.6 mol% methanol) at the top of column to column C2. The bottom (B3) is separating C5s product stream.

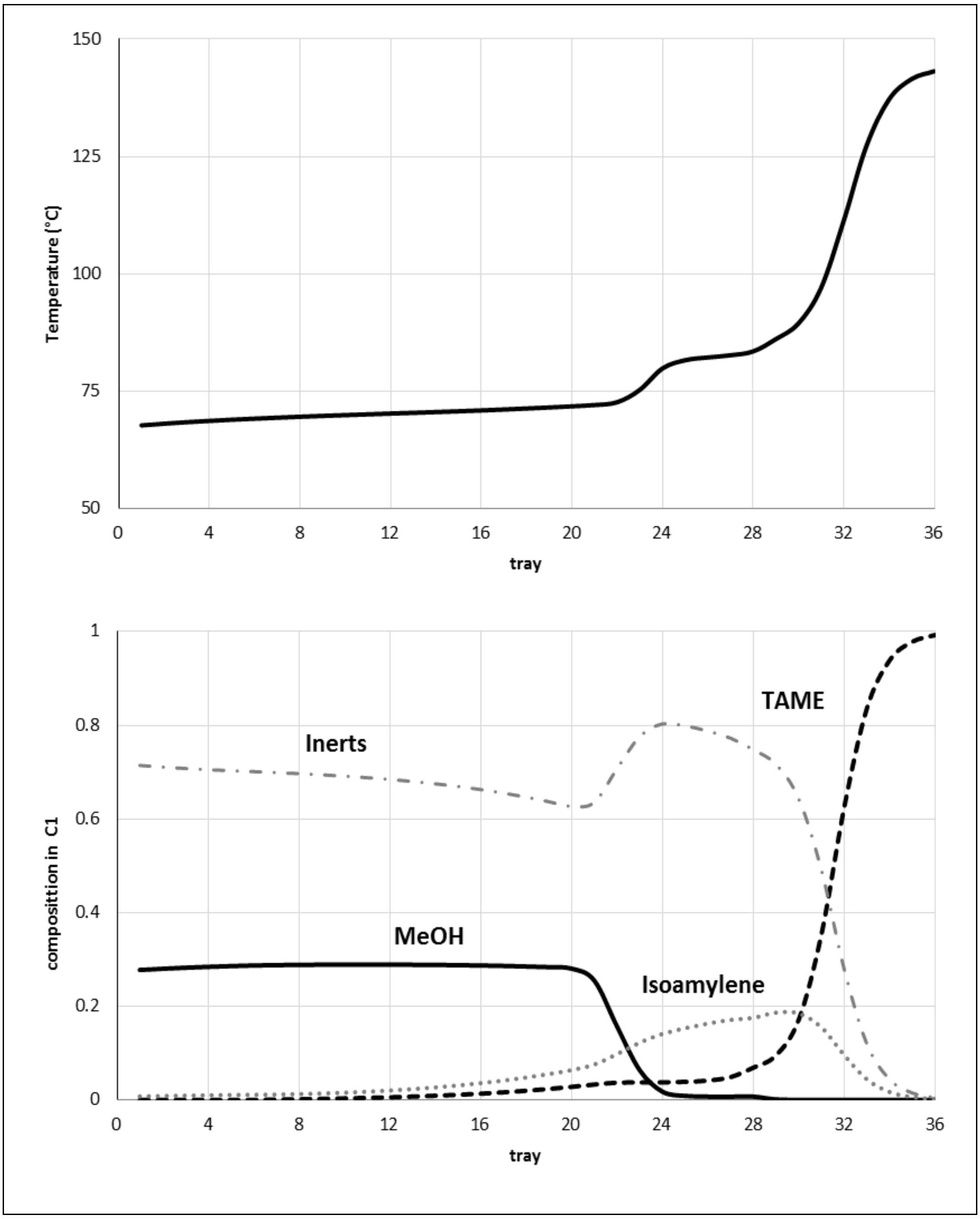


Figure 4.1 Temperature and composition profile of column C1

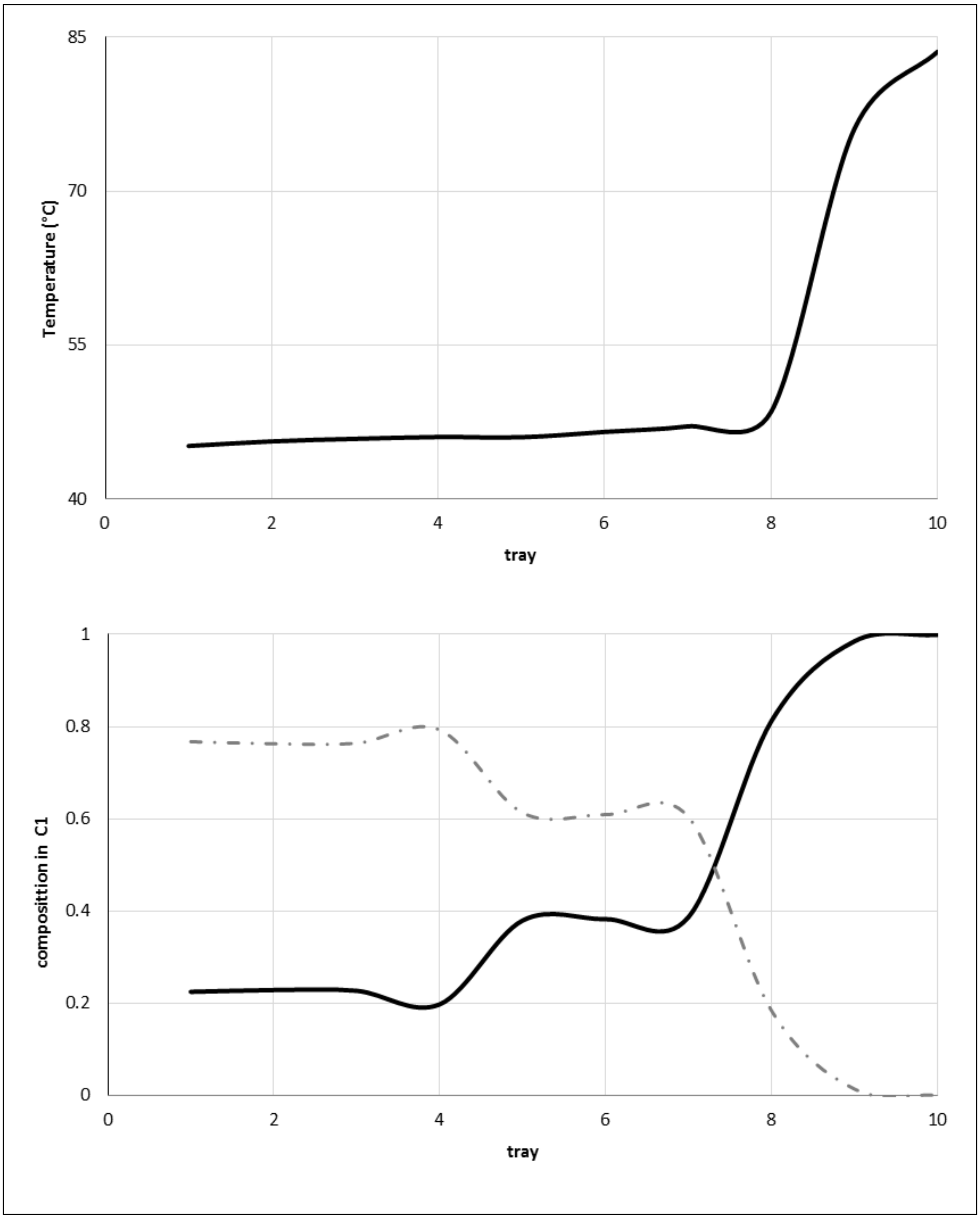


Figure 4.2 Temperature and composition profile of column C2

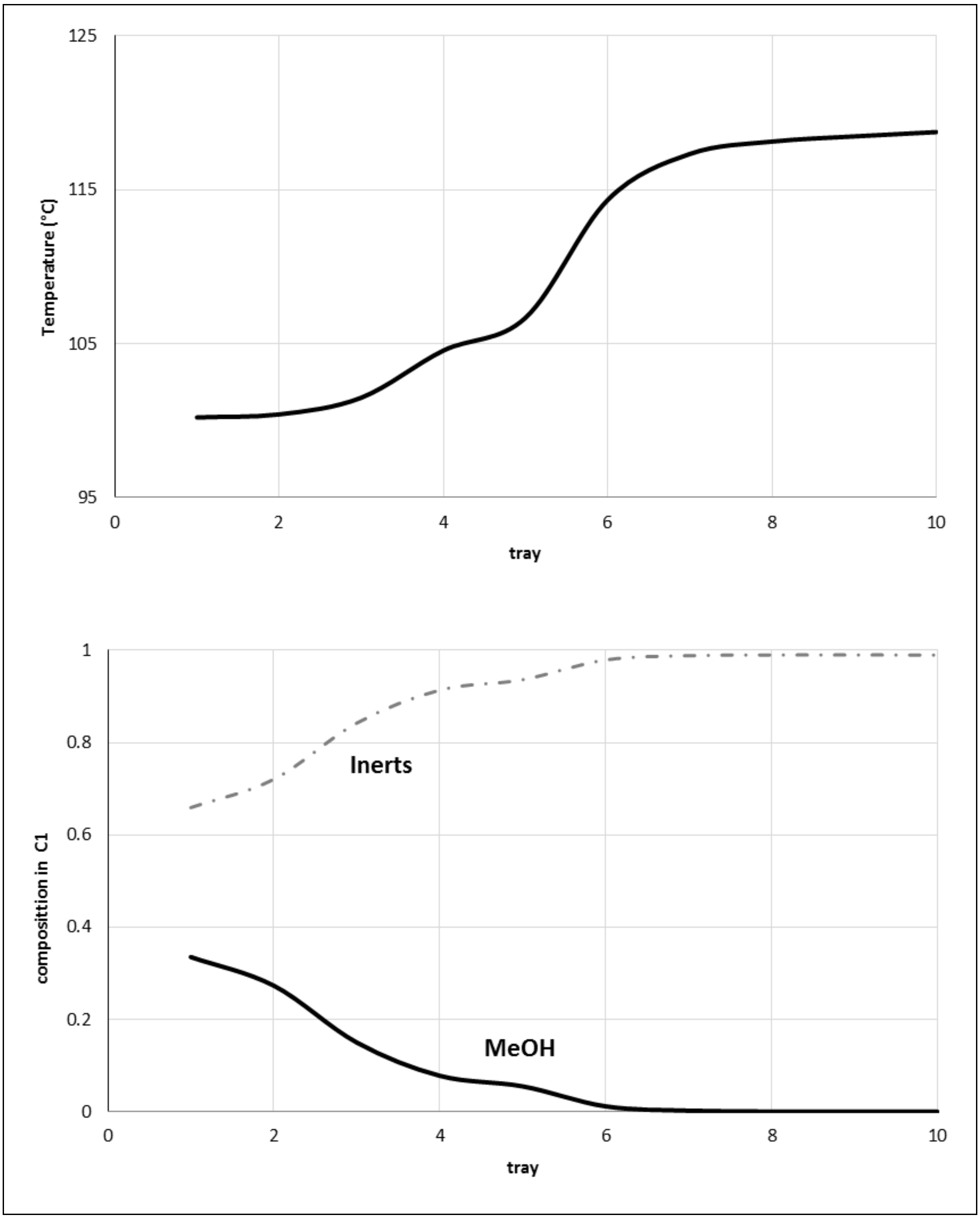


Figure 4.3 Temperature and composition profile of column C3

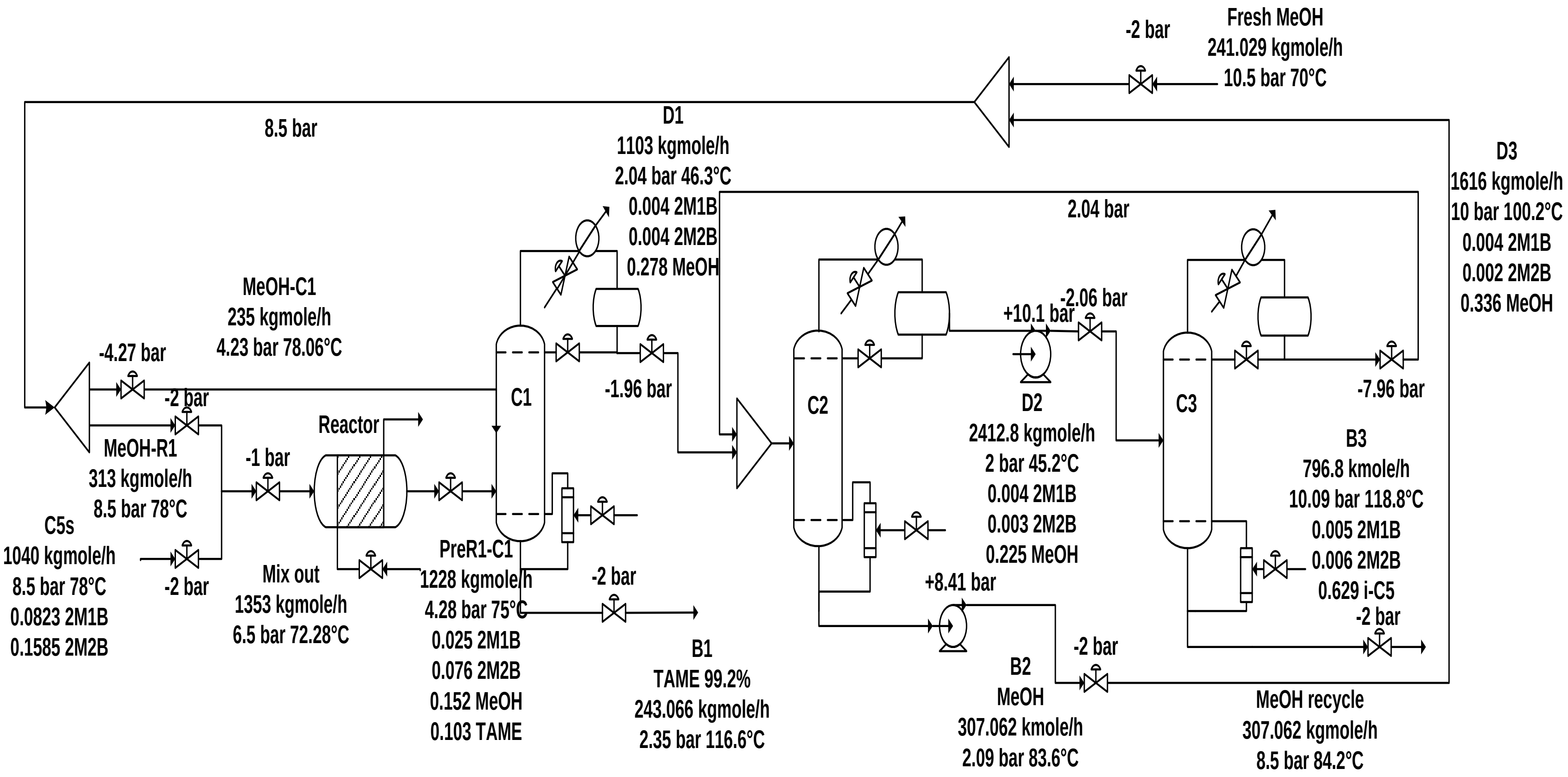


Figure 4.4 *tert*-Amyl Methyl Ether Process flowsheet

4.4 Plantwide Control Design Procedures

The new plantwide control design procedure emphasis on maintaining the plant operating conditions, i.e. establishing a fixture plant. The amount of components is accounted by regulating the material quantifiers which are location within the plant indicating the amount of the components. The material quantifier is a more general term than the material inventory. Additionally, the entered disturbance must be forced to leave the process plant at the nearest exits to avoid disturbance propagation through the plant. The plantwide control structure design is indeed a structural decision about placing control loops though out the plant to above objectives. It is divided into two levels: plant level and unit level designs. The new design procedure is carried out in eight steps, as following:

Step 1: Gather relevant plant information and control objective including constraints for control. Before initiating work on the control structure design, is it necessary to obtain all information relevant to process control. The process objectives and constraints will determine the lower/upper bounds on the control variables as well as set points on quality variables.

Step 2*:* Plant Analysis.

2.1 Control degree of freedom (CDOF).List manipulated variables (control degree of freedom, CDOF).

List all control variables:

I. An independent stream must have a control valve (1 DOF) you cannot place two control valves on a single stream.
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. For example, an isothermal reactor need heat input to keep its temperature constant, while an adiabatic reactor has zero degree of freedom.
V. A flash separator has two degree of freedom.
VI. A simple distillation column has five degree of freedom.

How to pair manipulated and controlled variables:

VII. A control and manipulated variables must have strong causal relationship (high gain)
VIII. The manipulated variables should not be far from the control variables (zero or minimal dead time)
IX. The time constant of the quality loops should be short and the time constant of the inventory loops should be longer.
X. The manipulated variables should not be saturated for the whole range of the disturbances.

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

2.2 Heat pathway.

Three different "heat pathways" introduced in Luyben (1997) is also useful in plant analysis from a plantwide perspective. The first pathway is from inside the process and flows out to the environment heat generated by exothermic reactions and by degradation of mechanical work. A second pathway carries heat from utilities into the process and to the environment. The third pathway is internal to the process. The heat flow is circular and its magnitude depends upon the heating and cooling needs and the amount of heat integration implemented. The level of heat circulated of the third pathway can be adjusted to optimize the energy used (step 7). The heat pathway is used to design control loops to reject the disturbances or to maintain the product qualities.

The fourth pathway is introduced here. This pathway is accounted for the enthalpies entered and leaved the plant via process stream. The third pathway can be optimized by adjusting its enthalpy level. This is done in step 4.1.

2.3 Material pathway.

The concept of material pathway is introduced here. The pathway is the flow path of a component from an entry point or an originated point to an exit point or an end point. The material pathway is useful for component balance and in control design as discussed in section 3 and section 4.2.

2.4 Material quantifier.

The notion of material quantifier is also introduced here. In order to regulate a component balance in a process plant, a place representing the amount of material in the plant must be identified to provide its handle. A material balance for each component must be satisfied. From the viewpoint of individual units, chemical component balancing is not a problem because exit streams from the unit automatically adjust their flows and compositions. However, when we connect units together with recycle streams, the entire system behaves almost like a pure integrator in terms of the reactants. For example, we want to minimize the loss of reactants exiting the process since we would lose its value. This means we must ensure that most of reactant fed to the process is consumed by the reactions. If reactants increase, the reactor conditions must be adjusted to consume more reactants. In the case that increasing one reactant composition will decrease the other reactant composition with an uncertain net effect on reaction rate. If this case is not effectively handled, the process will shut down when manipulated variable constraints are encountered in the separation section. Luyben (1997) gives a more complete discussion of this phenomenon. The features of material recycle and chemical component inventories mentioned above which have profound implications for a plant's control strategy (Luyben, 1997) can be handled quite readily by making use of quantifiers. By locating a quantifier, we can regulate the quantity of a component quantified by using its handle.

2.5 Reaction section

Practical aspects of industrial reactor control should be studied to obtain necessary information for reactor section control design. Since relatively little literature on chemical kinetics and reactor engineering has been written on the practical aspects of industrial reactor control (Luyben, 1998).

2.6 Separation section

The sensitivity test is suggested to be done on the changing of composition, total flow, temperature, and component flow while keeping the reboiler heat duty and reflux flow or reflux ratio constants. This sensitivity test is to spot the tray with the largest changes in temperature from the initial steady state. This is the exact situation happen right after the disturbance entering the column, when the column temperatures are controlled by manipulating the reboiler heat duty and reflux flow or reflux ratio. Hence the trays with largest changes may be good locations to control.

Step 3: Establish fixture plant.

The principal idea of establishing a fixture plant is first to have an entire plant fluid-filled and a material-balanced. This idea is similar to creating *hydraulic* control structure proposed by Buckley [7]. By establishing a fixture plant we mean creating a material-balanced process plant:

3.1 keep the materials entered and reentered fixed.

$$q_i\ (t)+q_r\ (t) = \text{constant} \tag{1}$$

This leaves the recycle streams free to adjust; one degree of freedom is added to the process.

If the composition of the recycle streams differ from the fresh feed stream significantly, each stream are separately controlled:

$$q_i\ (t) = \text{constant} \tag{2}$$

$$q_r\ (t) = \text{constant} \tag{3}$$

In this settlement, the flow of recycle stream cannot be used to regulate, e.g., the level of the reflux drum.

3.2 Regulate the production rate.

3.2.1) Consume the limiting reactant. The limiting reactant should be totally consumed at the reactor for the economic reason. Determine the most appropriate manipulate variable to control this, i.e. the reactor temperature, the reactor pressure, or the reactor holdup.

3.2.2) Regulate the production rate. The product rate can be regulated through 3.2.1. If this is done and the production rate does not reach the objective or the production demand, the limiting reactant feed rate must be increased. The reaction information about the accumulation or depletion of the limiting reactant must be used to determine the control strategy. However the design constraint may limit this strategy concerning increasing the reactant feed rate.

3.3 adjust the flow of exit material streams (products, by-products, and inert) according to their accumulations.

$$q_o(t) = q_i(t) - dq/dt \qquad (4)$$

3.4 Control the amount of the rest of the component at their quantifiers, i.e. the indicators of the representative accumulation, for the rest of the components and design the control loops to regulate their inventories in the plant. The quantifier can be volume (mass), pressure, or flowrate.

$$q_p(t) = -dq/dt \qquad (5)$$

$$q_p(t) = \text{constant} \qquad (6)$$

In retrospect, the material balances are checked in this step, since the control loops generated accomplish the plantwide material balances. Therefore, it is guaranteed the plantwide inventory will be regulated.

Step 4: Disturbance Management

In this step, the disturbances are handled by configuring the control loops employing the principle of disturbances management:

4.1 Heat Disturbance Management

The Heat disturbance is divided into 2 categories. Heat Disturbance Category 1 (HDC1) is the heat disturbance that does not directly effect on product qualities, such as heat disturbance in a process stream toward to a heater, a cooler, or a process-to-process heat exchanger. Heat Disturbance Category 2 (HDC2) is the heat disturbance that will affect the product qualities, such as heat disturbance in a process stream toward to a reactor or a separator.

4.1.1) Direct the thermal disturbances that are not directly related to quality to the environment via the next and nearest exit points, usually heaters or coolers, to keep the thermal conditions of process stream fixed. 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 thermal disturbance that related to quality in order to maintain the product specification constraints.

4.2 Material Disturbances Management.

The configuration of the control loops depend on the desired material pathways. The pathways can be obtained by analyzing the results of the material disturbance tests. The material disturbances can be generated at reactors and separators, besides coming with feeds and recycle streams. So if the feeds and recycle streams are fixed, the only places that alter the material (total or component) flowrates are the reactors and the separators. At reactor, its inlet temperature is adjusted in order to keep the reactor component flowrate or its composition in outlet stream. The decision of whether how to choose to control the component flow or the composition or not to control is based on the profit maximization or the smooth operation policies.

The control structure we select must reject the disturbance to the desired pathways. As in the case of heat disturbance management, we direct the material disturbances to the environment via the next and nearest exit points, usually separators, to keep the material conditions of process stream fixed.

Step 5: Design the rest of the control loops.

5.1 Design the control loops for the remaining control variables, i.e. the rest of the inventories.

5.2 Adding enhanced controls, i.e. cascade, feed forward controls.

Step 6: 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 7: Optimize economics and/or improve control performance.

For example, the controls scheme/structure of the reactor (e.g. temperature/composition sensor location), the control scheme of the distillation column (e.g. reflux to feed ratio control), the optimal operating temperatures of the reactors, the recycle flowrates, the sequence of separation, etc. If the opportunity of optimization exists, we might backtrack to the previous step as dictated.

Step 8: Validate the designed control structures by rigorous dynamic simulation. The measures can be costs, raw material and energy consumptions, control performances of the total plant or some selected loops, etc.

CHAPTER V

THE DESIGN CONTROL STRUCTURE OF *TERT*-AMYL METHYL ETHER PROCESS

In this research, Wongsri's plantwide control structure design procedure was applied to pressure-swing *tert*-amyl methyl ether (TAME) process. Two new control structures obtained were evaluated and compared with the control structure of Luyben (2004). In commercial process simulator, dynamic simulation for a flowsheet with a tubular reactor would not operate properly. Therefore, Al-Arfaj and Luyben (2004) presented to a tubular reactor was replaced by two continuous stirred tank reactors in series. Both reactors were operated at 82°C and volumes 10 m^3 as shows in Figure 5.1.

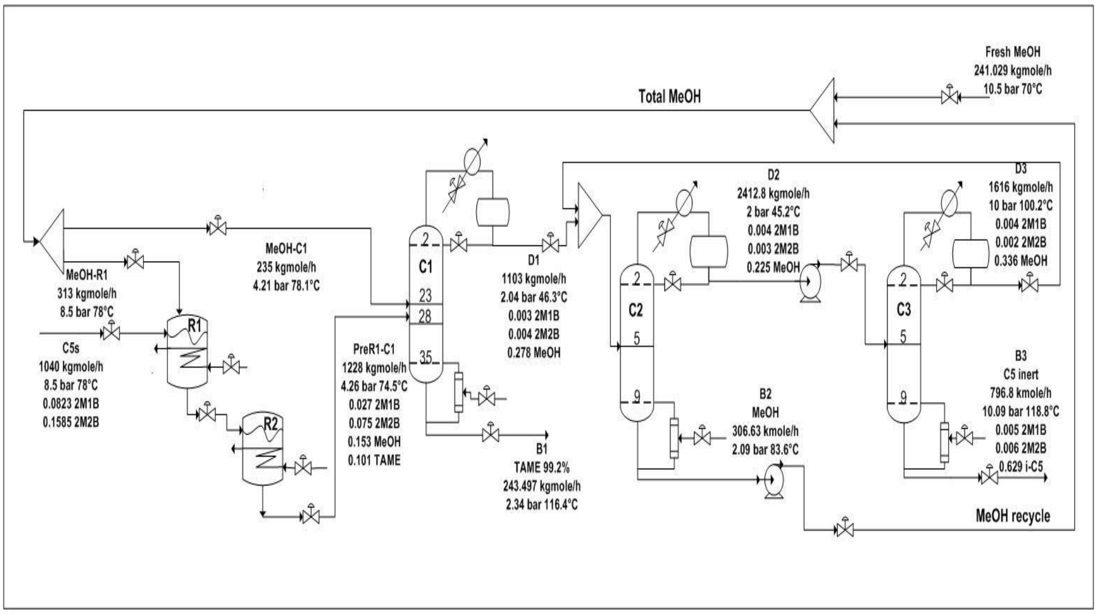


Figure 5.1 The flowsheet of *tert*-amyl methyl ether with CSTRs in series

5.1 New control structures

The new control structure design was determined as follows:

***Step 1**:* Gather relevant plant information and control objective including constraints for control.

Plant information:

1. Operating temperatures in reactor R1 and R2 are 82 ˚C.
2. Column C1 (Reactive distillation column) operates at 4 bar.
3. Concentration of TAME out of column C1 is better than 99.1mol%.
4. Column C2 (Methanol recovery column) operates at 2 bar.
5. Methanol out of bottom column C2 is better than 99.9 mol%.
6. Column C3 (C5s column) operate at 10 bar.

Control objectives:

1. The plant operation must be smooth and stable.
2. The control structures designed must be able to reject disturbances efficiently.
3. The purity of TAME product is more than 99.1mol%.
4. The production rate is about 217,408 tons/year.

Step 2: Plant Analysis.

2.1 List Control degree of freedom (CDOF).

Table 5.1 Manipulated variables (control degree of freedom, CDOF).

Unit	**Manipulated variable**	**Quantity**	**CDOF**
Independent streams	Flowrate	3	3
Reactor	Outlet flow Cooling flow	2	4
Distillation column	Distillate flow Bottom flow Reboiler heat remove Condenser heat input	3	15
Total control degree of freedom			**22**

2.2 Heat pathway.

This step was to identify four heat pathways for *tert*-amyl methyl ether process were shown in Figure 5.2. The first pathway (Path#1) was generated by exothermic reactions of TAME production and by degradation of two pumps work then flows out to the environment. Second pathway (Path#2) was carried heat from utilities into all units in process to the environment. Third heat pathway (Path#3) was the head circulated in the process. The last pathway (Path#4) was accounted for the enthalpies entered with two fresh feed streams and leaved the plant via TAME and C5s production streams at bottom of column C1 and C3, respectively.

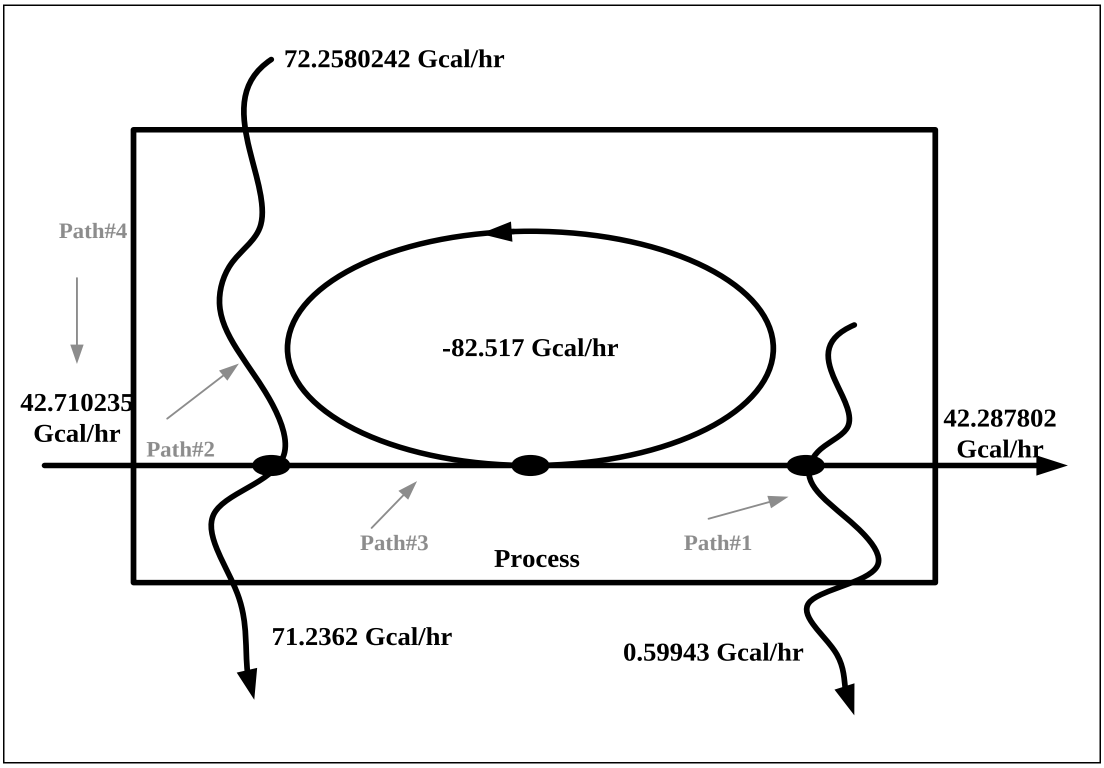


Figure 5.2 Heat pathways of *tert*-amyl methyl ether process

2.3 Identify material pathway.

Figure 5.3-5.6 shows pathways of all materials in this process. The dashed line was represented road of each material. The C5s fresh feed consist of isoamylene and inerts, all of isoamylene had been used in reaction section and inerts left the process at bottom of C3. Methanol was recycled in process. The production (TAME) occurred in prereactors and reactive distillation column then it was saparated at bottom of column C1.

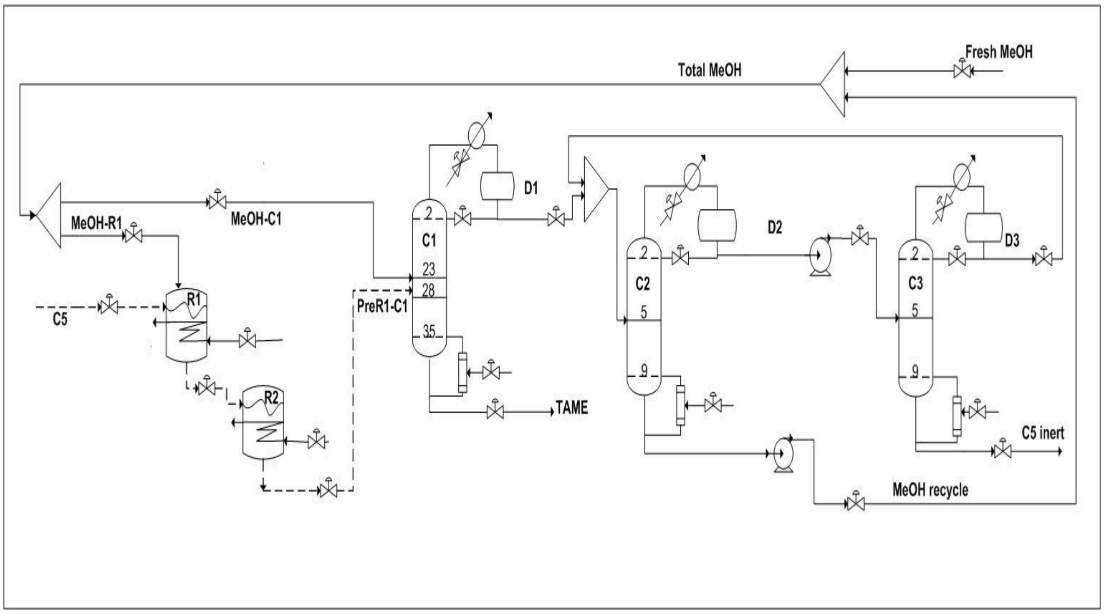


Figure 5.3 Pathway of isoamylene

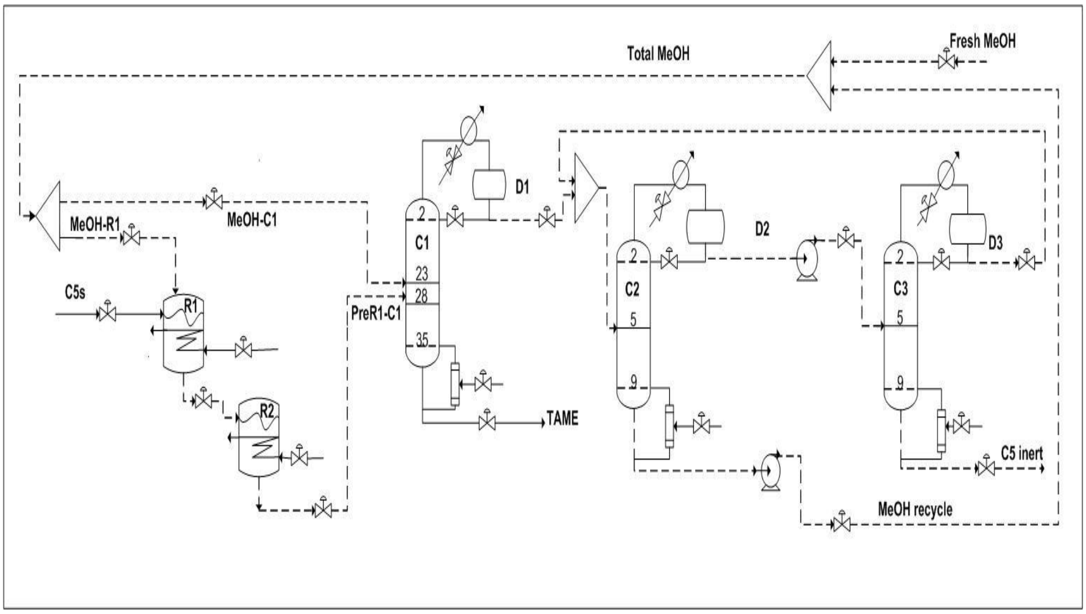


Figure 5.4 Pathway of methanol

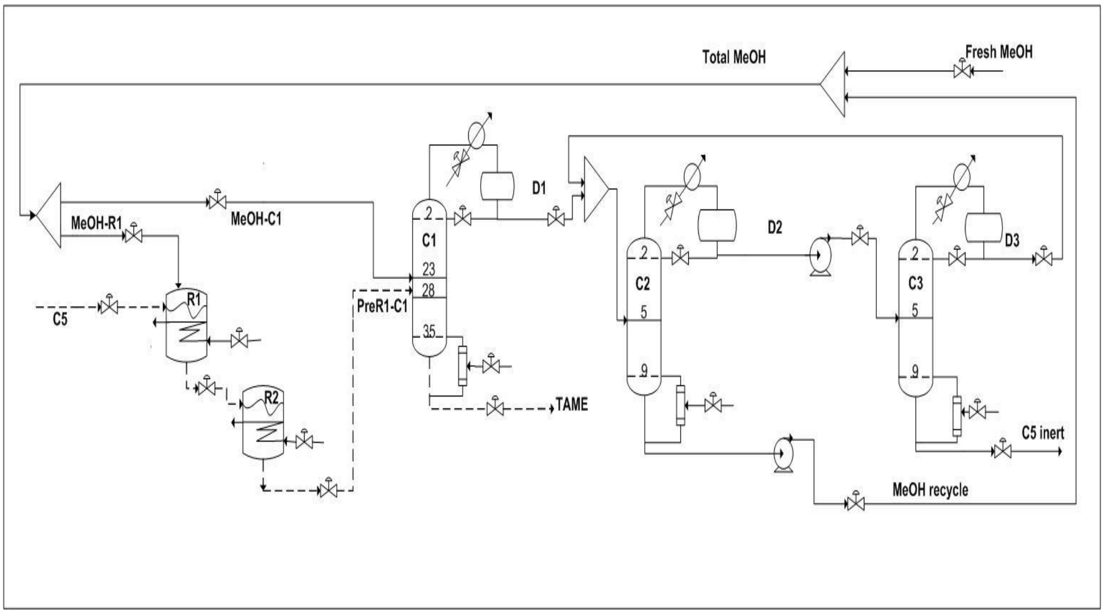


Figure 5.5 Pathway of *tert*-amyl metyl ether

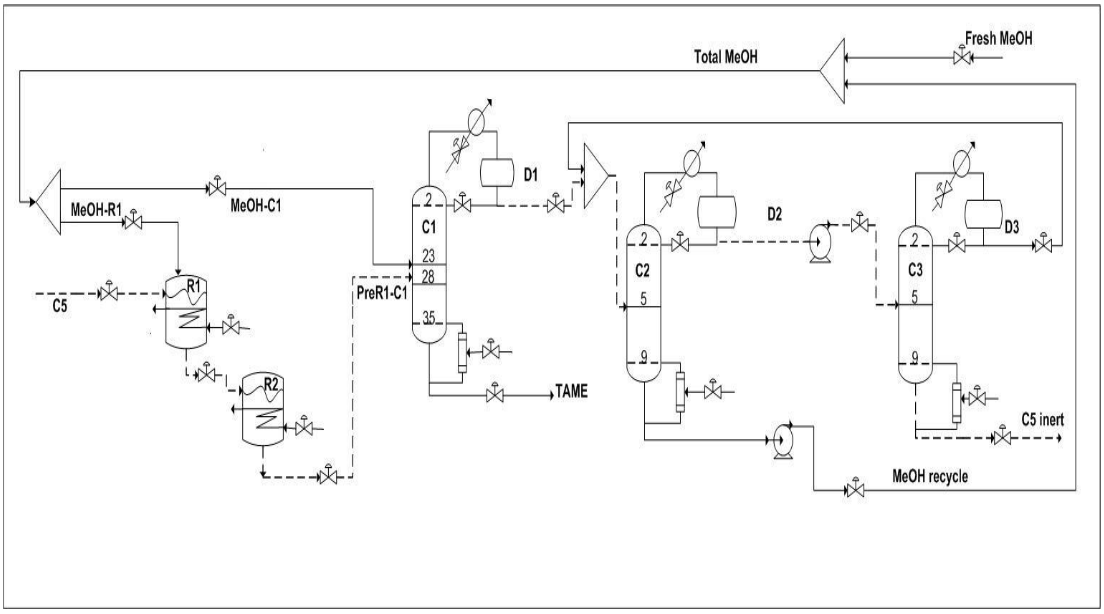


Figure 5.6 Pathway of inerts

2.4 Identify material quantifier.

Figure 5.7-5.10 shows quantifier of all materials in process. First, isoamylene quantifier was determined in C5s fresh feed. Second, methanol quantifier, the best place for representation was the place where fresh feed and recycle combined. Third, TAME quantifier was the liquid level of bottom of C1. The last, inerts quantifier located in the liquid level of bottom of C3.

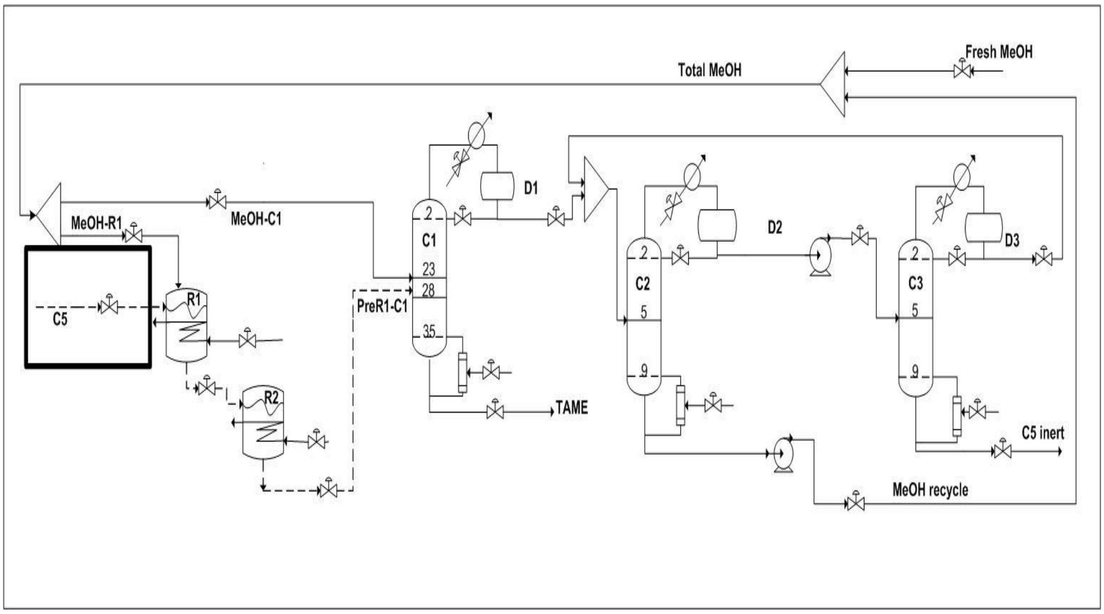


Figure 5.7 Quantifier of isoamylene

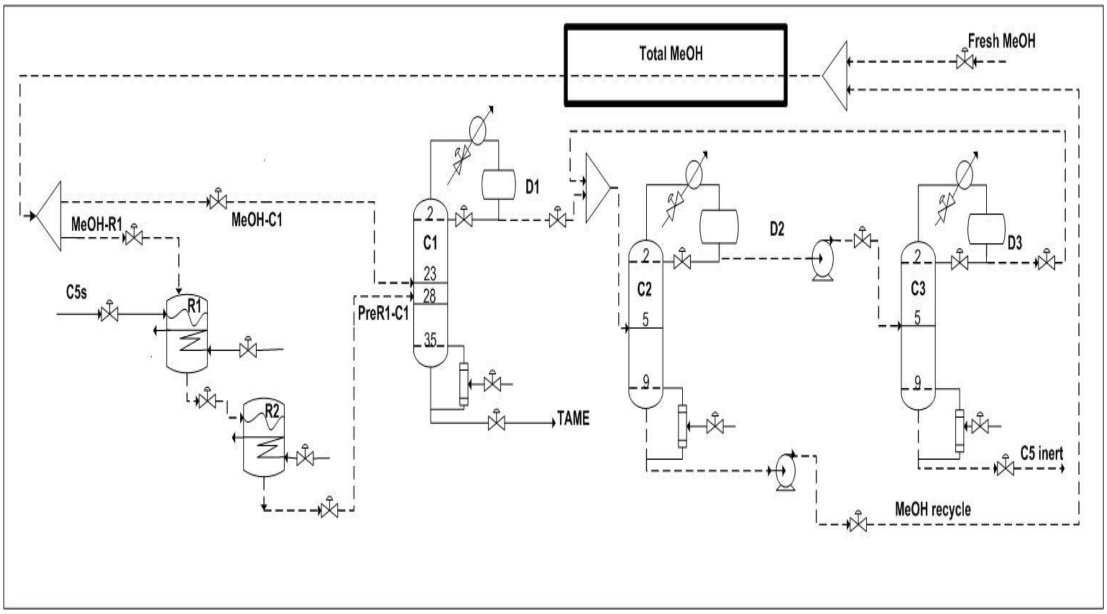


Figure 5.8 Quantifier of methanol

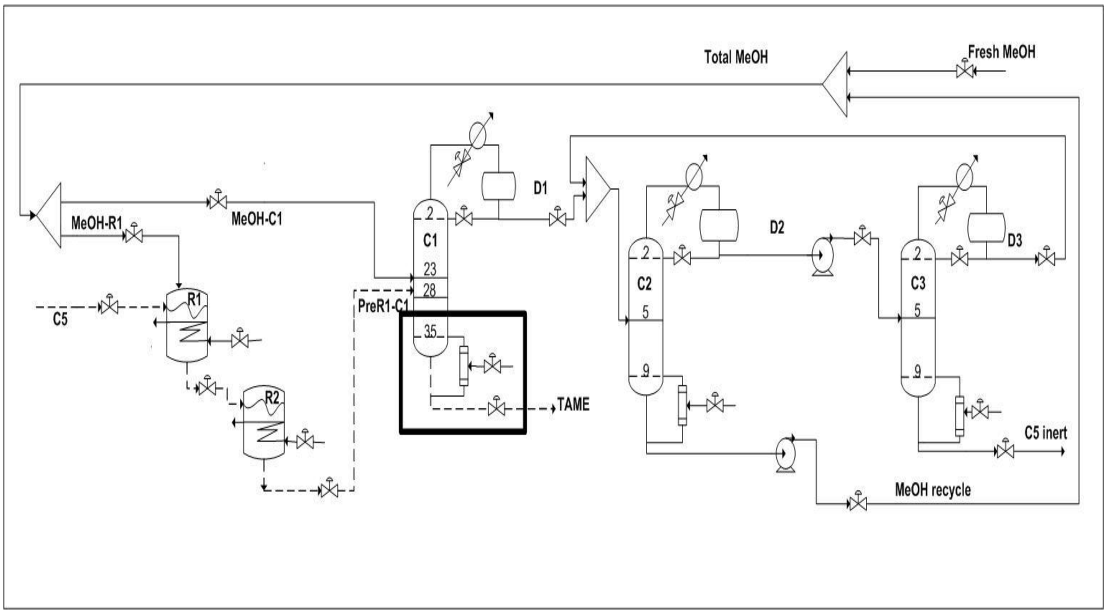


Figure 5.9 Quantifier of *tert*-amyl methyl ether

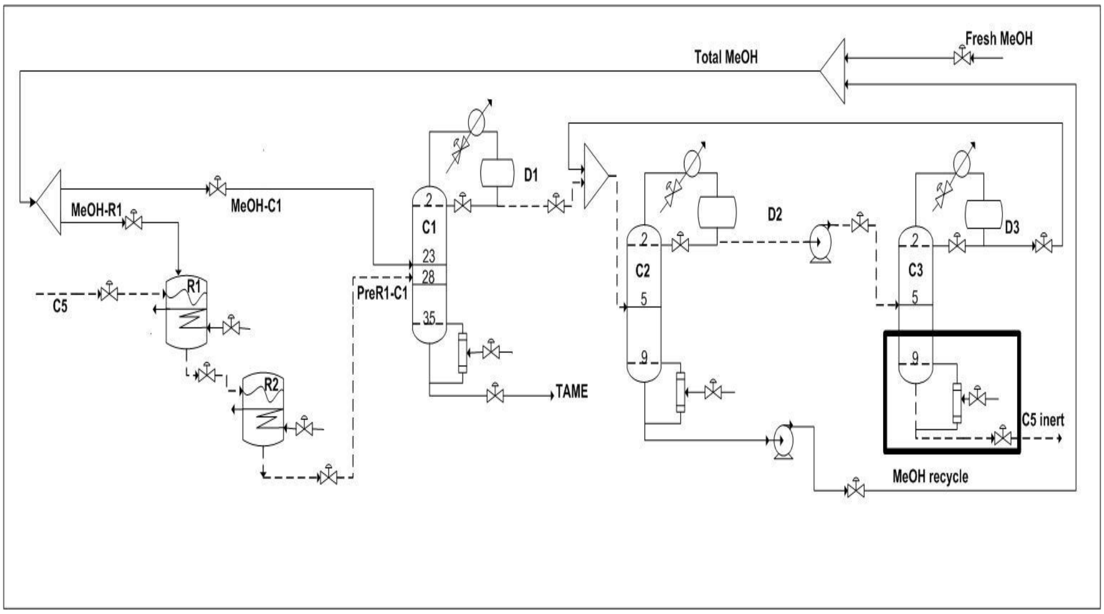


Figure 5.10 Quantifier of inerts

2.5 Reaction section.

2M1B + methanol ↔ TAME (etherification) (1)

ΔH_{rxn} = -34440 kJ/kmol

2M2B + methanol ↔ TAME (etherification) (2)

ΔH_{rxn} = -26760 kJ/kmol

2M1B ↔ 2M2B (isomerization) (3)

ΔH_{rxn} = -7670 kJ/kmol

When ΔH_{rxn} is heat of reaction.

All equations of reaction were exothermic reaction. It occurred in both continuous stirred tanks and reactive distillation column.

2.6 Separate section (Disturbances tests to find the best place to detect the disturbances.)

The disturbances tests at steady state were considered for finding the best place to detect the disturbances. It was possible to achieve a good product quality by controlling the temperature at that tray. In this work, the best place to detect the disturbances was determined from two methods. First, the sensitivity test is suggested to be done on the changing of feed flow, feed composition, feed temperature, and feed component flow while keeping the reboiler heat duty and reflux ratio constants. Table 5.2 shows temperature profile in column C1, C2, and C3 at steady state. Column C1 the largest changes in temperature from initial steady state was tray 34.

For column C2, the temperature profile of all disturbances tested had the same response as Table 5.3. Tray 9 was the location where the largest changed both positive and negative changed.

Table 5.4 shows the temperature profile in Column C3. The best place to detect the disturbances in sensitivity test was tray number 4. That had the most changing for Flow, Temperature, and component disturbances.

Table 5.2 Temperature profile of the sensitivity test for column C1 when a.) C5s feed flow change, b.) C5s feed composition change, c.) C5s feed temperature change, and d.) C5s feed component flow change

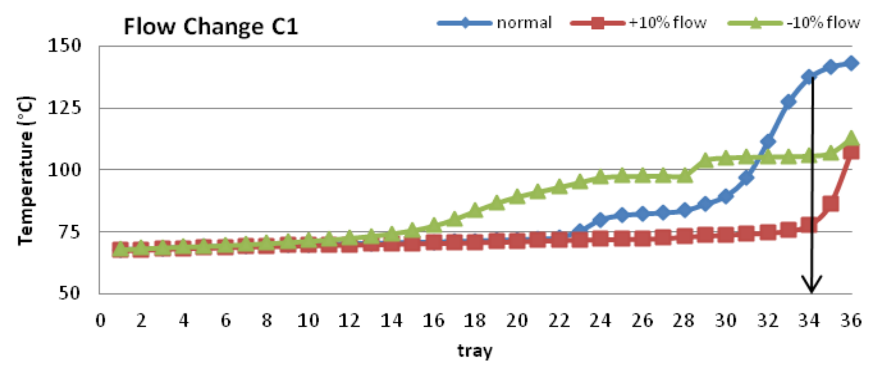
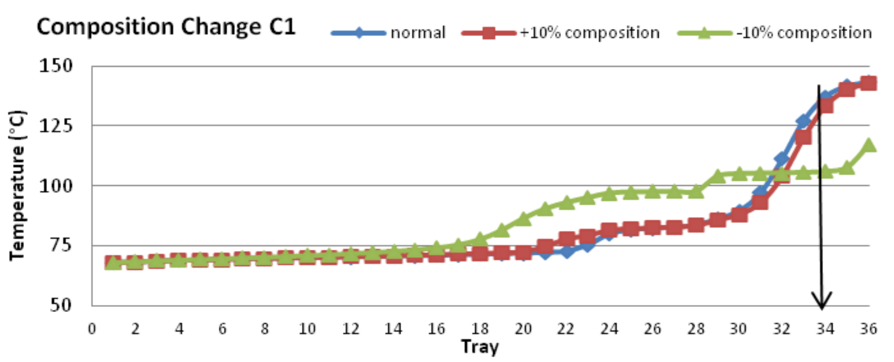
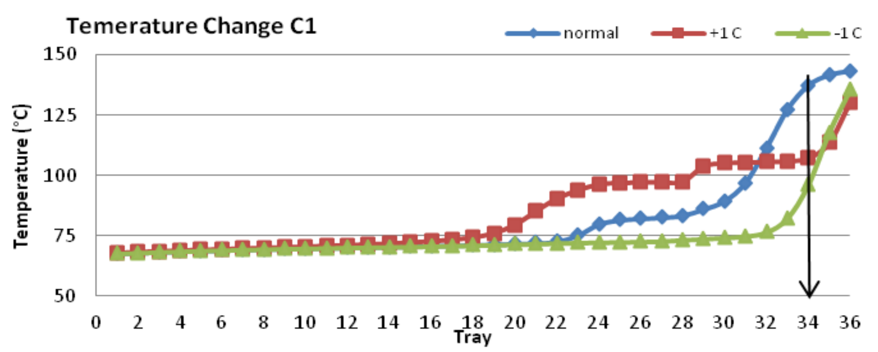
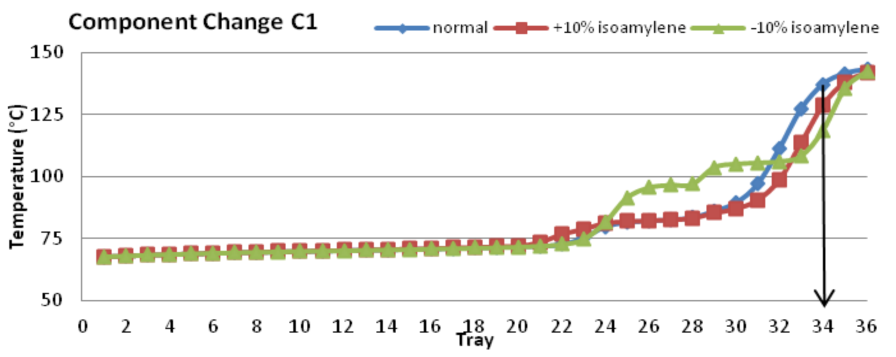
a.)	
b.)	
c.)	
d.)	

Table 5.3 Temperature profile of the sensitivity test for column C2 when a.) Feed flow change, b.) Feed composition change, c.) Feed temperature change, and d.) Feed component flow change

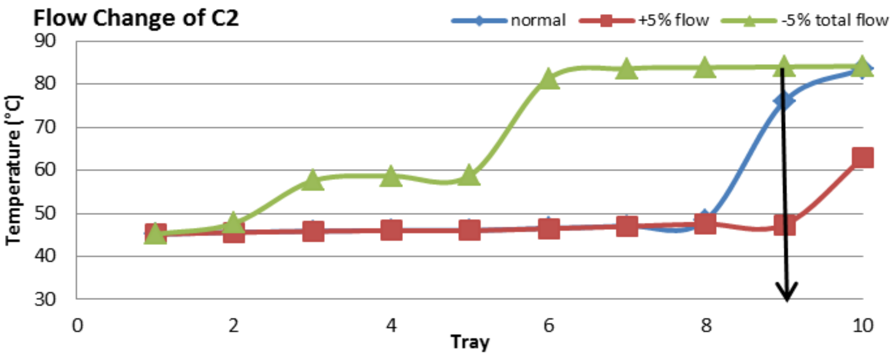
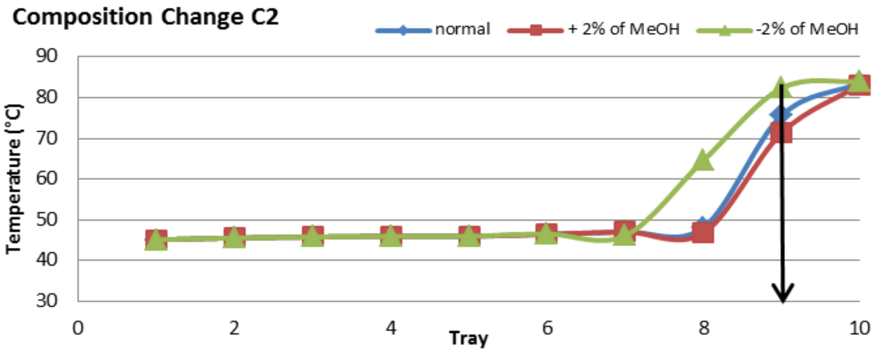
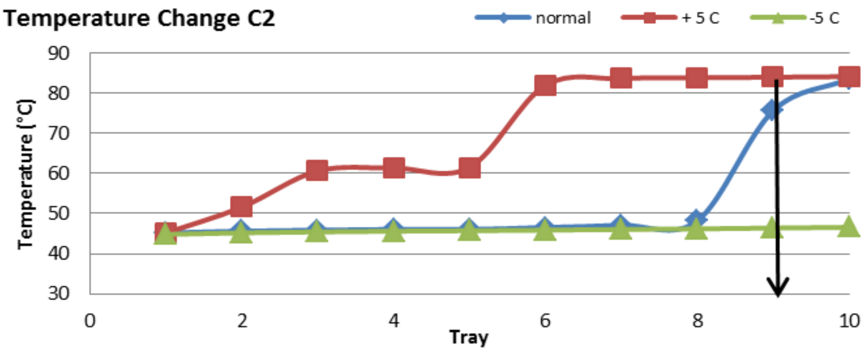
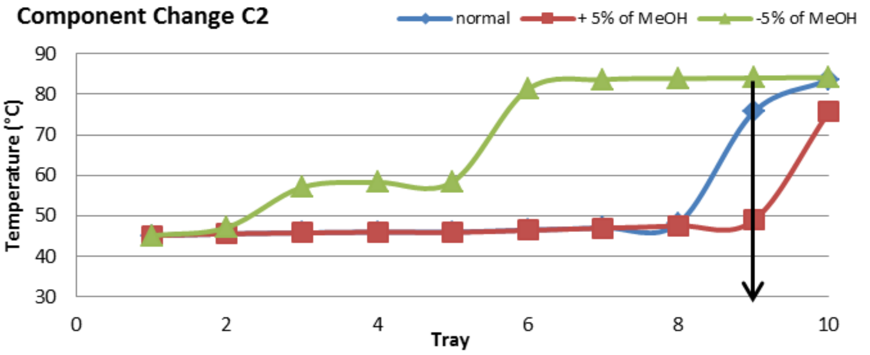
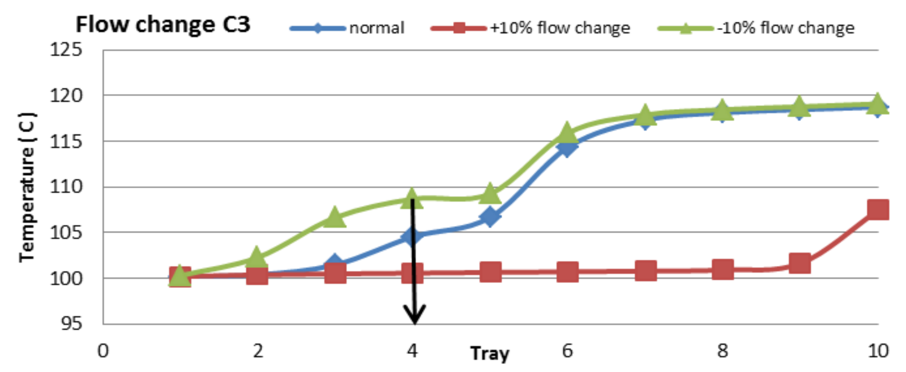
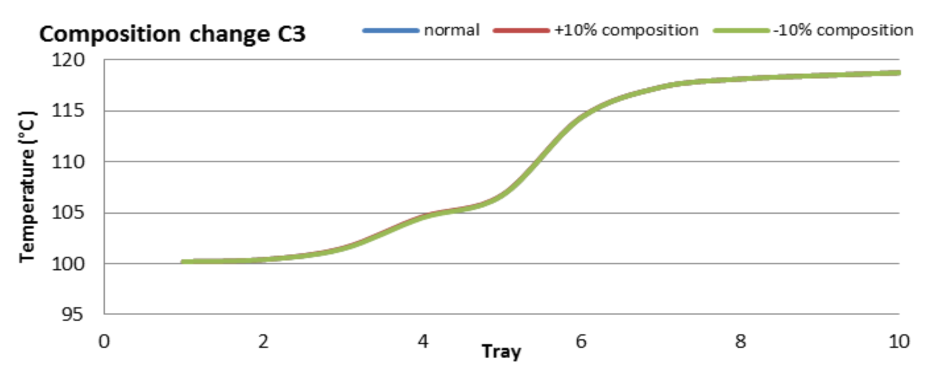
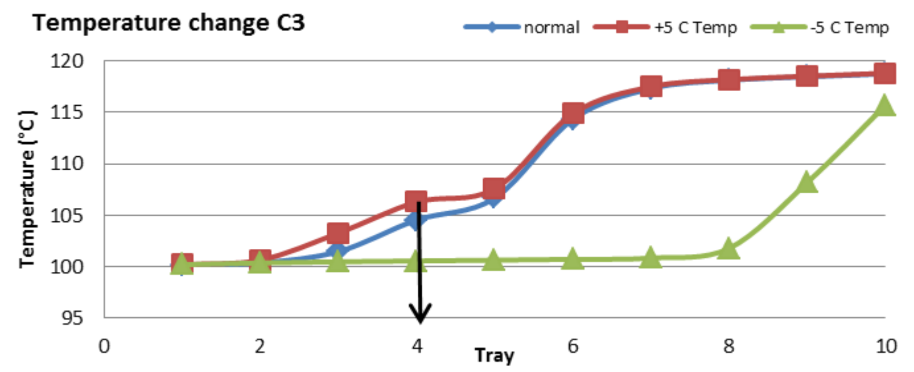
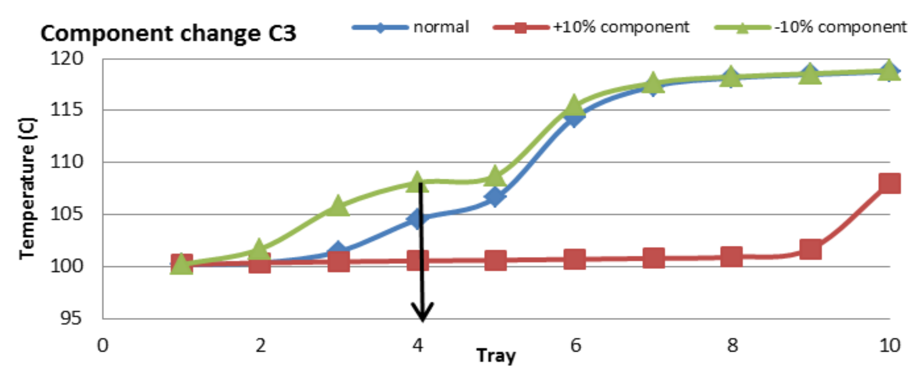
a.)	
b.)	
c.)	
d.)	

Table 5.4 Temperature profile of the sensitivity test for column C3 when a.) Feed flow change, b.) Feed composition change, c.) Feed temperature change, and d.) Feed component flow change

a.)	
b.)	
c.)	
d.)	

Another method, Luyben, 2011 presented method to selecting temperature location that remaining control variables are reflux and reboiler heat input. They fixed the reflux flow rate and made a small (0.1%) change in the reboiler heat input. The resulting changes in the tray temperatures from the original steady state were calculated. The tray with the largest changes in temperature may be a good spot to use for temperature control. In a commercial process simulator that was used with this work could not fixed reflux flowrate. Thus, reflux ratio was represented. From Table 5.5-5.7 shows resulting changes in the tray temperatures from the original steady state of three columns. Trays 32, 9 and 4 were the trays with largest changes of temperature profile in C1, C2, and C3, respectively.

Table 5.5 Temperature profile of open loop sensitivity analysis for column C1 when a.) Fix reboiler duty and vary reflux ratio, b.) Fix reflux ratio and vary reboiler duty

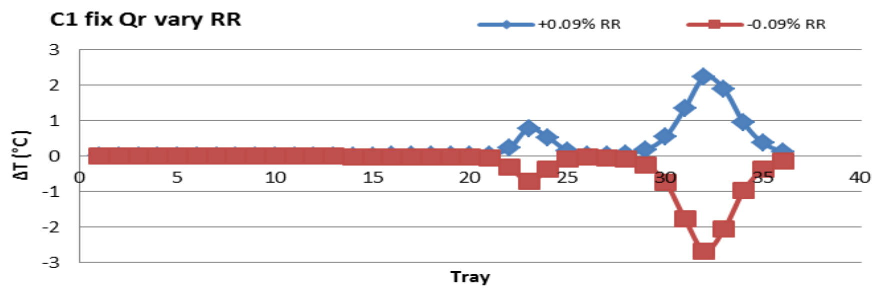
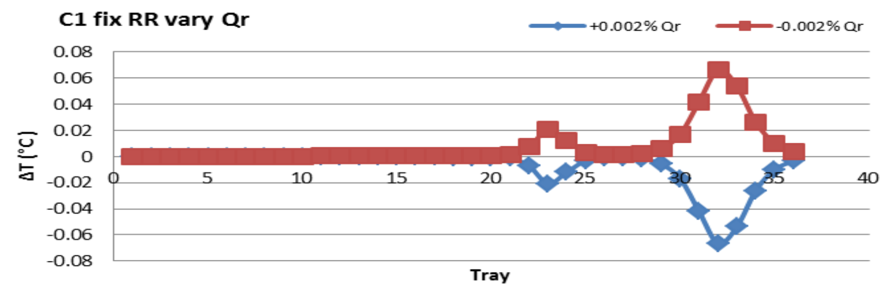
a.)	
b.)	

Table 5.6 Temperature profile of open loop sensitivity analysis for column C2 when a.) Fix reboiler duty and vary reflux ratio, b.) Fix reflux ratio and vary reboiler duty

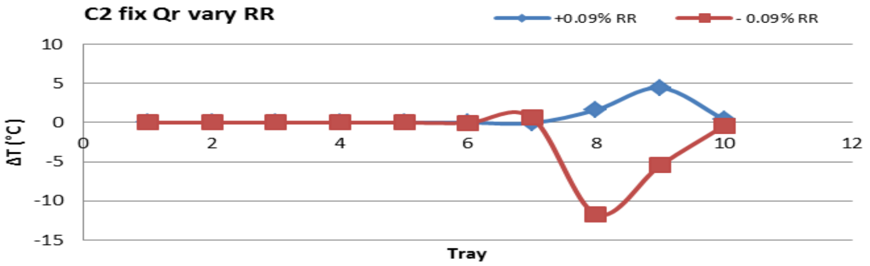
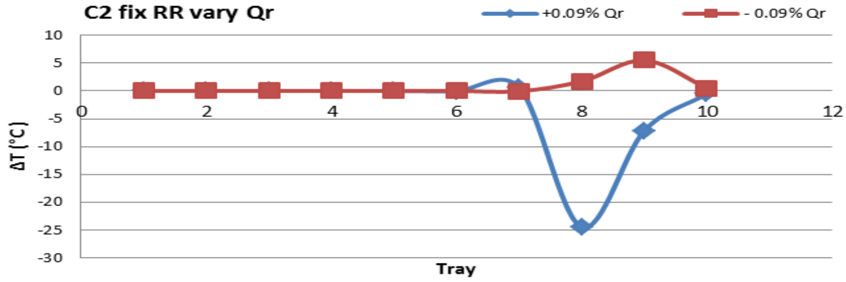
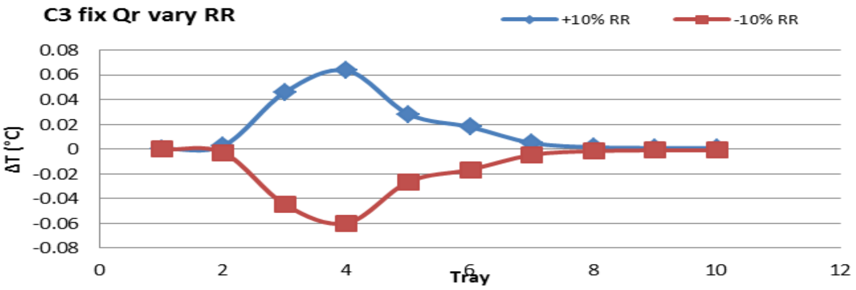
<table>
<tr><td>a.)</td><td>
</td></tr>
<tr><td>b.)</td><td>
</td></tr>
</table>

Table 5.7 Temperature profile of open loop sensitivity analysis for column C3 when a.) Fix reboiler duty and vary reflux ratio, b.) Fix reflux ratio and vary reboiler duty

<table>
<tr><td>a.)</td><td>
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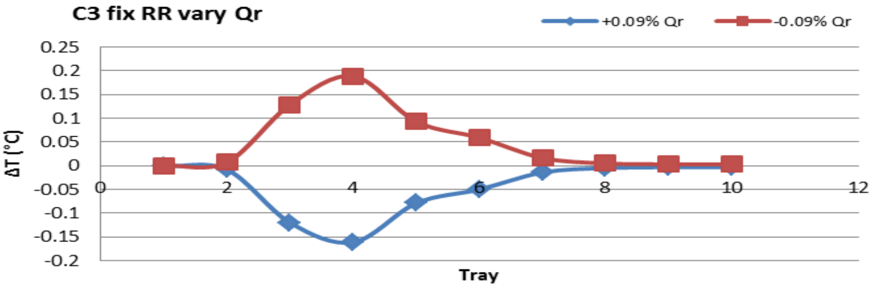
<tr><td>b.)</td><td>
</td></tr>
</table>

From two methods, the largest change of temperature in reactive distillation column (C1) was not the same tray. Therefore, the dynamic simulation was considered for comparing the best location for control temperature. Figure 5.11 shows the diagram of column C1. In dynamic simulation test, other control loops were installed as the same. All of the tests were done by step changed at 1.5 hours. The results show in Table 5.8-5.11. From the ±10% total flow changing and ±5°C temperature changing in PreR1-C1 stream, both control structure gave the purity of TAME approach the set point but tray 32 closer than tray 34. On the other hand, ±10% composition and component of isoamylene in PreR1-C1 stream were examined. Control temperature on tray 34 provided the better product composition than tray 32, explicitly. So tray 34 was the best location for control temperature in column C1 because it gave a TAME purity close to the specification for all disturbances test.

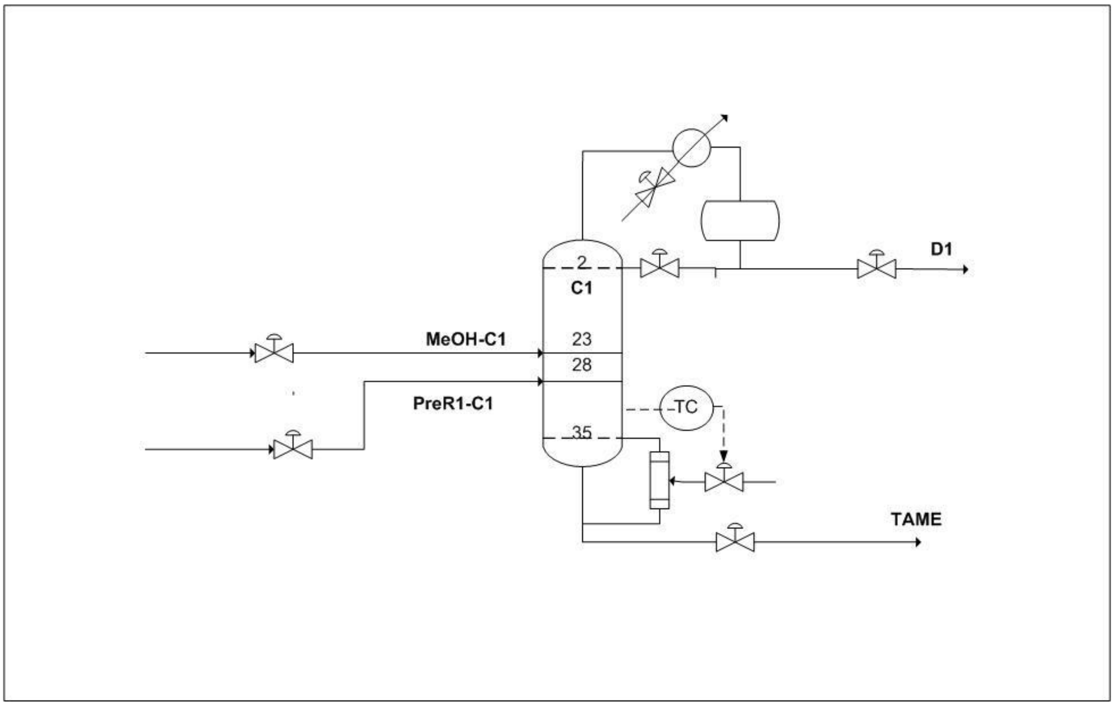


Figure 5.11 Diagram of column C1

Table 5.8 Dynamic responses of total feed flow changes for column C1 between tray 32 and tray 34

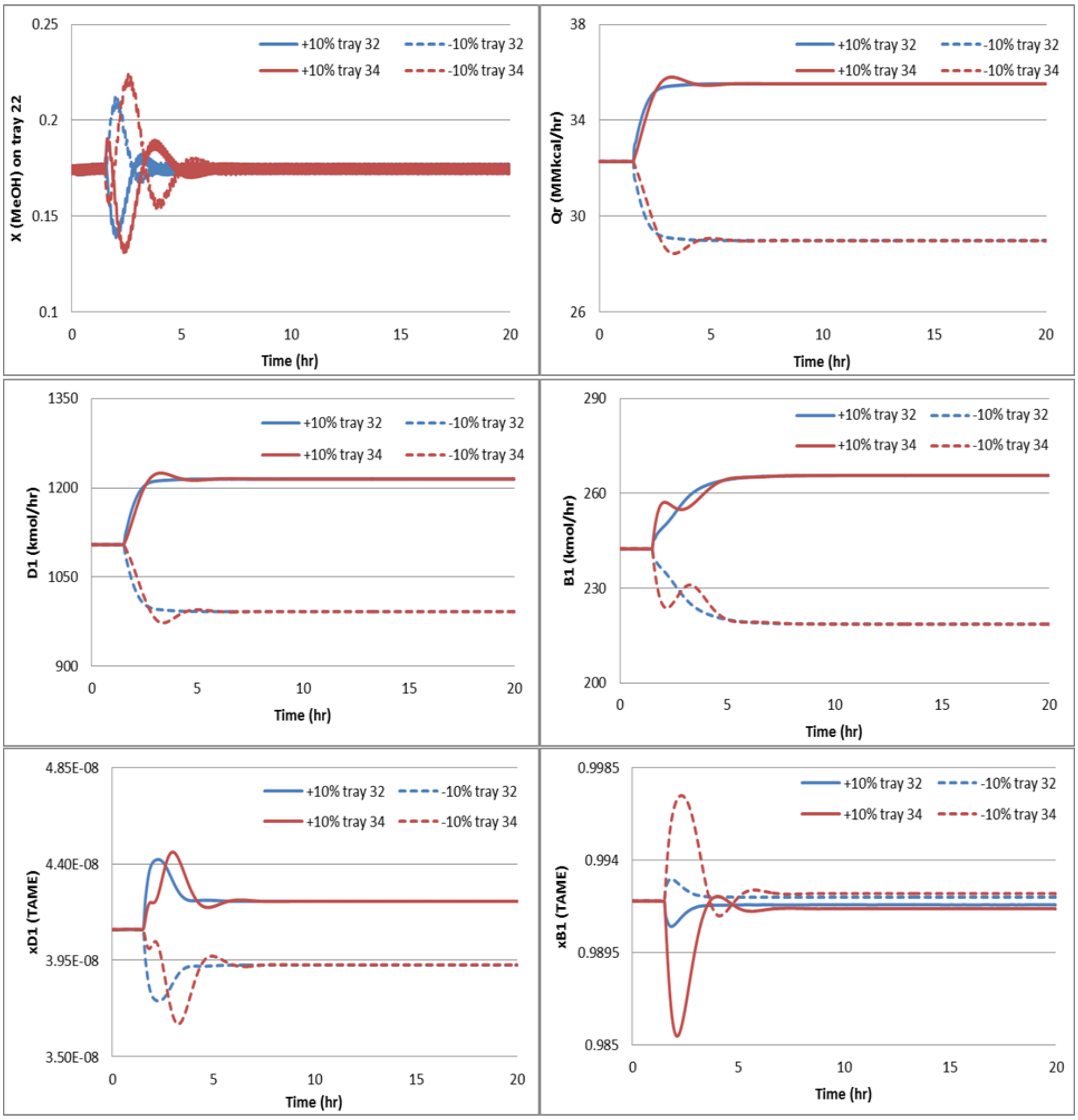


Table 5.9 Dynamic responses of isomylene composition changes for column C1 between tray 32 and tray 34

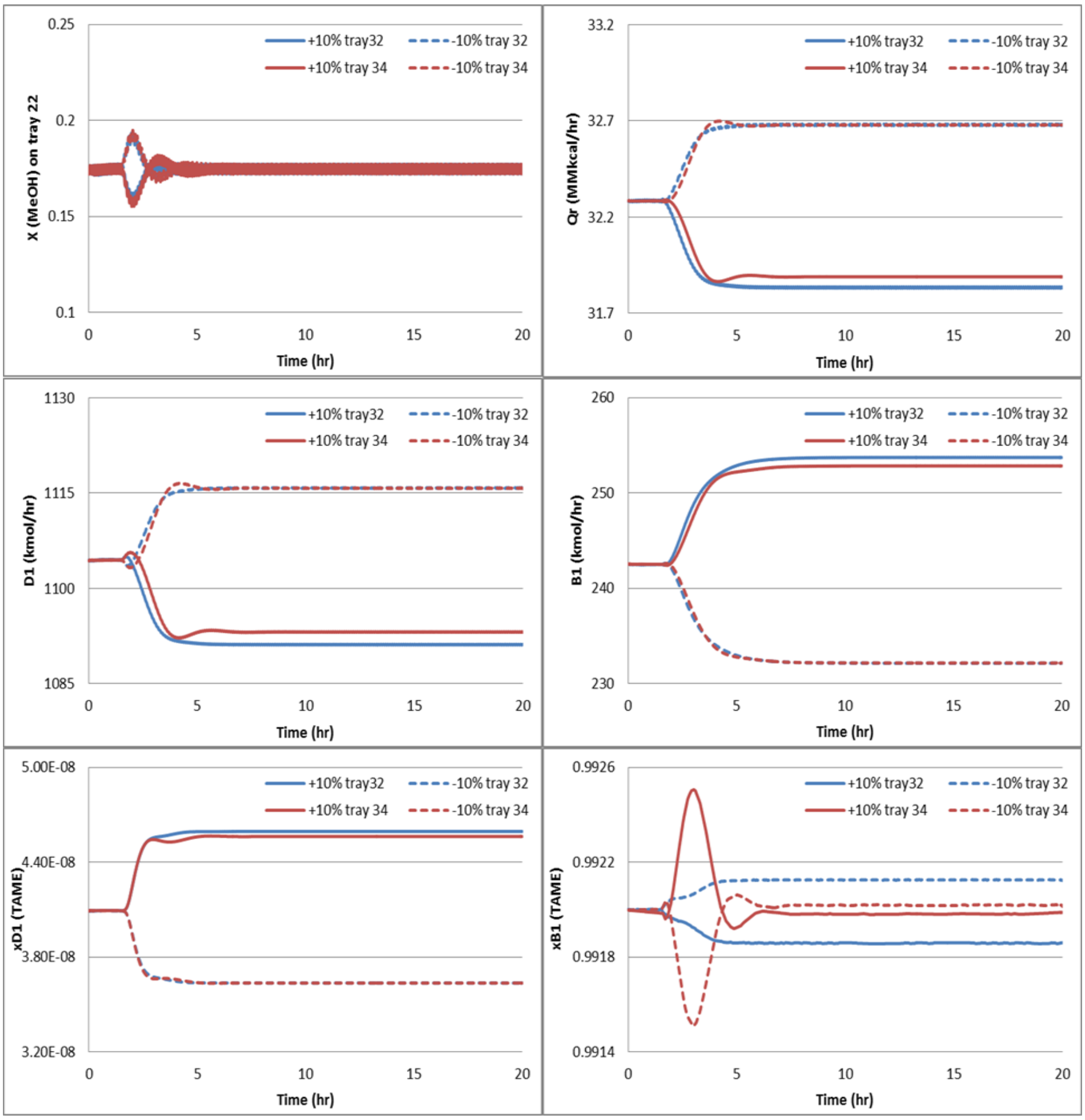


Figure 5.10 Dynamic responses of feed temperature changes for column C1 between tray 32 and tray 34

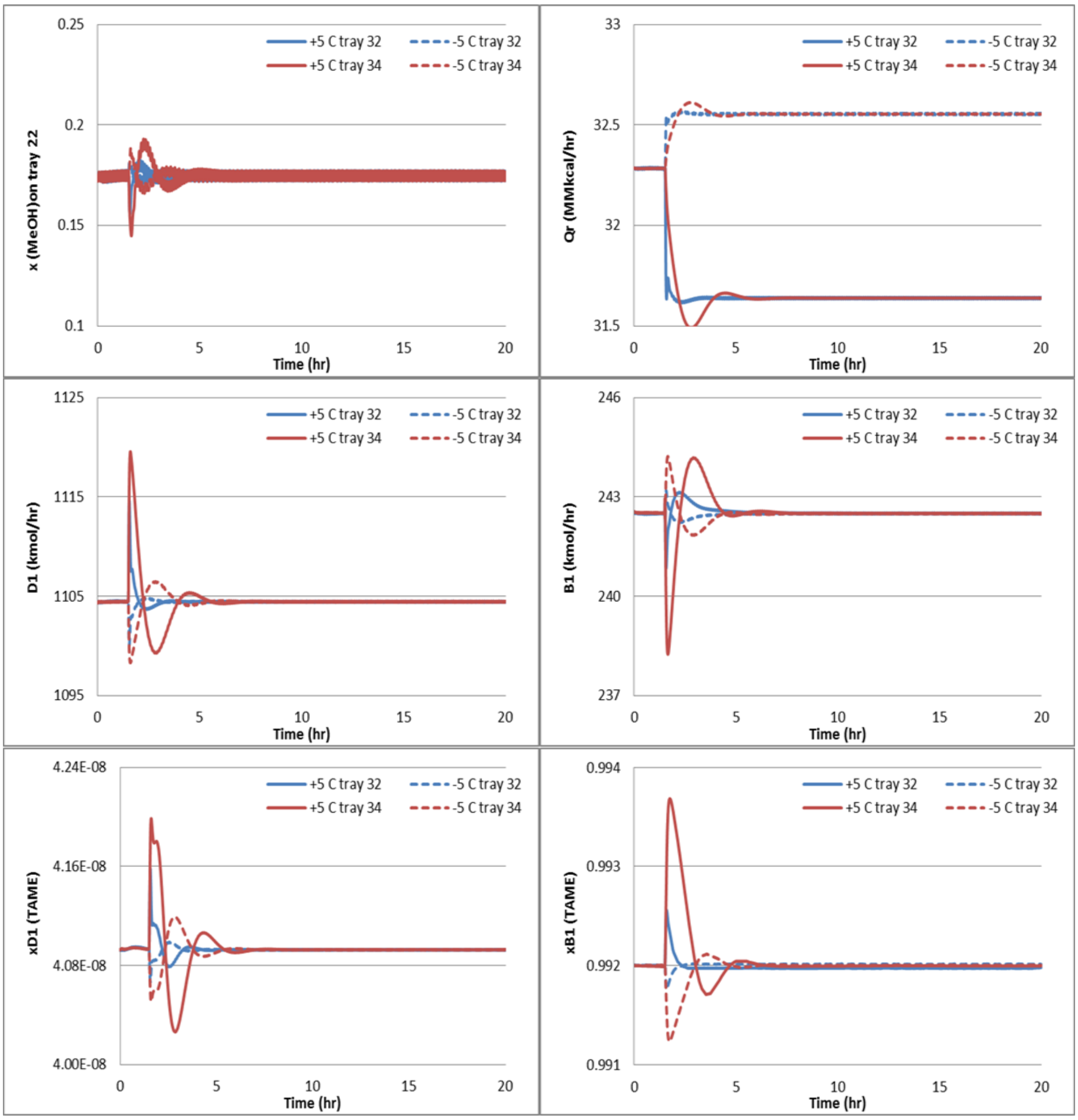
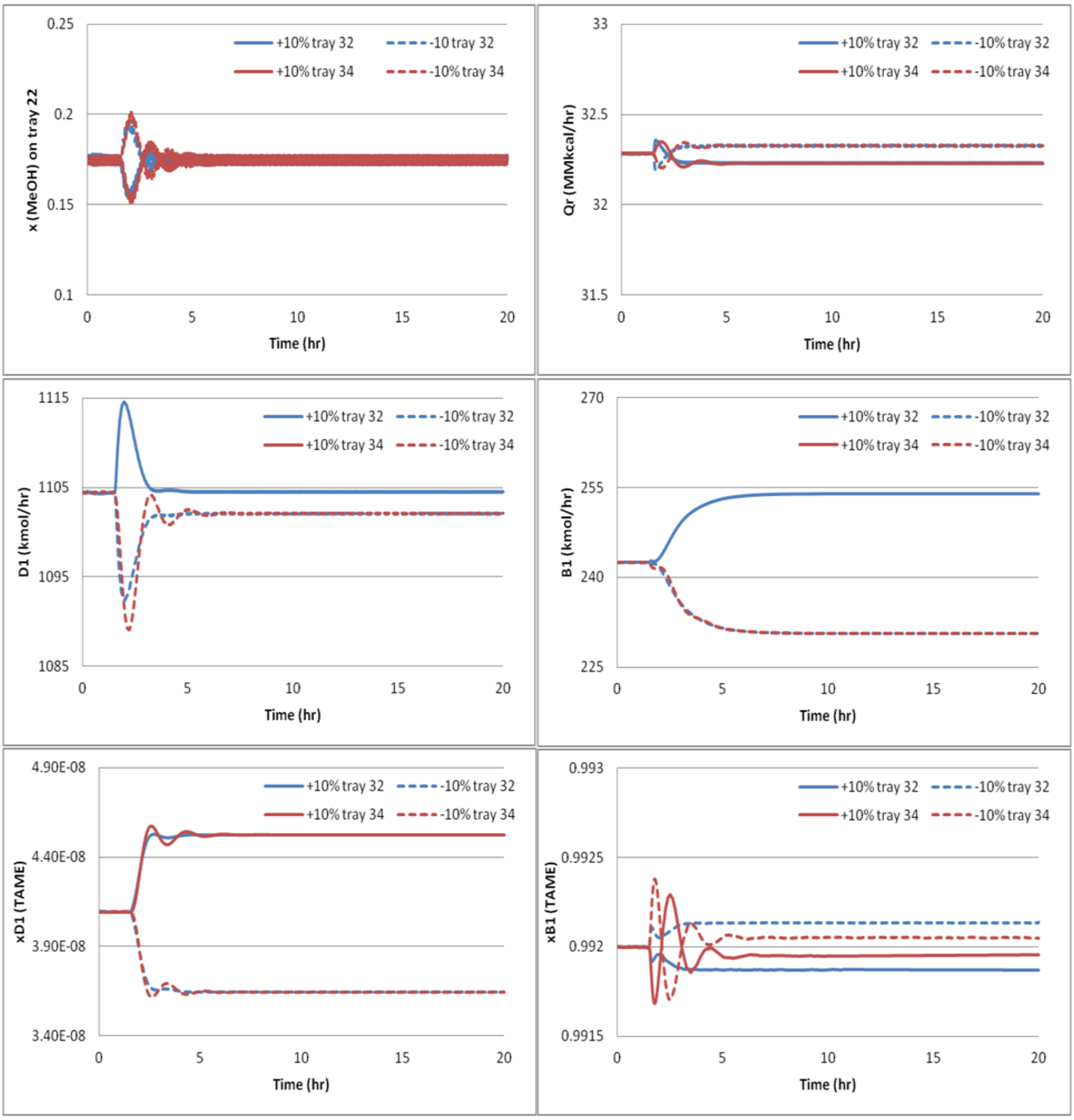


Figure 5.11 Dynamic responses of isoamylene Component changes for column C1 between tray 32 and tray 34



Step 3: Establish fixture plant.

3.1 Keep the materials entered and reentered fixed.

The raw materials were very important for demand production. In regulation, the C5s fresh feed to the first reactor was fixed to be constant. The total methanol flow (fresh feed mixed with recycle stream) was controlled by adjusting a valve of fresh feed. Then, the total methanol was split to two streams that feed to first reactor and reactive distillation column, respectively. The flowrate of methanol to first reactor was controlled to be constant as following Figure 5.12.

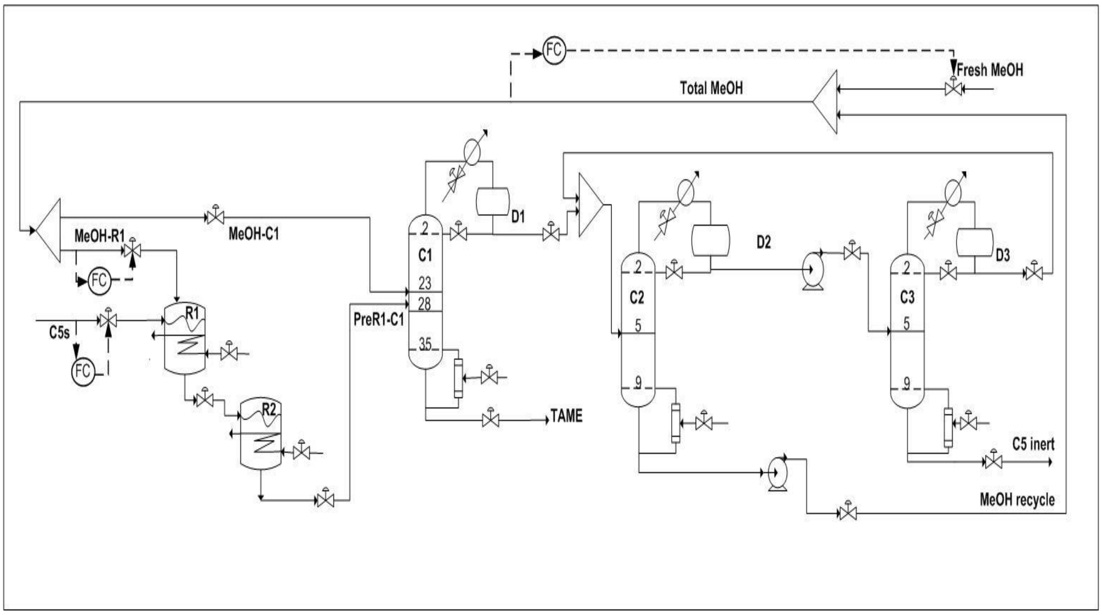


Figure 5.12 Control structure design in step 3.1

3.2 Regulate the production rate.

3.2.1 The limiting reactant was consumed by measuring the composition of methanol on tray 22in reactive distillation column (C1) then sending to adjusted total flowrate of methanol as following Figure 5.13. In addition, the limiting reactant could be consumed by adding ratio control between flowrates of methanol that feed to C1 with component of isoamylene in PreR1-C1 stream, as shows in Figure 5.14.

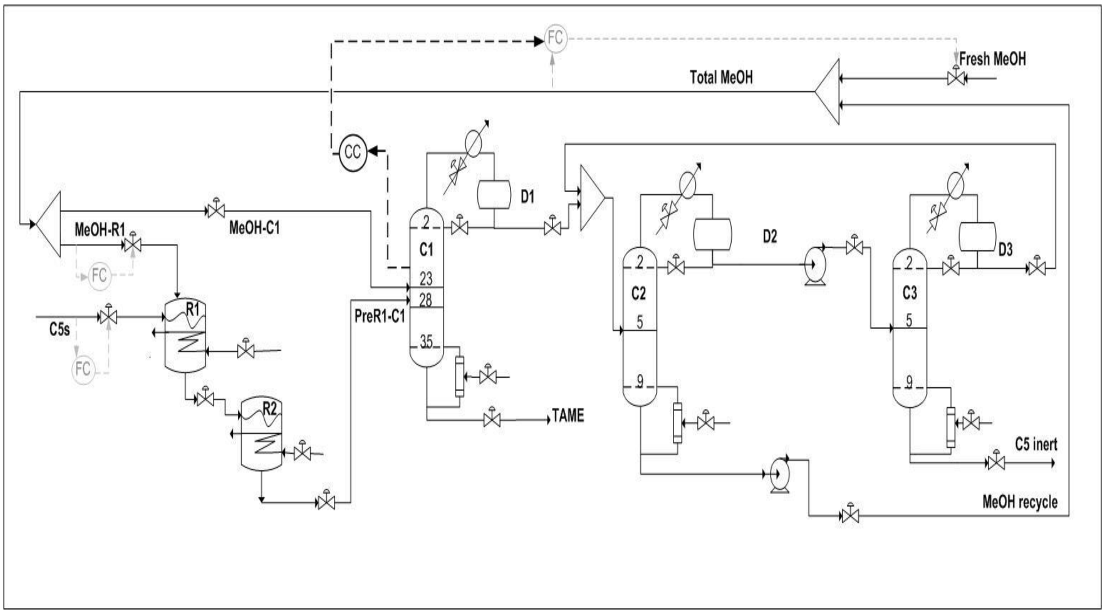


Figure 5.13 Control structure design in step 3.2.1 (1)

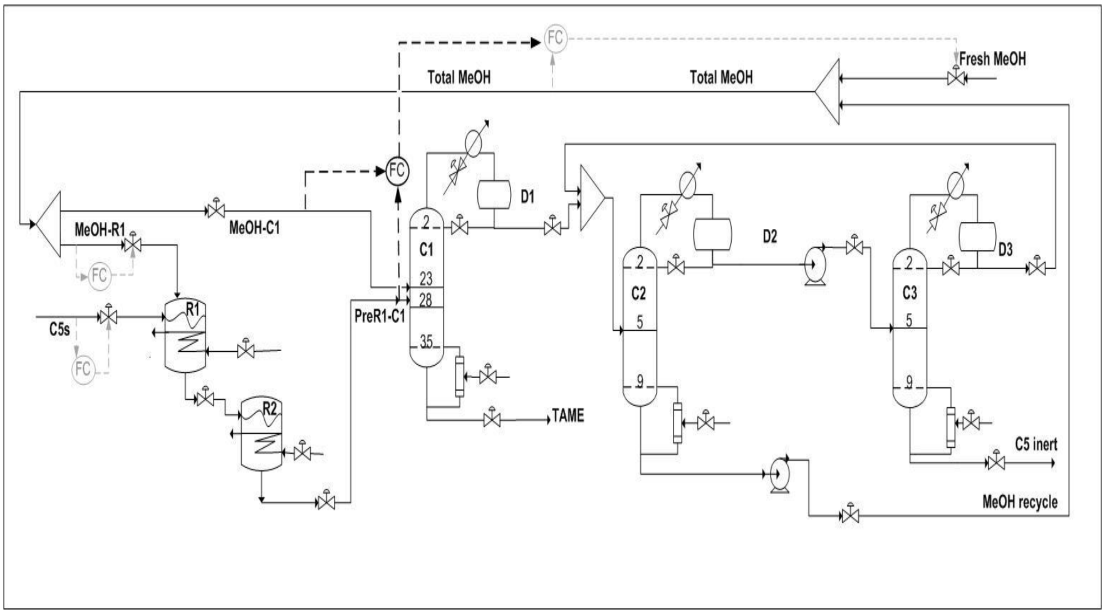


Figure 5.14 Control structure design in step 3.2.1 (2)

3.2.2 If the plant needs to produce on demand, the production rate might be regulated by manipulating feed of limiting reactant (C5s) as following Figure 5.15.

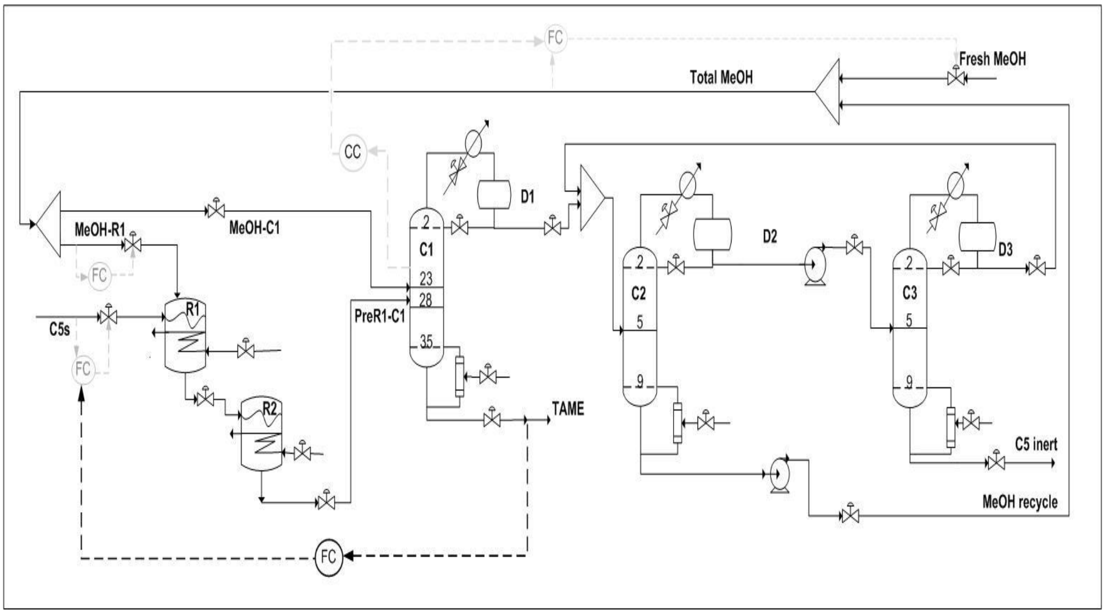


Figure 5.15 Control structure design in step 3.2.2

3.3 Adjust the flow of exit material streams (products, by-products, and inert) according to their accumulations.

The exit material stream in the process was at two end points, the bottom product of C1 (TAME product) and C3 (inert stream), respectively. Figure 5.16 shows the liquid levels of reboiler in both columns which were controlled by adjusting flow of TAME product and inert stream, respectively.

3.4 Control the amount of the rest of the component at their quantifiers.

There is no other component left for quantification control because the components at their quantifiers were controlled in previously step. Show as Figure 5.17.

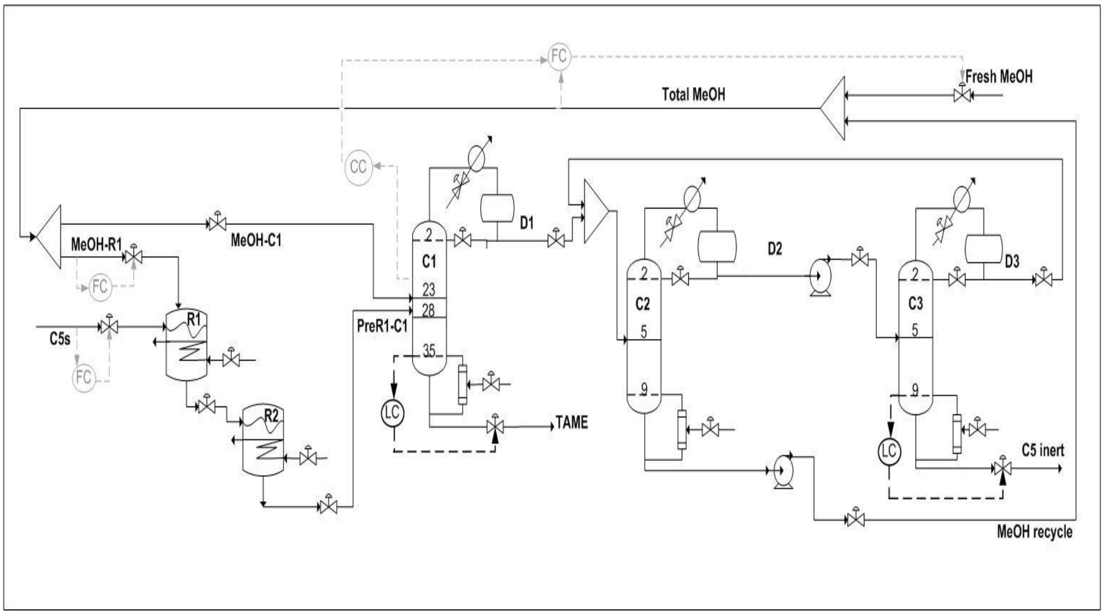


Figure 5.16 Control structure design in step 3.3

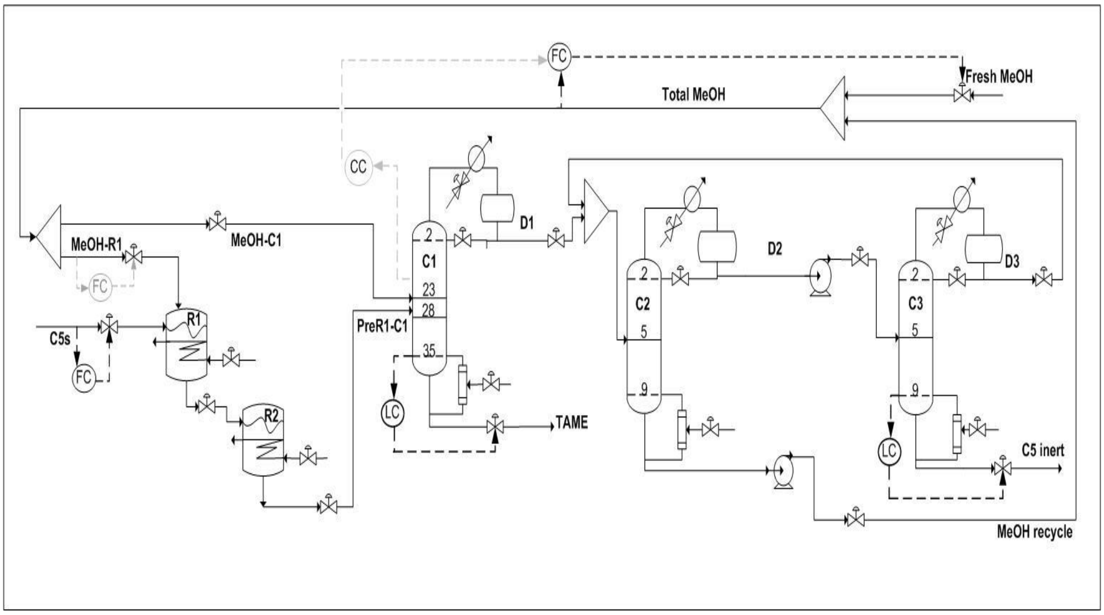


Figure 5.17 Control structure design in step 3.4

***Step 4**:* Handling the disturbances.

4.1 Heat Disturbances.

The thermal disturbance in this process was controlled manipulating cooling water and reboiler duty of reactors and columns. The locations in columns where controlled temperature were determined by step 2.6. This managing related to quality in order to maintain the product specification constraints. Figure 5.18 shows handling the heat disturbance in the process.

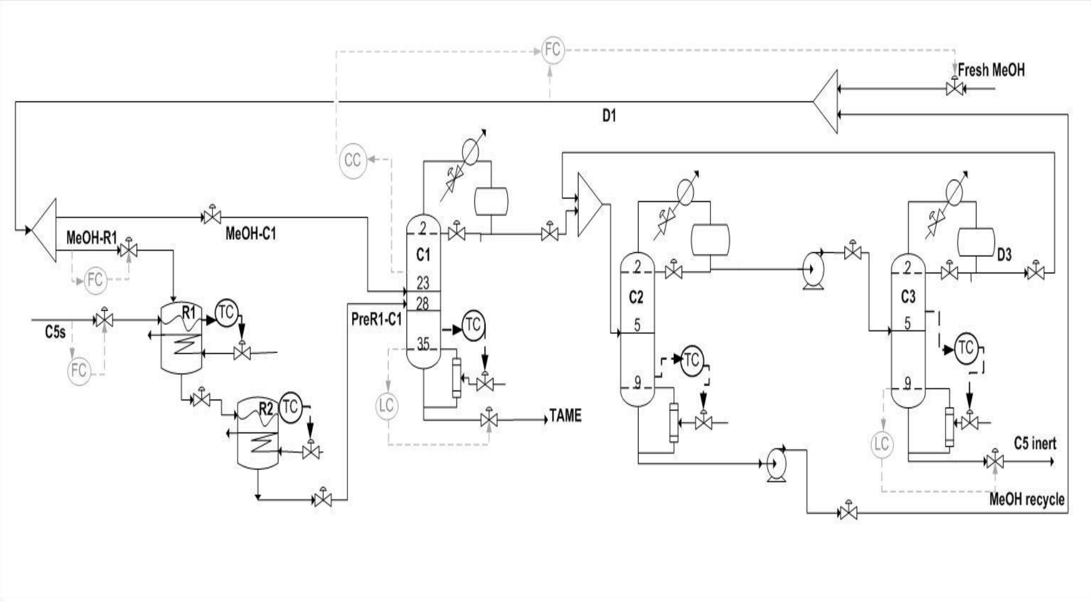


Figure 5.18 Control structure design in step 4.1

4.2 Material disturbances.

The configuration of the control loops depend on the desired material pathways. The pathways can be obtained by analyzing the results of the material disturbance tests. Isoamylene was controlled by adding ratio control with methanol that feed to reactor. Temperature control loops in all columns was used for controlling other material disturbances that were excess methanol, product, and inert, as following Figure 5.19.

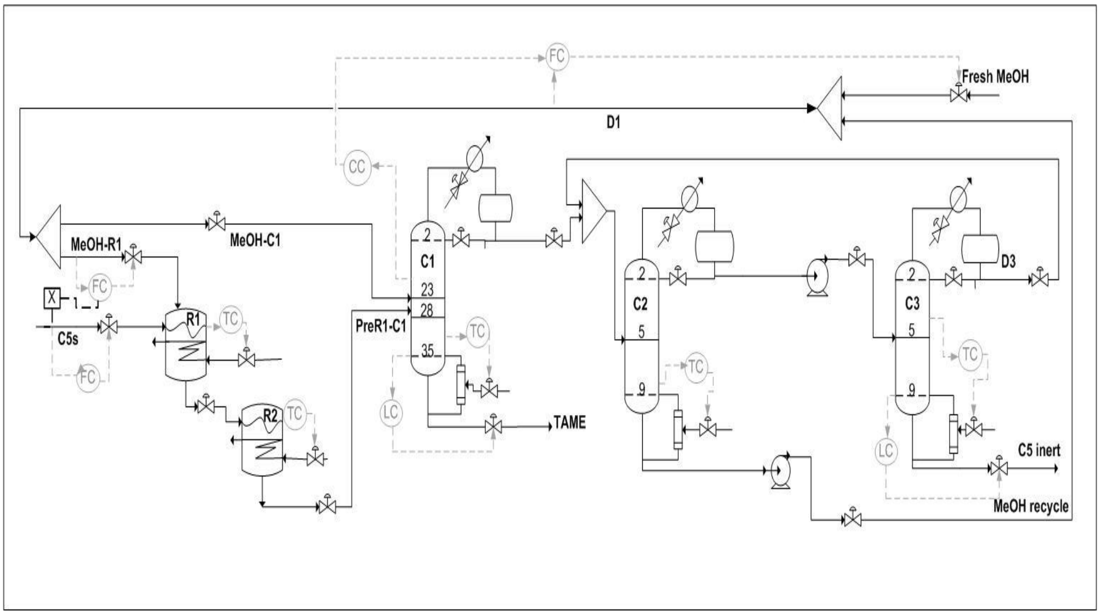


Figure 5.19 Control structure design in step 4.2 from pathway

Fixing reflux flow, reflux ratio or reflux to feed.

A series of dynamic simulation runs were made in which the effects of changes in composition, temperature, total flow and component flow of distillation column feed for selecting reflux flow, reflux ratio, or reflux to feed control.

1. Reactive distillation column (Column C1)

Diagram of column C1 was shown Figure 5.11. PreR1-C1 stream was selected to change disturbances. tert-Amyl methyl ether was focused in the column.
Dynamic response of column C1 for differential fixing was presented in Table 5.12-5.15. Step changing was examined at 1.5 hours. Red line, back line, and blue line were represented for reflux flow control, reflux ratio control, and reflux to feed control, respectively. The disturbance first test, total flowrate of PreR1-C1 stream was increased 10% that affected to increasing distillate rate and bottom rate. The TAME composition at bottom rate closed to it specification for all loops reflux control. The resulting was opposite when reducing total flowrate.

A second, composition of isoamylene was changed ±10% in PreR1-C1 feed.

When, isoamylene were added. It affected to increase the forward reaction, and increase the production rate at the bottom column because this column was reactive distillation column. Fixing the reflux ratio kept TAME composition close to the target value.

The third, variation of the temperature ± 5 °C in PreR1-C1 feed gave the same response for all fixing. Reflux ratio gave the smallest deviation of all variables in this test.

Finally, the component test was altering ±10% isoamylene flowrate. This test gave the same result total flow test and component test. Therefore, the reflux ratio control was the best fixing because it can be maintained TAME purity very close to its specification for all disturbances.

Table 5.12 Dynamic response of column C1 when change total feed flowrate

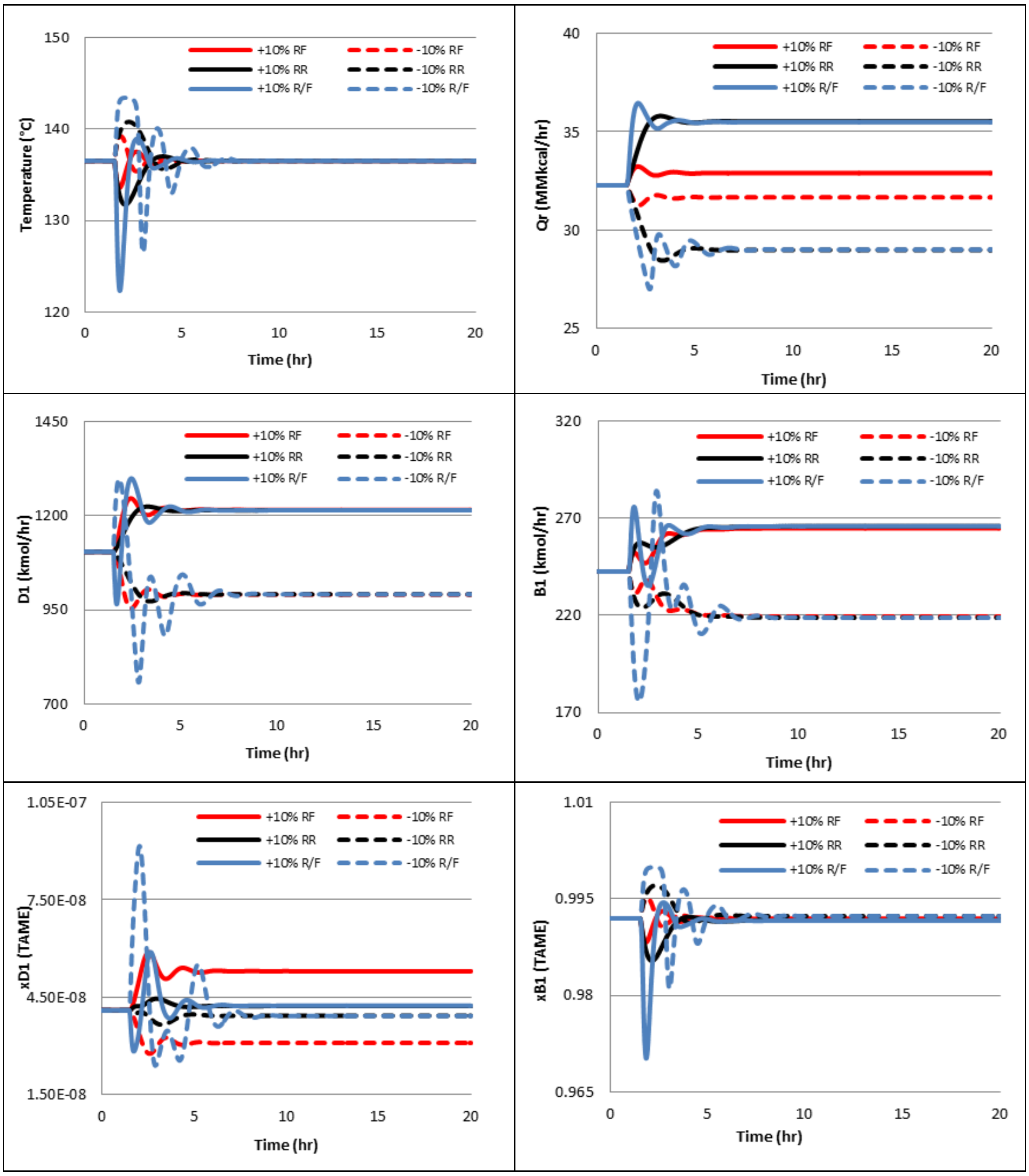


Table 5.13 Dynamic response of column C1 when change feed composition

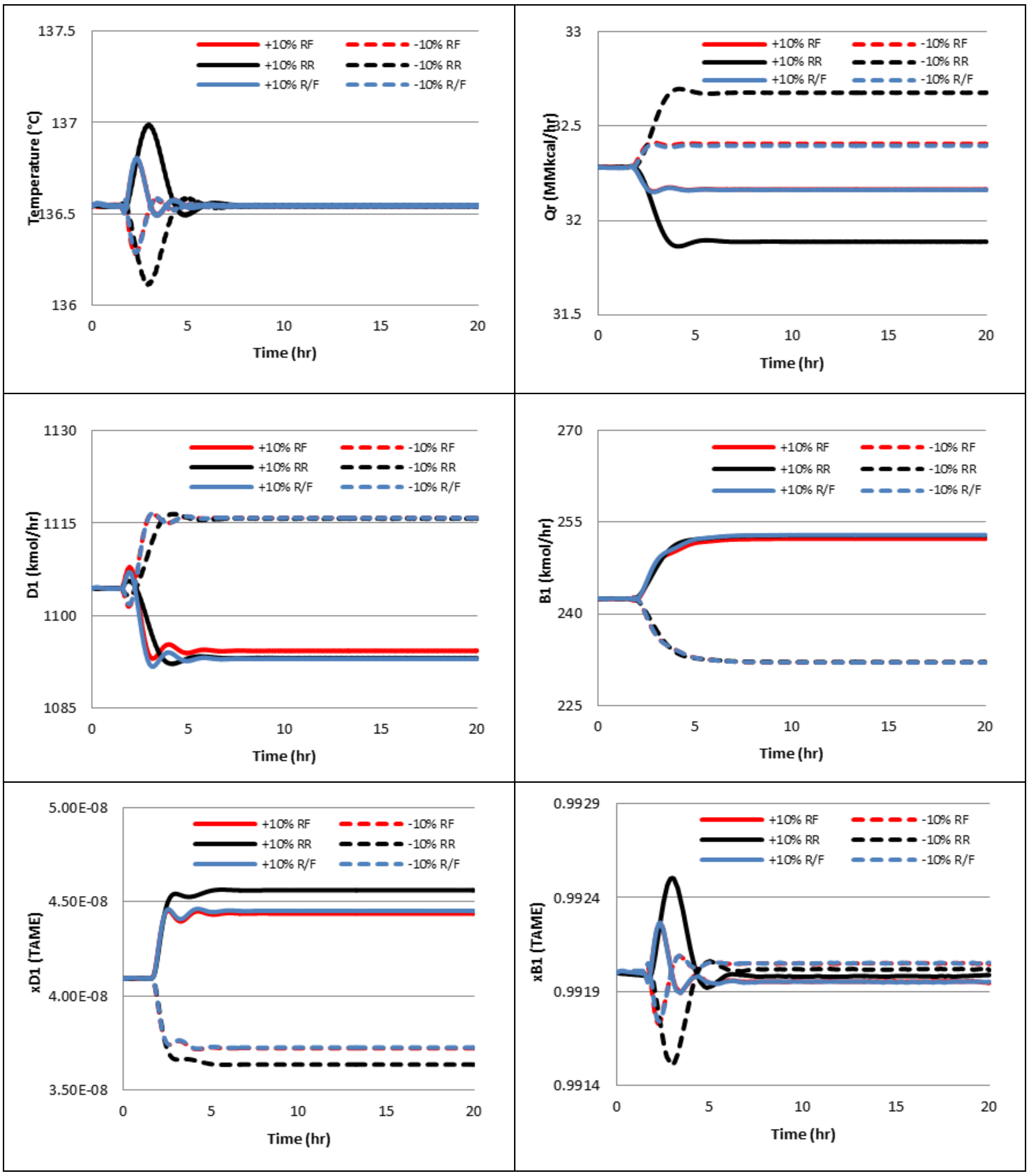


Table 5.14 Dynamic response of column C1 when change feed temperature

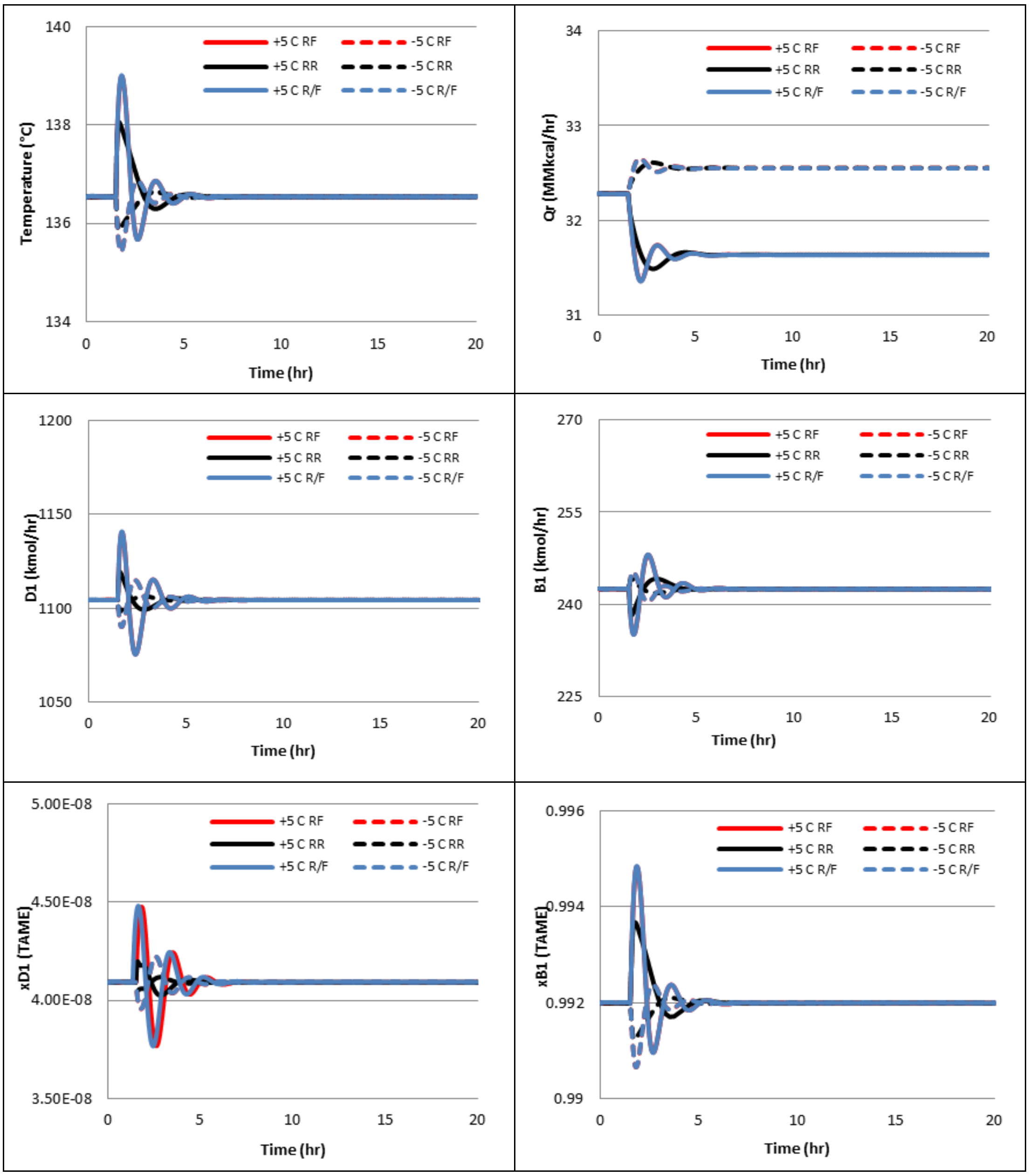
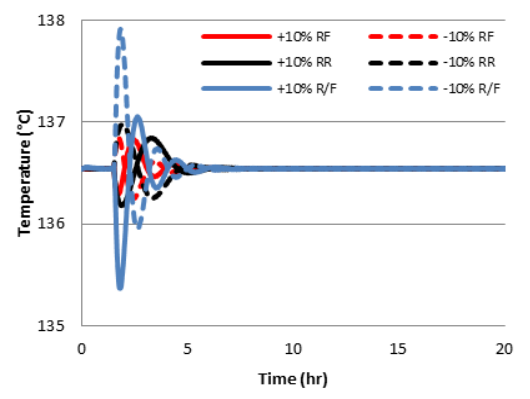
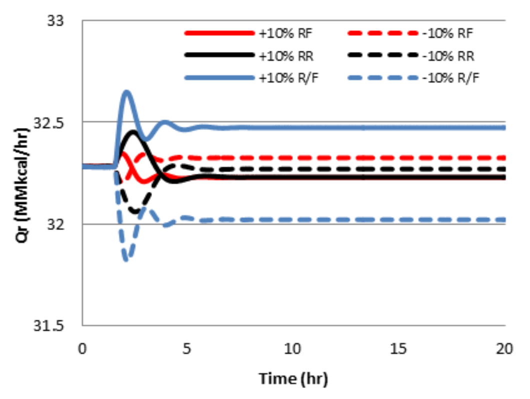
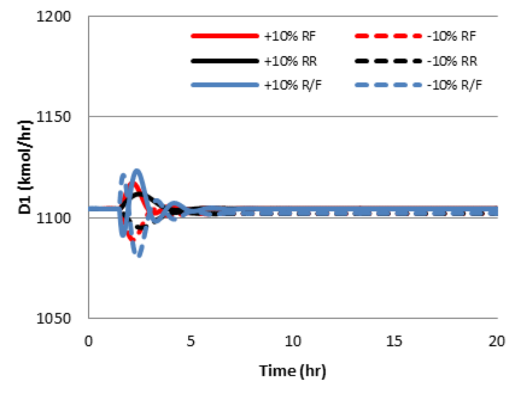
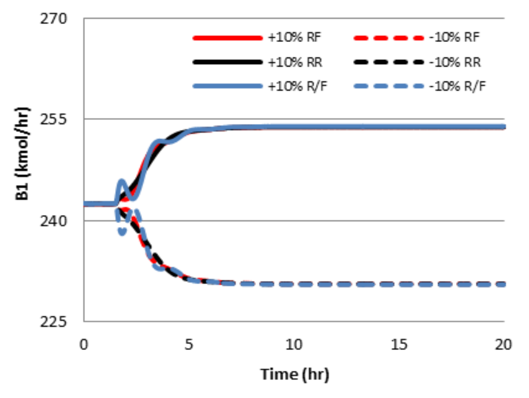


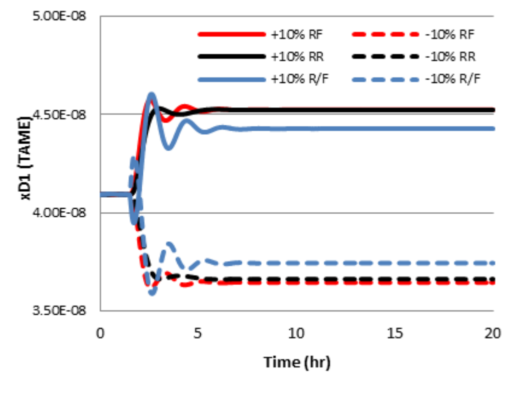
Table 5.15 Dynamic response of column C1 when change feed component flow

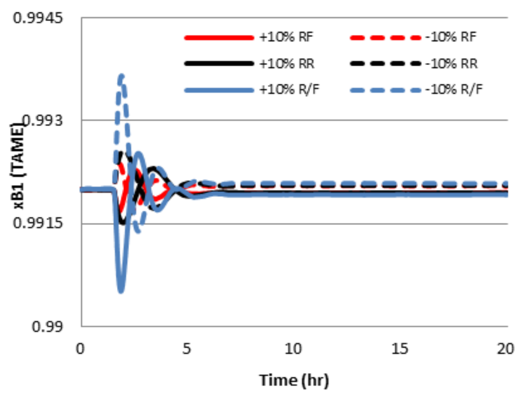












2. Methanol recovery column (Column C2)

Figure 5.20 shows diagram of methanol recovery column. The feed consist of methanol and inerts. This column focused the methanol at bottom of column for recycle back to process. Table 5.16-5.19 present the response to positive and negative changes of flow, composition, temperature, and component for feed flowrate changing.

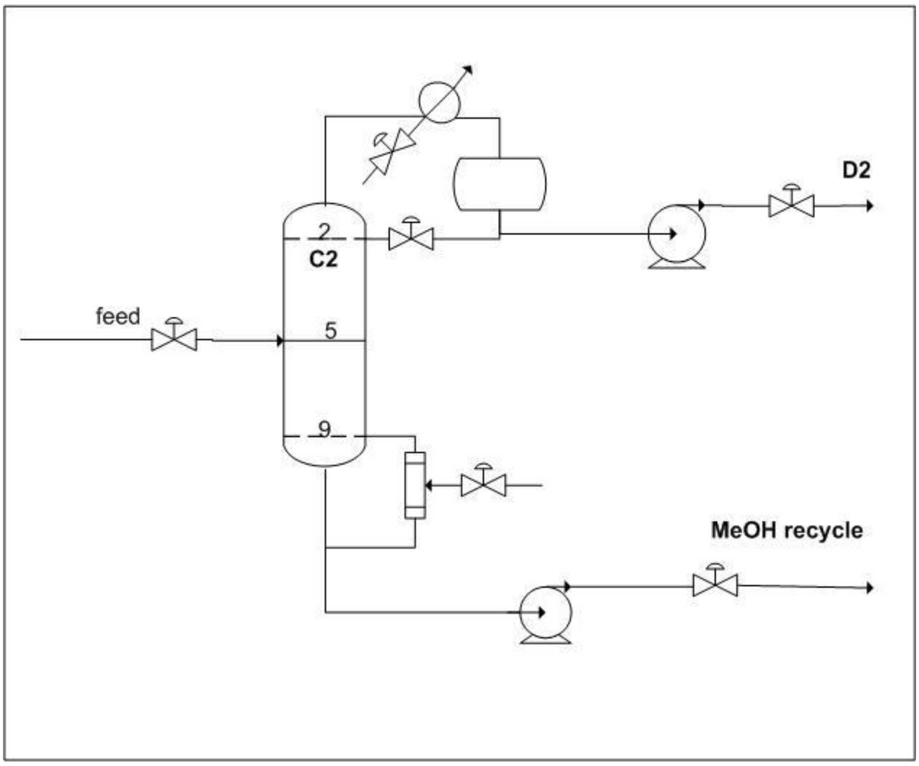
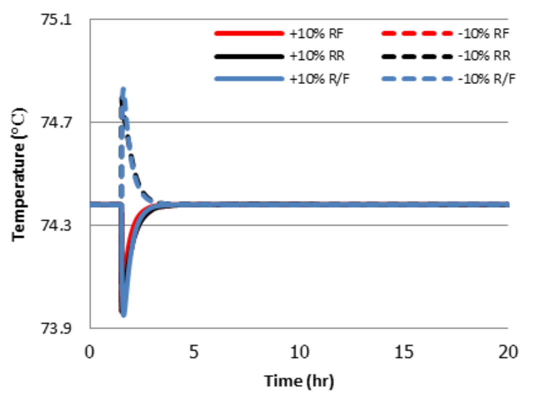
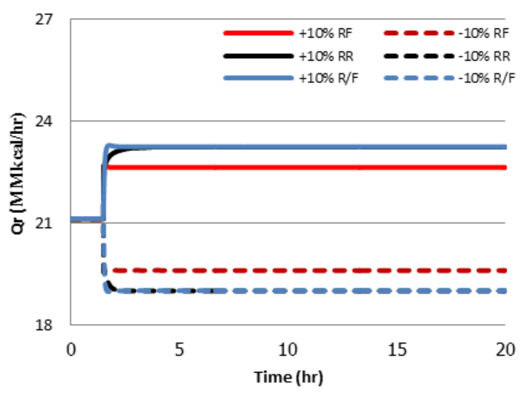


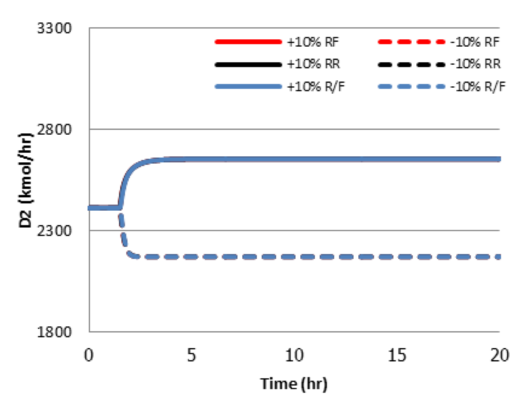
Figure 5.20 Diagram of column C2

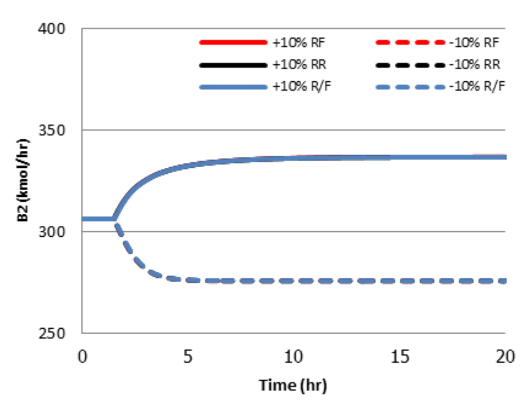
When, the total flow was altered. Distillate rate and bottom rate was affected by the mass balance rules. The fixing reflux flow used the smaller reboiler duty than other fixing and gave the best methanol composition. For changing methanol composition result same as total flow changing. The temperature disturbance and the component disturbance, the response went to the same way in all fixing. Consequently, the reflux flow fixing was selected to control in this column.

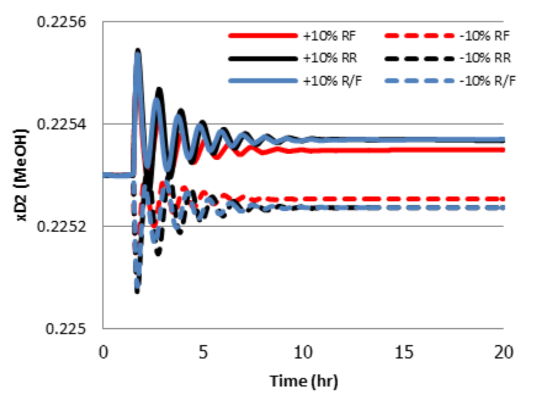
Table 5.16 Dynamic response of column C2 when change total feed flowrate











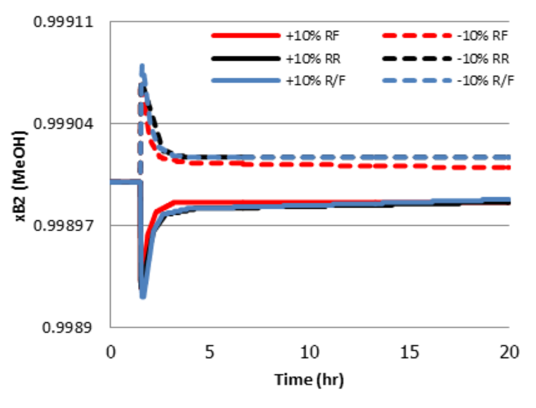
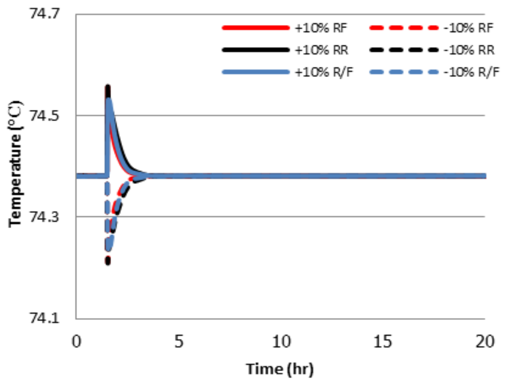
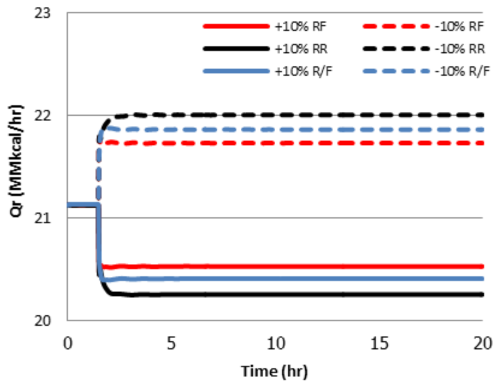
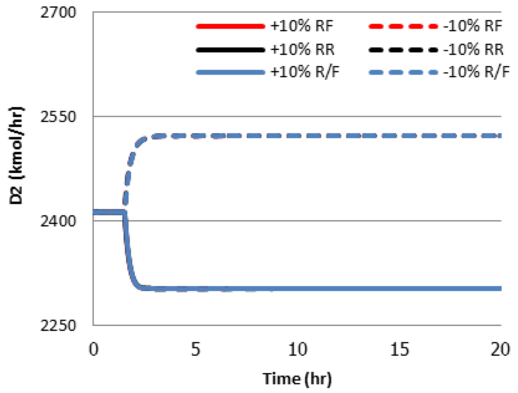
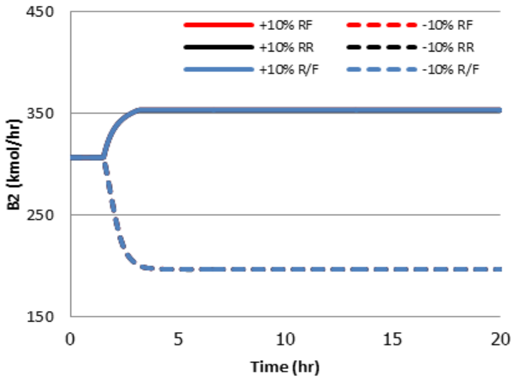


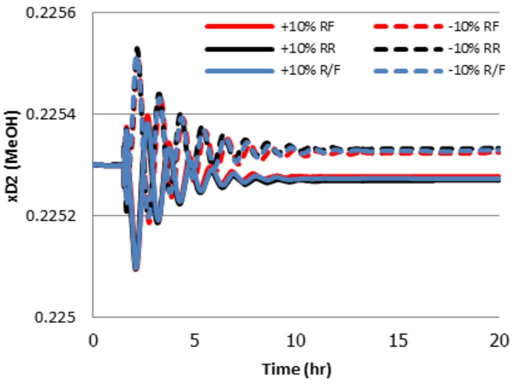
Table 5.17 Dynamic response of column C2 when change feed composition











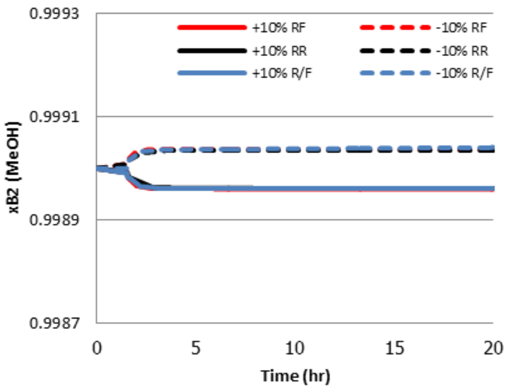


Table 5.18 Dynamic response of column C2 when change feed temperature

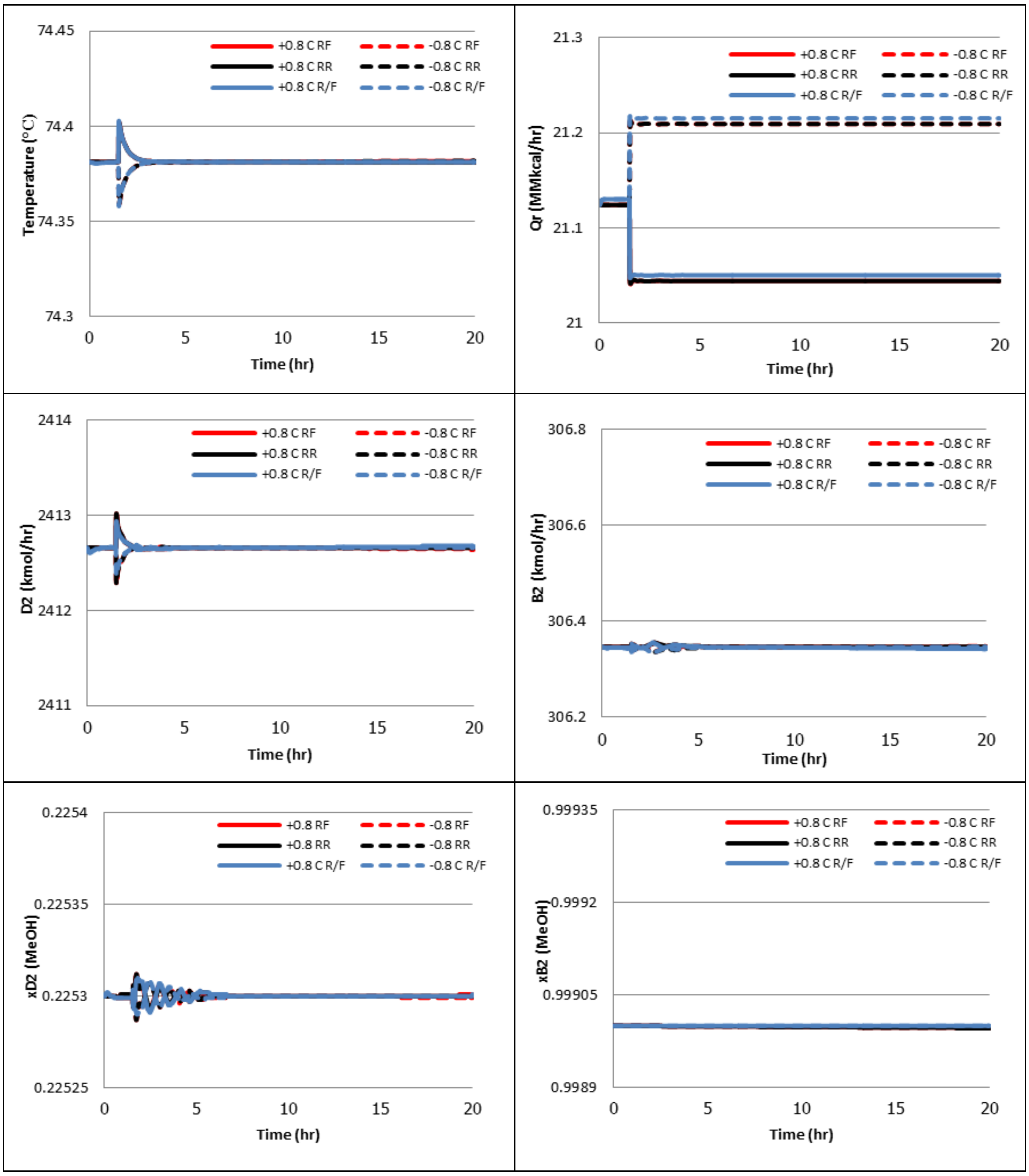
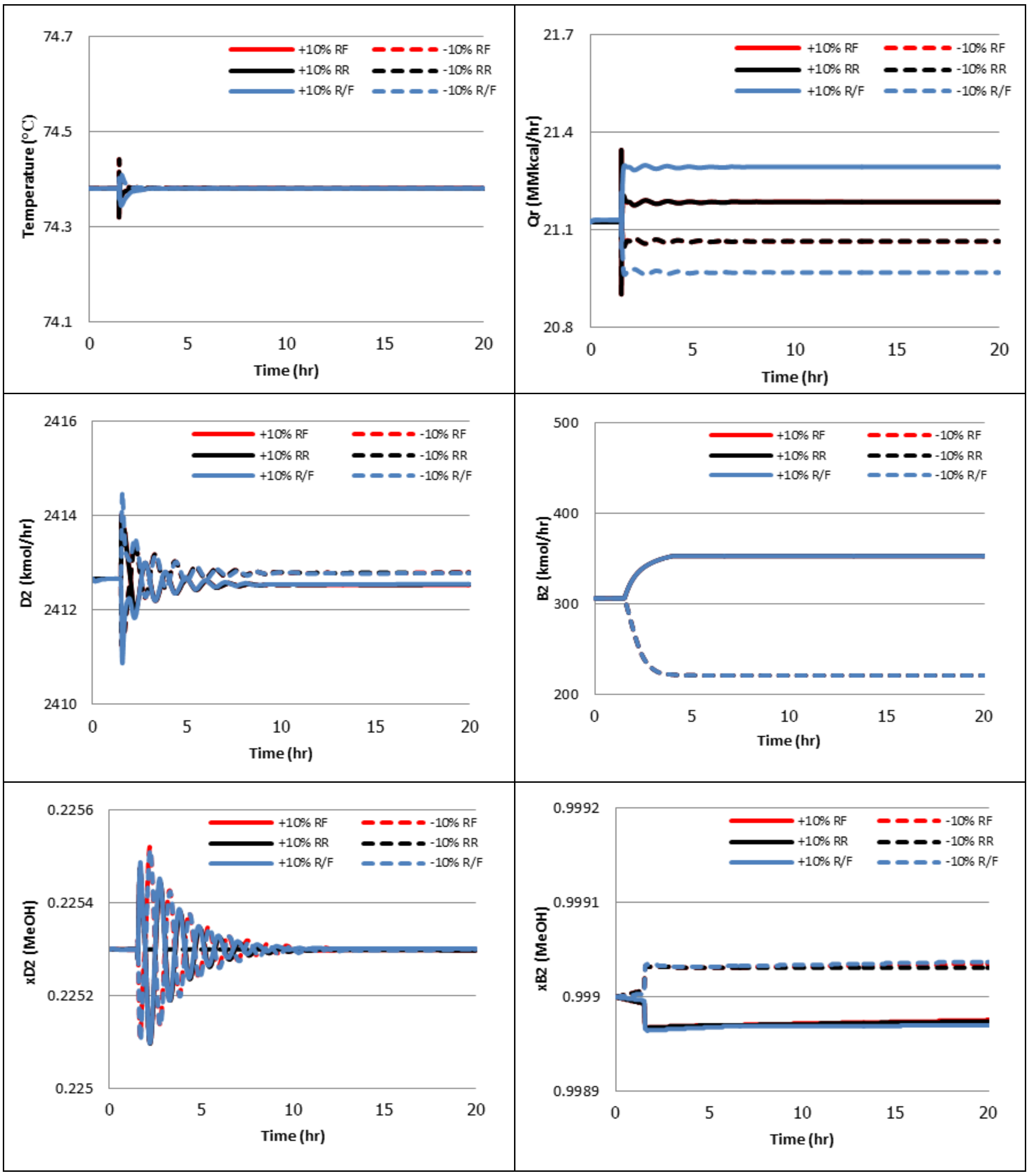


Table 5.19 Dynamic response of column C2 when change feed component flow



3. Column C3

For column C3, methanol in distillate stream was recycled back to separate in column C2. Inerts was left from bottom of column, as Figure 5.21. Purity of methanol was focus. The fixing of reflux ratio could be maintained methanol purity very close to its specification more than other fixing as Table 5.20-5.23.

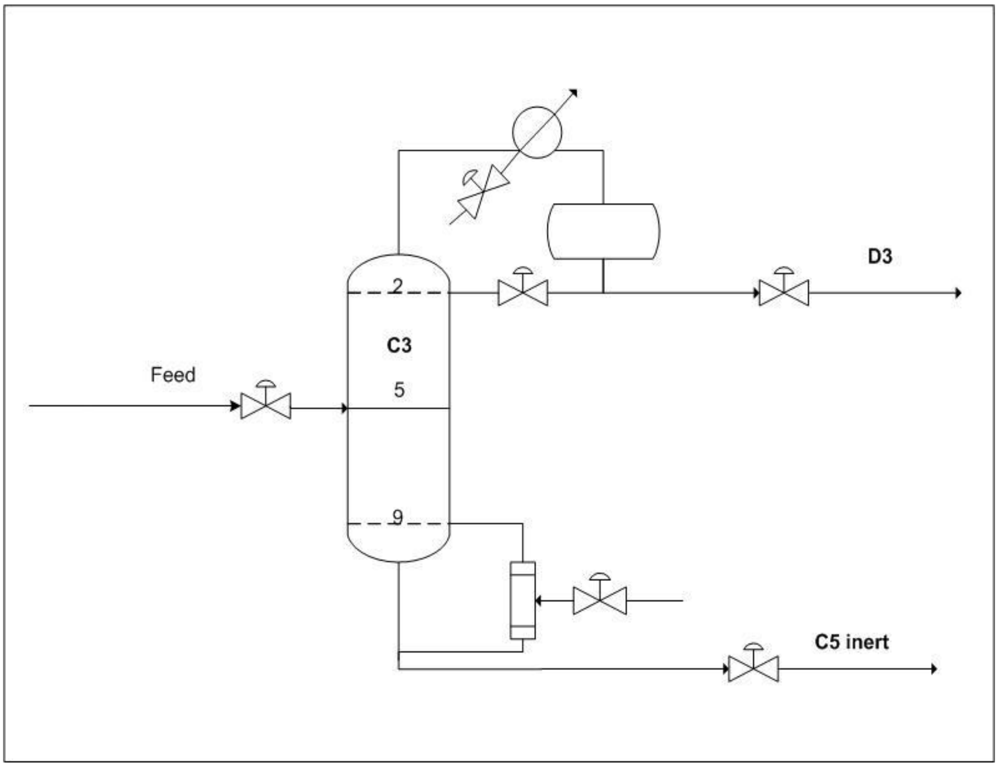


Figure 5.21 Diagram of column C3

Table 5.20 Dynamic response of column C3 when change total feed flowrate

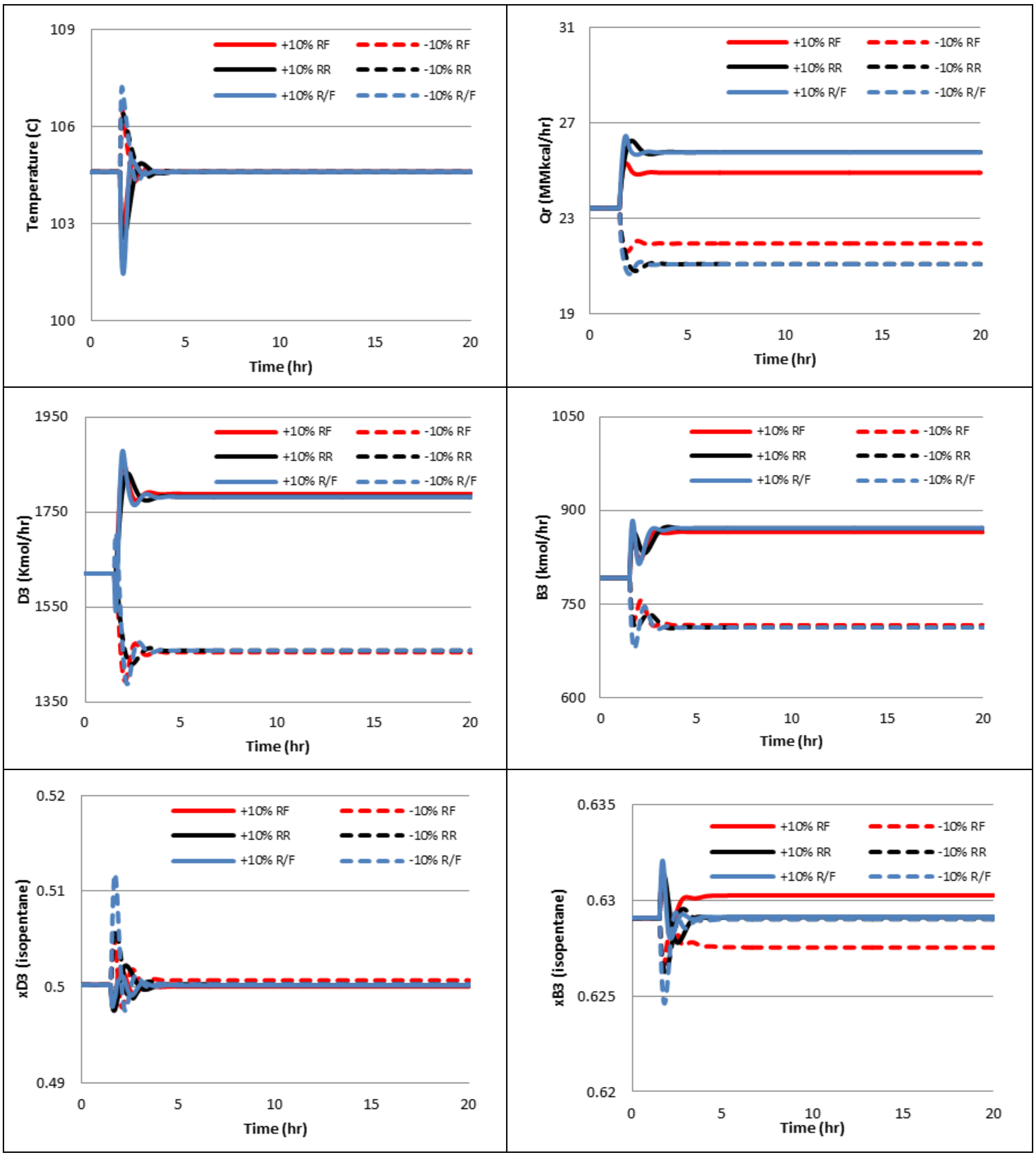


Table 5.21 Dynamic response of column C3 when change feed composition

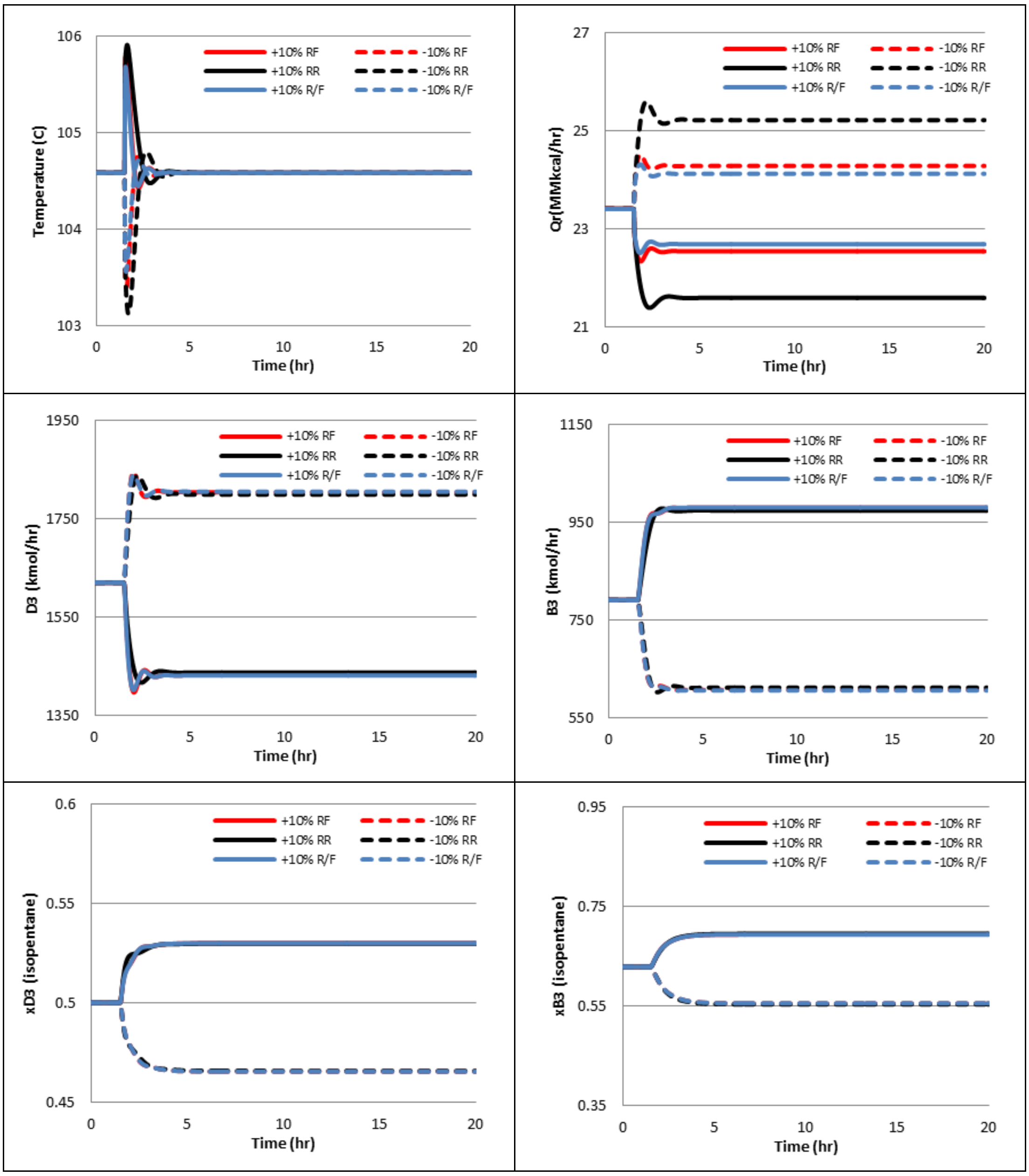


Table 5.22 Dynamic response of column C3 when change feed temperature

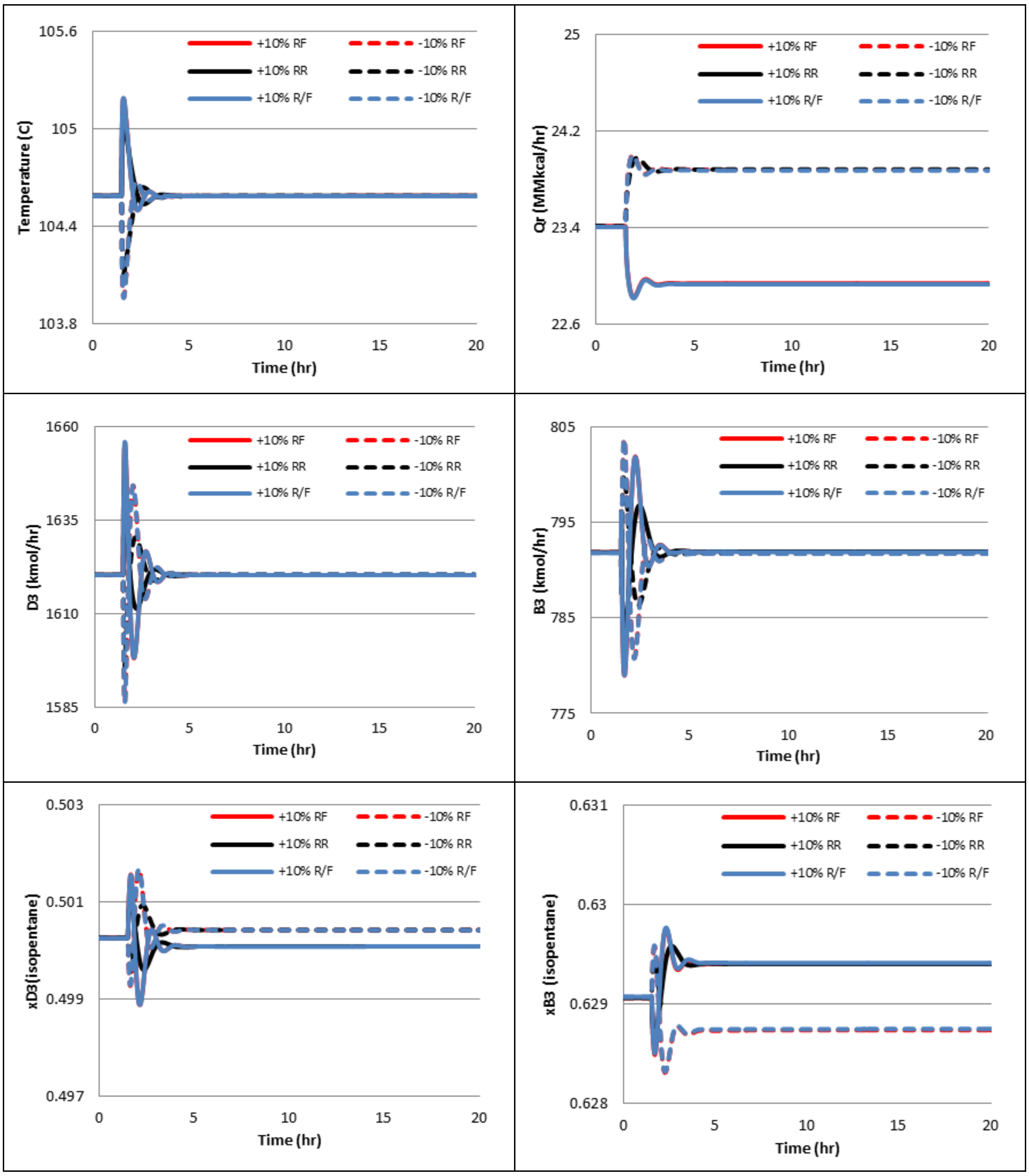
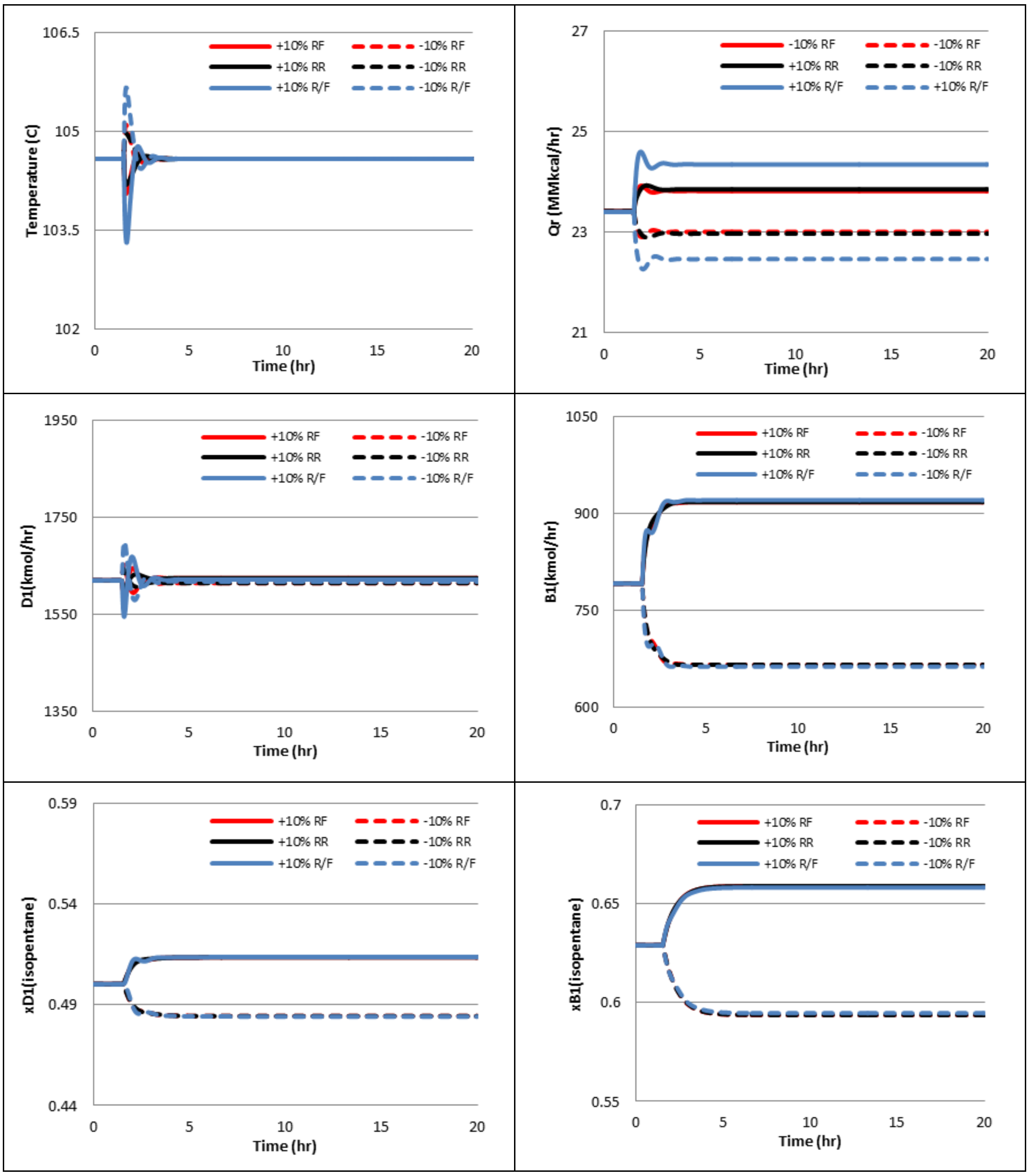


Table 5.23 Dynamic response of column C3 when change feed component flow



From the disturbances tests in all columns, Figure 5.22 shows the control loops were selected.

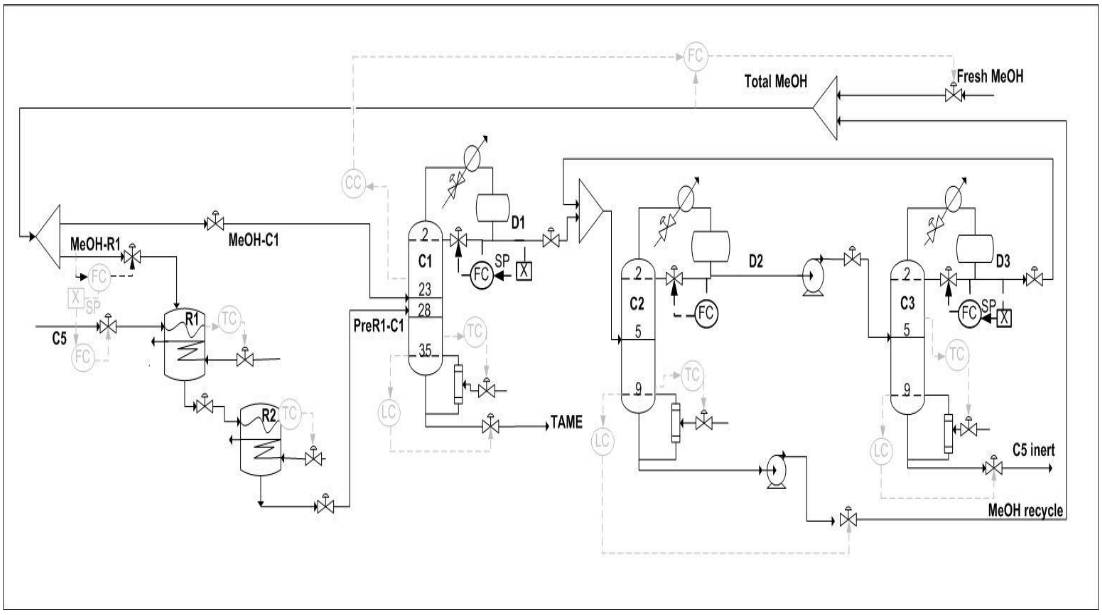


Figure 5.22 Control structure design of distillation column in step 4.2

Step 5: Design the control loops for the remaining control variables or adding enhanced controls, i.e. cascade, feed forward controls.

The rest control loops were added in this step including pressure controls and level controls of reactors and columns as shows in Figure 5.23.

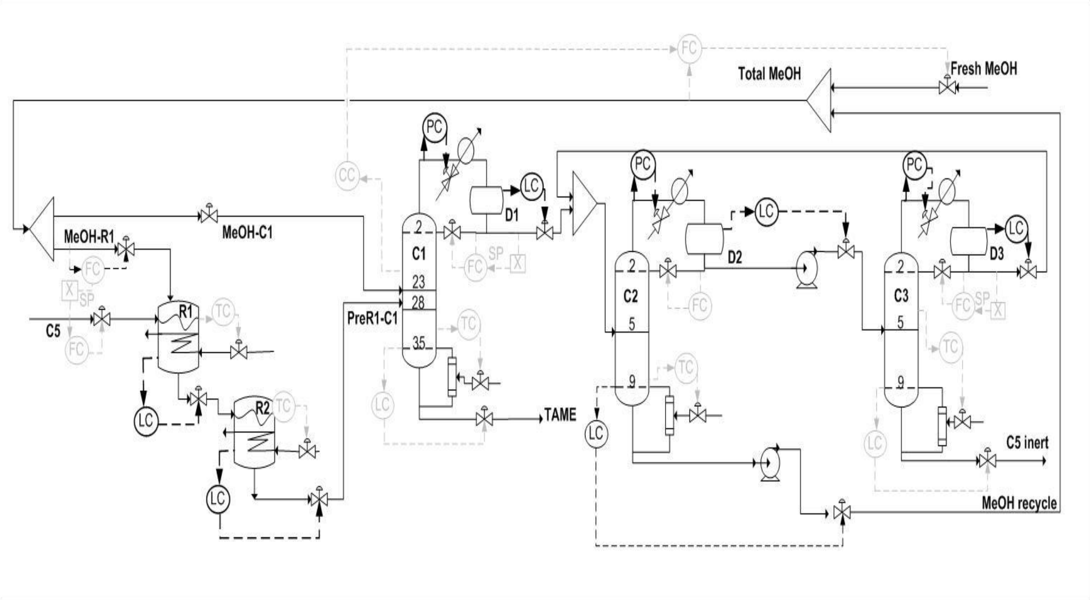


Figure 5.23 Control structure design in step 5.

***Step 6**:* Energy management via heat exchanger networks.

The energy for *tert*-amyl methyl ether (TAME) process was not feasible enough to design any heat integrated networks.

***Step 7**:* Optimize economics and/or improve control performance.

This process had been optimized. In 1999, the steady-state designs of a prereactor and a reactive-distillation system for the production of *tert*-amyl methyl ether (TAME) was studied by Subawalla and Fair. Then, in 2004 Al-Arfaj and Luyben extended this work to design a complete plant with methanol recovery using a pressure-swing azeotropic separation method.

Furthermore, the PID controllers were used in temperature controls and concentration control for the new control structure design. All control structures were designed in Figure 5.24-5.26. Reference control structure (Base case) was presented by Al-Arfaj and Luyben (2004) as shown in Figure 5.24. The new design control structures 1-2 (NNCS1-2) were show in Figure 5.25 and 5.26, respectively.

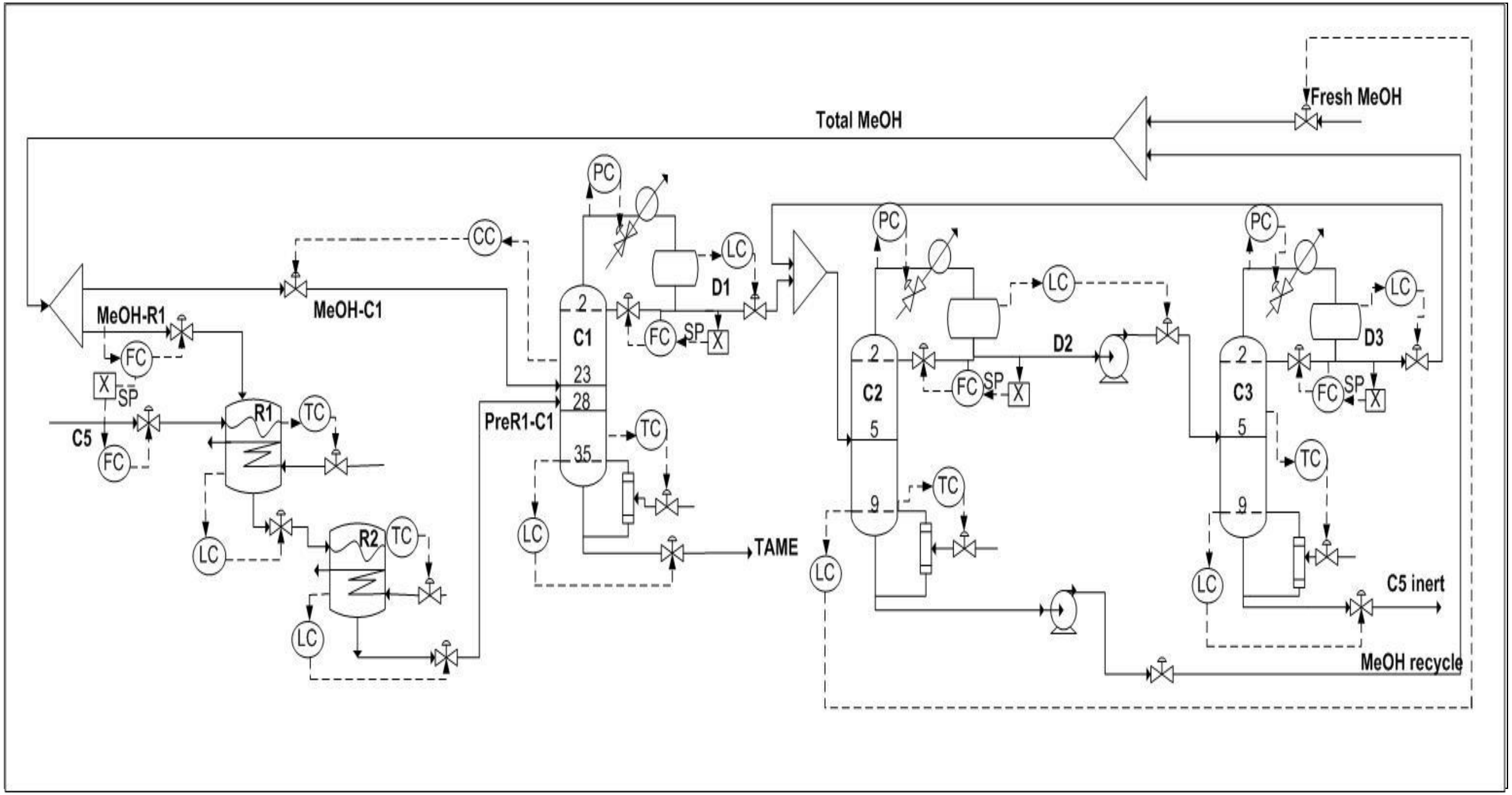


Figure 5.24 Reference control structure (Base case) of *tert*-amyl methyl ether process

Table 5.24 Control structure lists of base case

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP
Methanol feed	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	√
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	√
Reactor R1	TC	Temperature	Reactor duty	PI	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Reactor R2	TC	Temperature	Reactor duty	PI	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 32	Reboiler duty	PI	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	
	CC	Composition tray 22	Methanol feed flowrate to C1	PI	Reverse	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 9	Reboiler duty	PI	Reverse	√
	LC	Reboiler level	Bottom flowrate	PI	Direct	
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 4	Reboiler duty	PI	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	

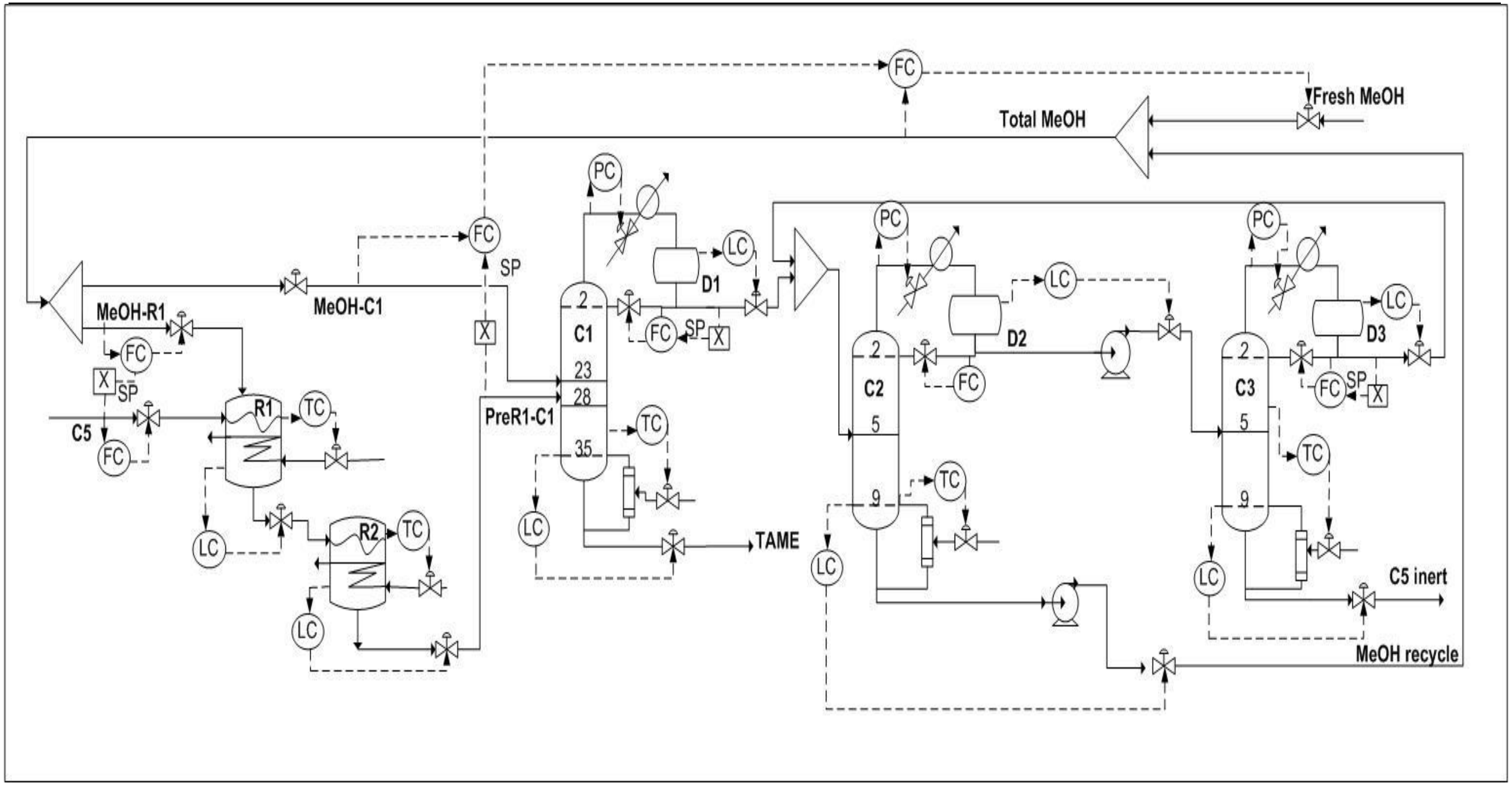


Figure 5.25 The new control structure 1(NCS1) of *tert*-amyl methyl ether process

Table 5.25 Control structure lists of new control structure 1 (NCS 1)

Equipment	**Control**	**Controlled variable**	**Manipulated variable**	**Type**	**Action**	**SP**
Methanol feed	FC	Total flowrate	Feed flowrate	PI	Reverse	√
	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	√
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	√
Reactor R1	TC	Temperature	Reactor duty	PI	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Reactor R2	TC	Temperature	Reactor duty	PI	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 34	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	
	FC	Flowrate of 2M1B in PreR1-C1 Stream	Methanol feed flowrate to C1	PI	Reverse	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux flow	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 9	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	PI	Direct	
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 4	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	

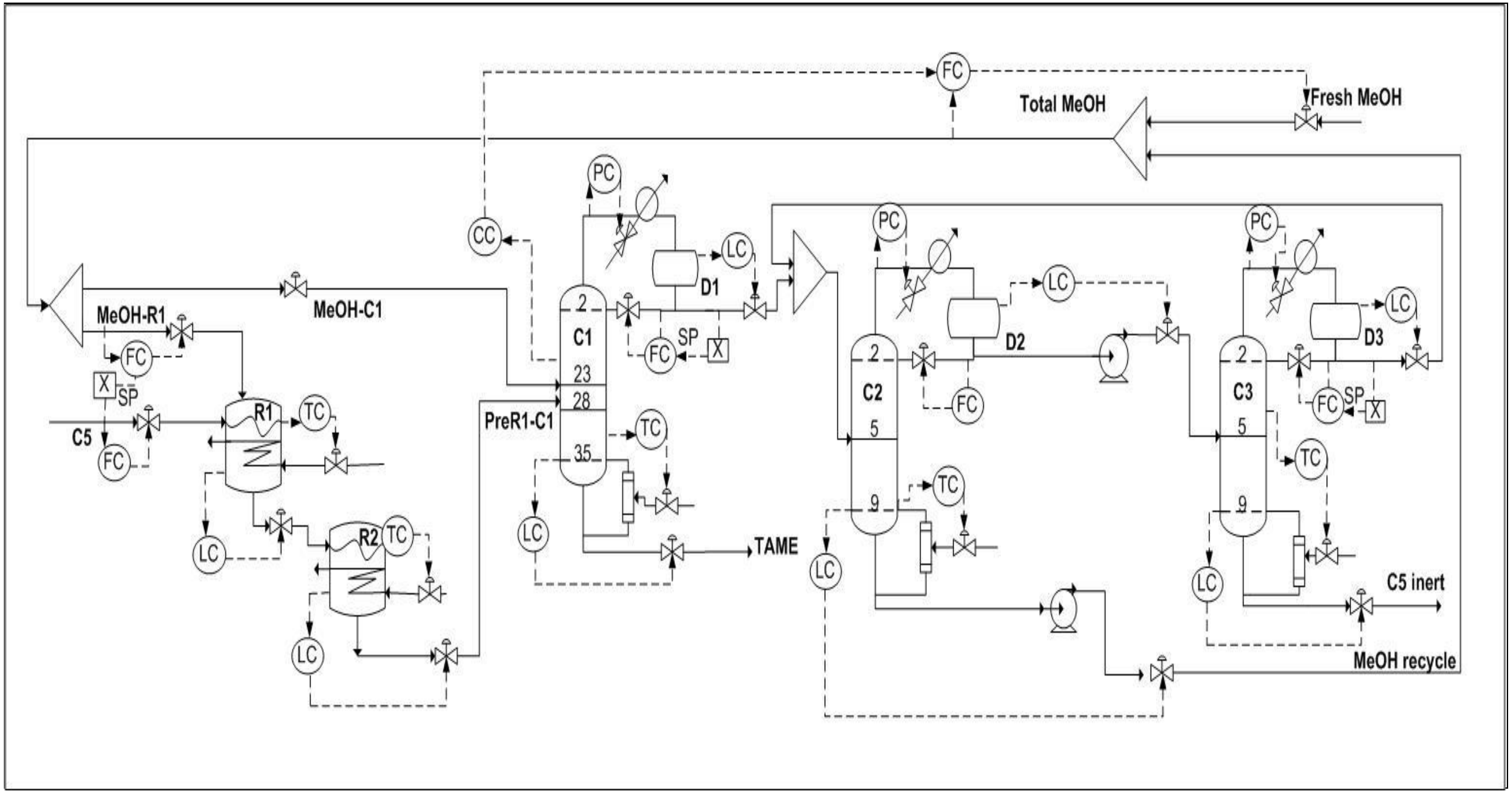


Figure 5.26 The new control structure 2 (NCS2) of *tert*-amyl methyl ether process

Table 5.26 Control structure lists of new control structure 2 (NCS 2)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP
Methanol feed	FC	Total flowrate	Feed flowrate	PI	Reverse	√
	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	√
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	√
Reactor R1	TC	Temperature	Reactor duty	PID	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Reactor R2	TC	Temperature	Reactor duty	PID	Reverse	√
	LC	Liquid level	Effluence flowrate	P	Direct	
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 34	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	
	CC	Composition tray 22	Methanol feed flowrate to C1	PID	Reverse	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux flux	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 9	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	PI	Direct	
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	√
	LC	Reflux drum level	Distillate flowrate	P	Direct	
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	√
	TC	Temperature tray 4	Reboiler duty	PID	Reverse	√
	LC	Reboiler level	Bottom flowrate	P	Direct	

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

The control performance of the total plant was tested by step changing of total flow, composition, temperature, and component of C5s feed flowrate at 1.5 hours. The dynamic responses of the variables for all control structures (Base case, NNCS1, NNCS2) were obtained by the commercial process simulator as following:

1. Total C5s feed flowrate change.

Total C5s feed flowrate was changed ±10% (±ΔF) at 1.5 hours. Flowrate of C5s increased from 1103.864 kmol/hr to 1143.8504 kmol/hr and decreased from 1103.864 to 935.8776 kmol/hr. Table 5.27 shows dynamic response of variables by total flow disturbance. All methanol streams depended mainly on the C5s feed flowrate. The shape of methanol fresh feed flowrate at the first period differed because the differential location to control. In base case the methanol fresh feed was adjusted from the liquid level in bottom of column C2 but in NCS1 and NCS2 were adjusted from the flowrate of methanol feed to column C1 and the methanol composition on tray 22 in column C1, respectively.

The temperature of reactor 1 (R1) and reactor 2 (R2) were suddenly increased in all case. In NCS2 has temperature deviation smaller than base case and NNCS1 because the effect of PID controller. The temperature deviation of column C1 in base case, NCS1, and NCS2 were about 5 °C, 1.5°C, and 1°C, respectively. It returned to set point in 3.5, 3 and 2 hours. The smallest deviation and minimize time to returned to set point for NCS2 were affected of PID controller same reactors. For column C2 and column C3, temperature control loops of new control structure (NCS1, NCS2) could handle in 5 hours.

Distillation and bottom flow of all columns depended on feed flowrate of each column. The product exited at bottom of column C1. When increasing C5s feed flowrate, in NCS1 the purity of product could not go to specification value in 20 hours and methanol at tray 22 of column C1 did not close to the set point because this control structure did not control the composition in column C1. For base case and NCS2, the purity went to new steady state in 3.5 hours.

Methanol at bottom column C2 was recycled to first reactor and column C1. The purity of methanol in this stream was maintained close to specification in all control structures. Distillate of column C3 was recycled to column C2. Methanol returned to the desired target in 5 hours. Base case and NCS1 reached a new steady state in 7 and 5 hours.

Table 5.27 The Dynamic responses of total feed flow changed

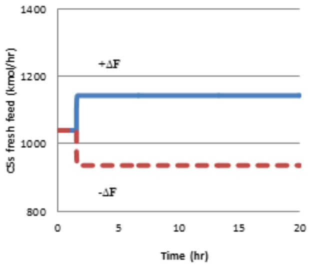
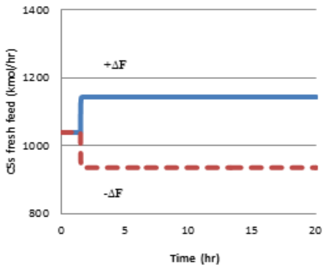
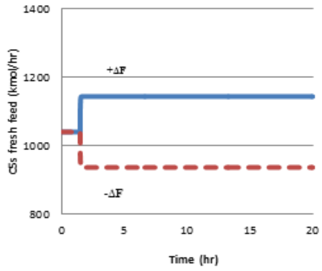
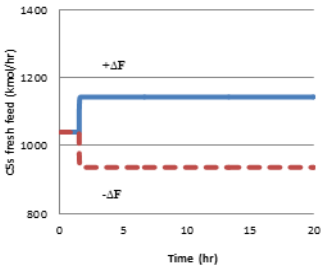
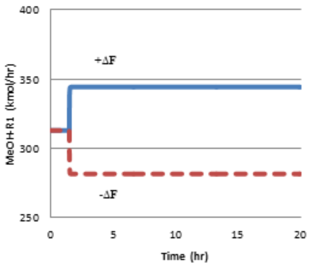
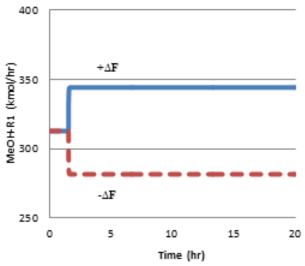
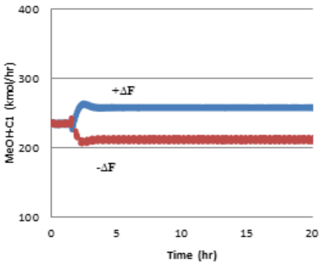
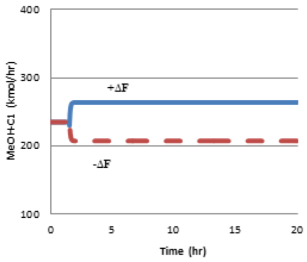
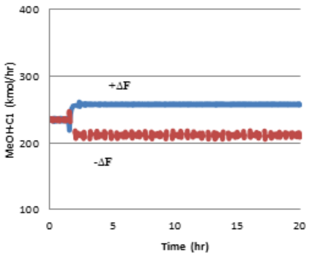
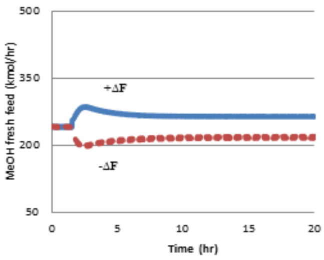
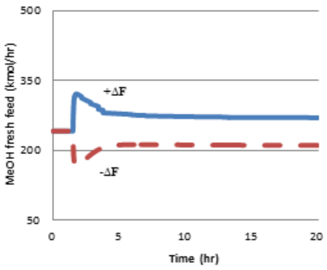
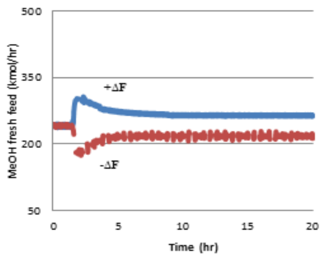
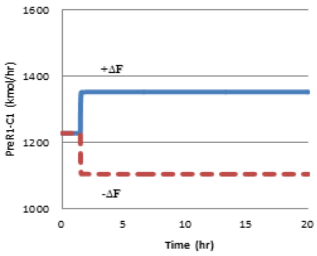
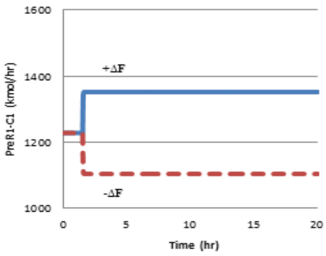
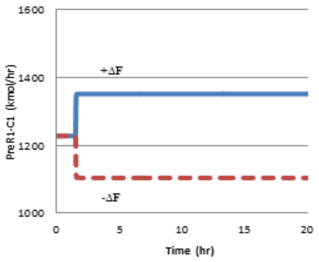
	Base Case	NCS1	NCS2
C5s fresh feed (kmol/hr)			
MeOH-R1 (kmol/hr)			
MeOH-C1 (kmol/hr)			
MeOH fresh feed (kmol/hr)			
PreR1-C1 (kmol/hr)			

Table 5.27 (continue) The Dynamic responses of total feed flow changed

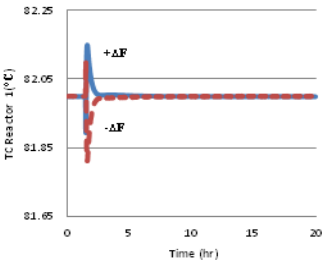
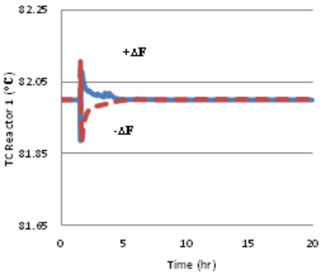
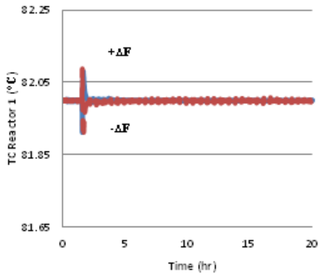
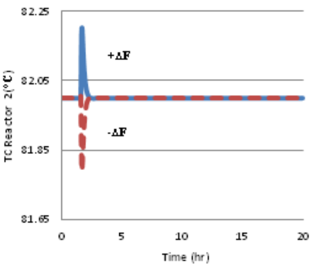
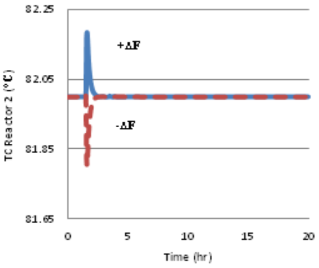
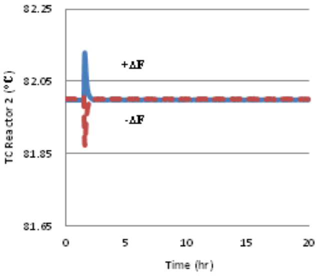
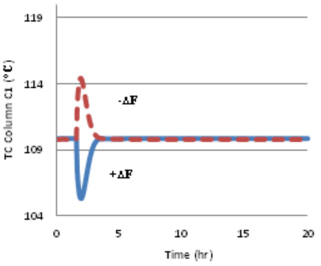
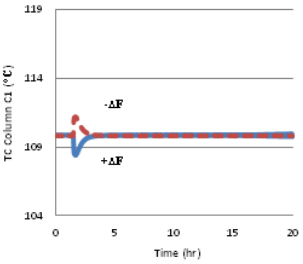
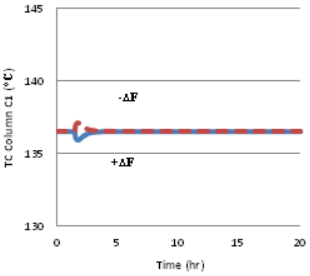
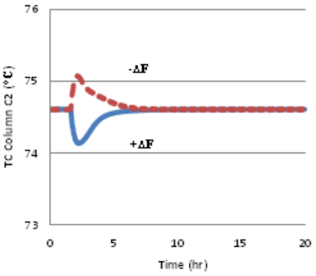
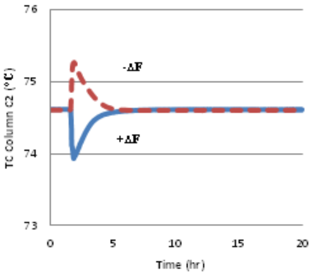
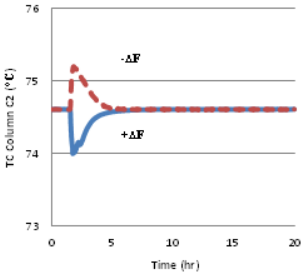
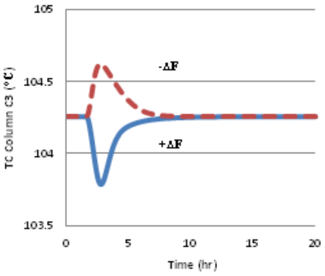
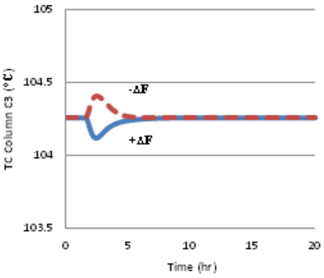
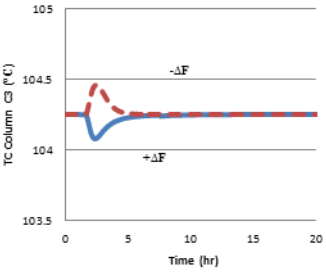
	Base Case	NCS1	NCS2
TC Reactor 1			
TC Reactor 2			
TC Column C1			
TC Column C2			
TC Column C3			

Table 5.27 (continue) The Dynamic responses of total feed flow changed

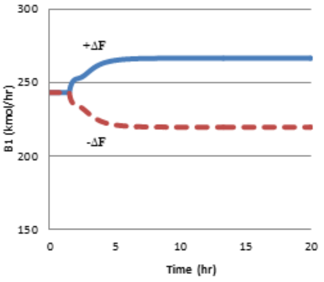
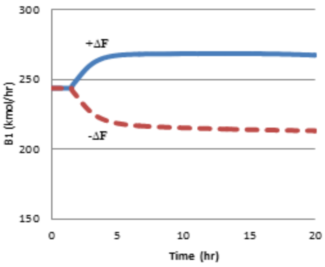
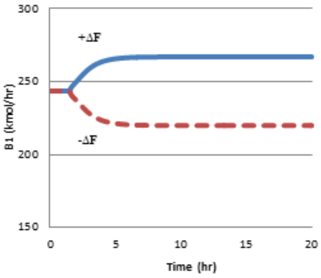
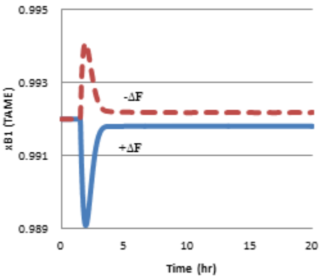
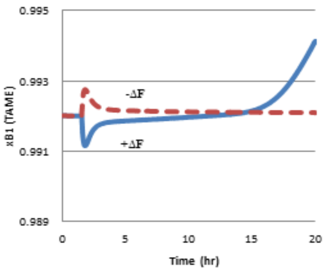
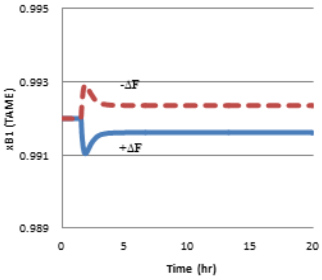
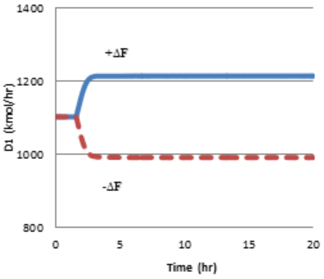
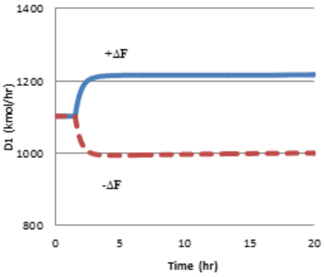
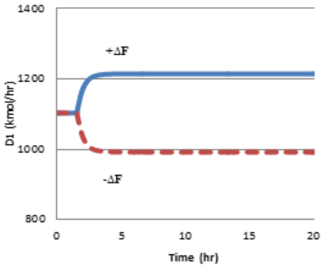
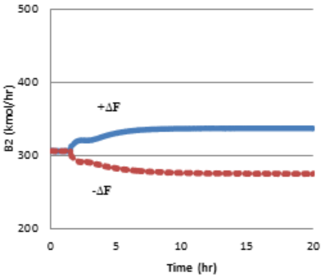
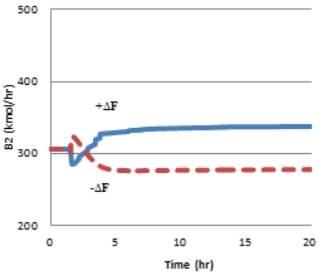
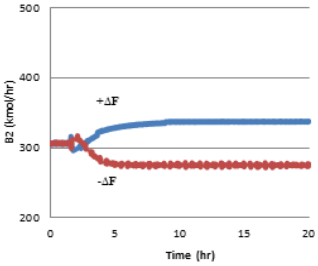
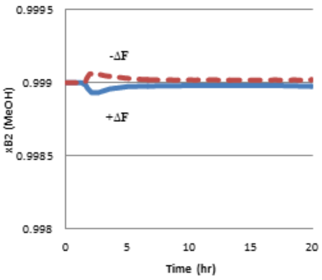
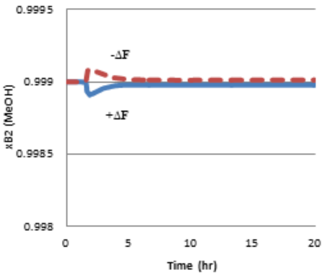
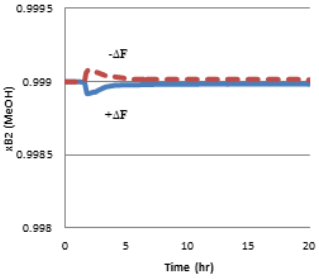
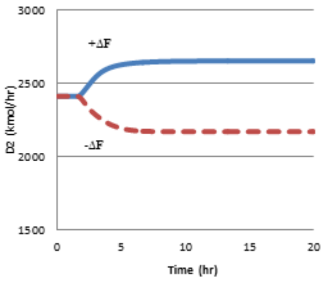
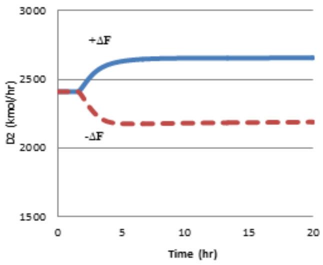
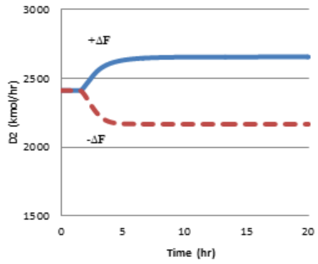
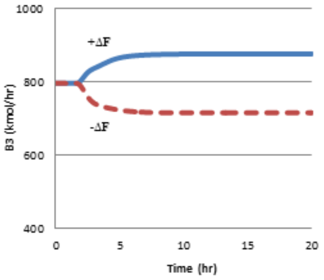
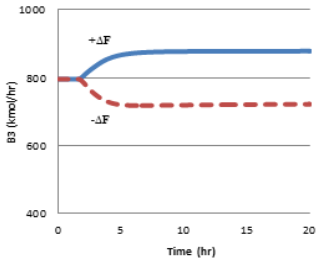
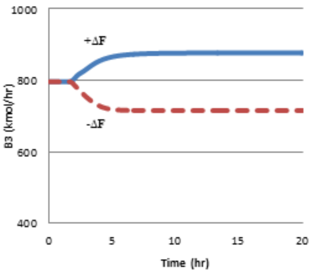
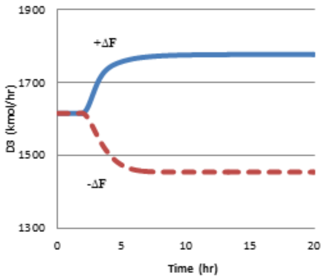
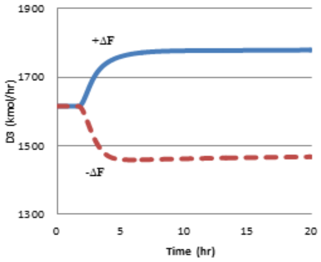
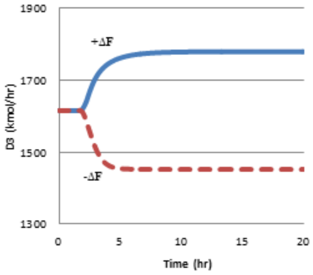
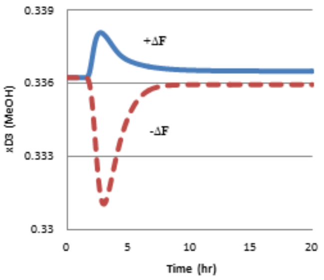
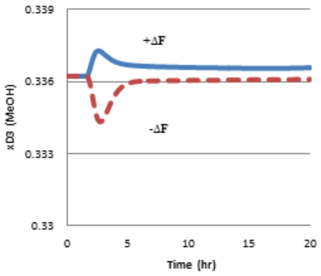
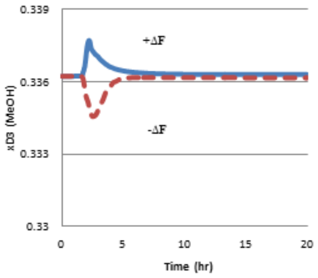
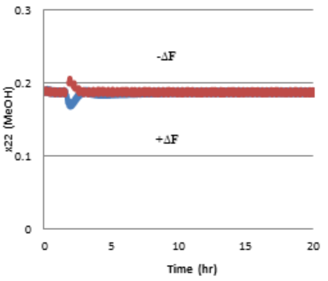
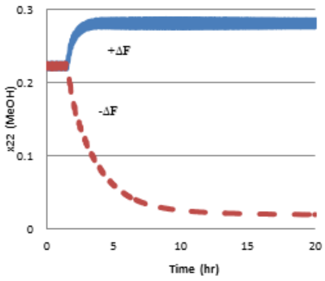
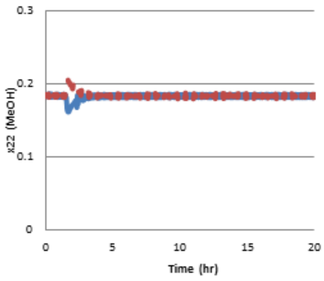
	Base Case	NCS1	NCS2
B1 (kmol/hr)			
xB1 (TAME)			
D1 (kmol/hr)			
B2 (kmol/hr)			
xB2 (MeOH)			

Table 5.27 (continue) The Dynamic responses of total feed flow changed

	Base Case	NCS1	NCS2
D2 (kmol/hr)			
B3 (kmol/hr)			
D3 (kmol/hr)			
xD3 (MeOH)			
X22 (MeOH)			

2. Composition of C5s fresh feed change.

Composition of isoamylene (2M1B, 2M2B) in C5s fresh feed were deviated ±10% (±ΔZ) from the nominal case. Table 5.28 shows the responses of increasing and decreasing 10 % of composition in C5s fresh feed. It was observed that the composition of isoamylene was increased 10% from the nominal case, affected to increase in temperature, reaction rate, and production rate, respectively. In another hand, when the composition of isoamylene was decreased, the results were reversed.

For temperature control loop, PID controller in NCS2 and NCS1 affected to small temperature deviation and took time to set point less than PI controller in base case. The purity of product in NCS2 gave the desired target, base case and NCS1 gave new steady state in 4 hours for base case, 10 hours for NCS1.

The composition of methanol in both recycle streams came to set point but in distillate rate of column C3, NCS1 and NCS2 went to specification value earlier than base case.

Table 5.28 The Dynamic responses of feed composition changed

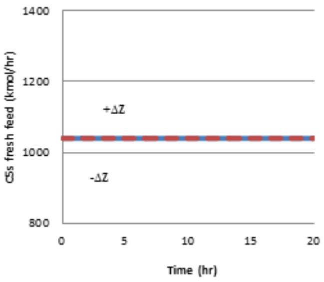
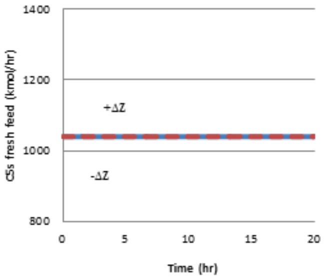
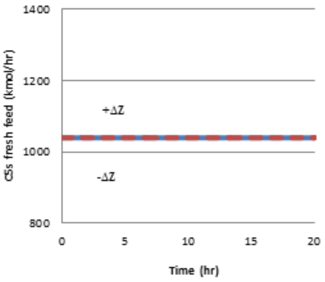
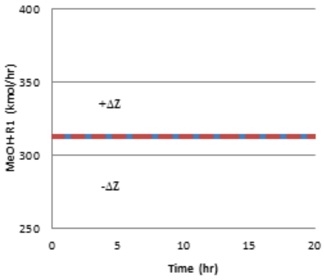
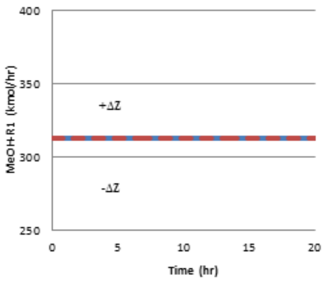
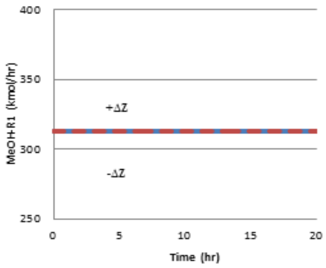
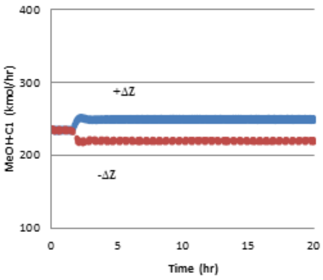
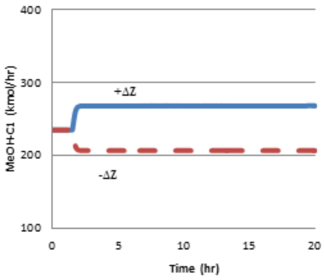
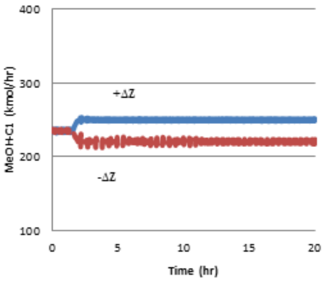
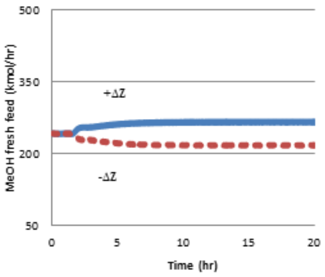
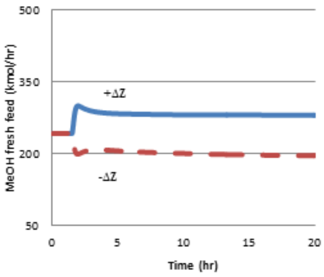
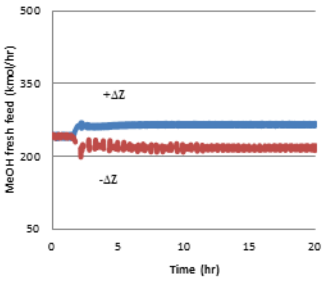
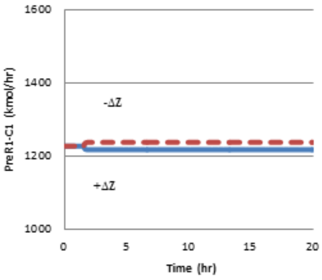
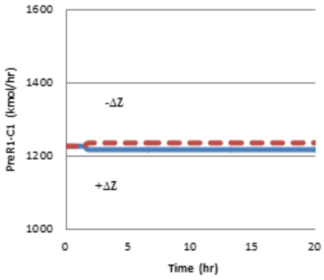
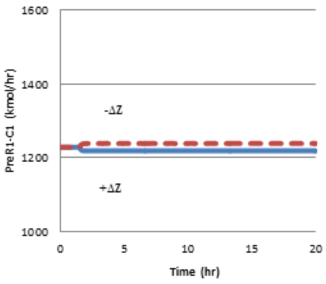
	Base Case	NCS1	NCS2
C5s fresh feed (kmol/hr)			
MeOH-R1 (kmol/hr)			
MeOH-C1 (kmol/hr)			
MeOH fresh feed (kmol/hr)			
PreR1-C1 (kmol/hr)			

Table 5.28 (continue) The Dynamic responses of feed composition changed

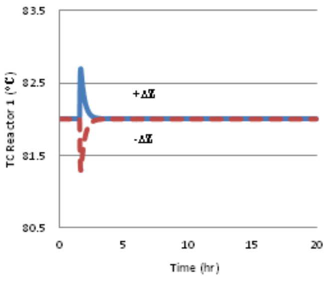
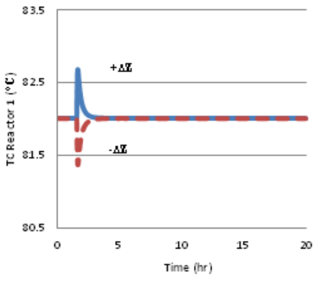
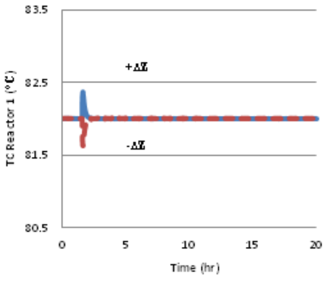
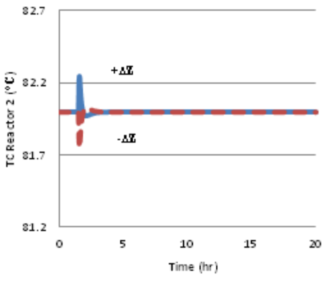
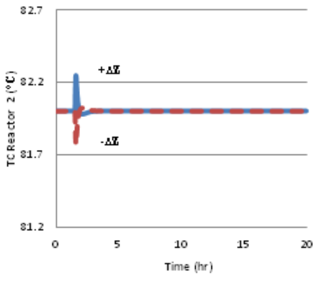
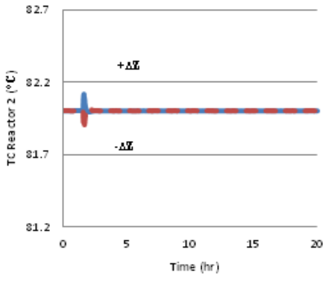
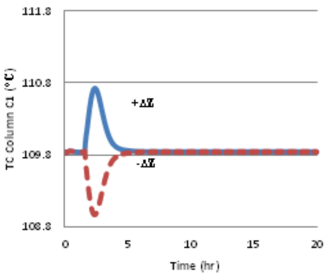
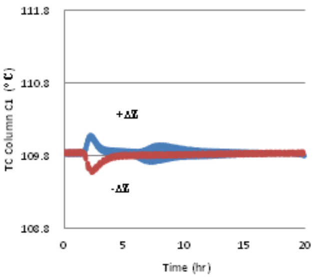
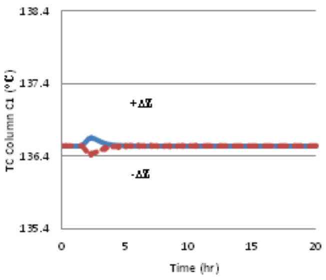
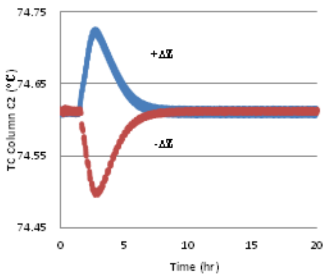
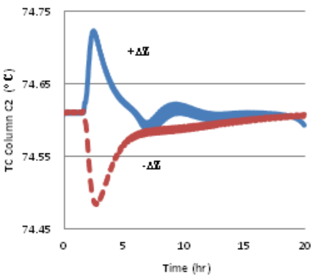
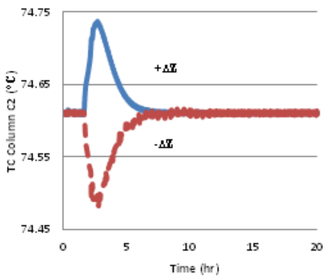
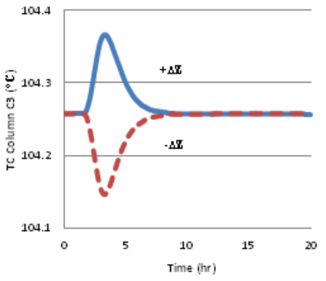
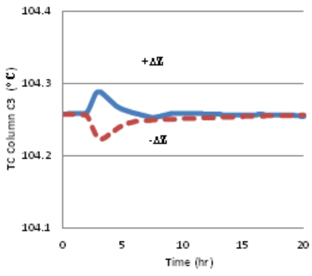
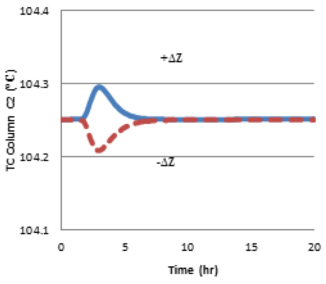
	Base Case	NCS1	NCS2
TC Reactor 1			
TC Reactor 2			
TC Column C1			
TC Column C2			
TC Column C3			

Table 5.28 (continue) The Dynamic responses of feed composition changed

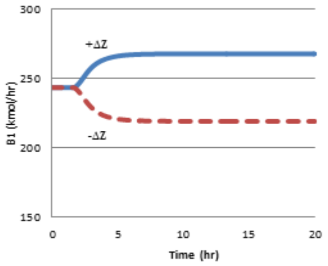
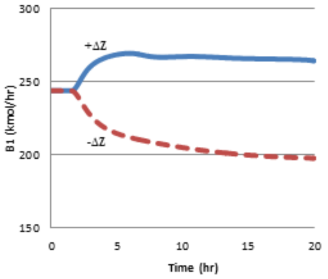
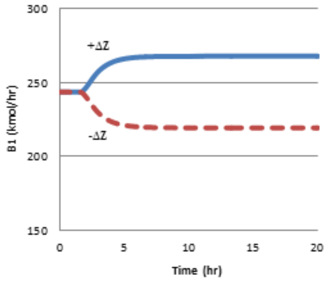
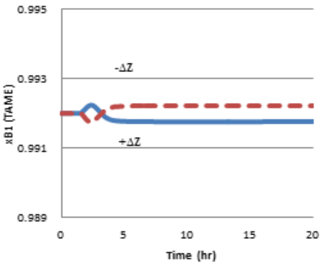
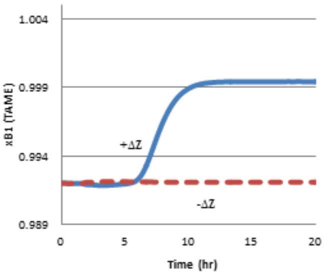
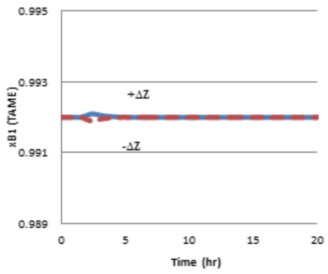
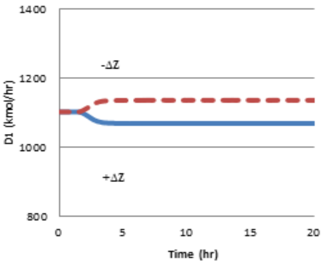
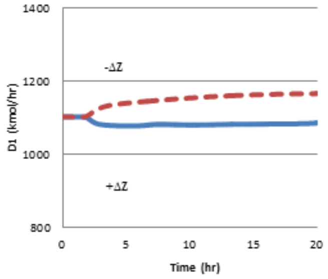
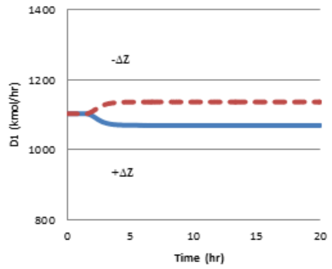
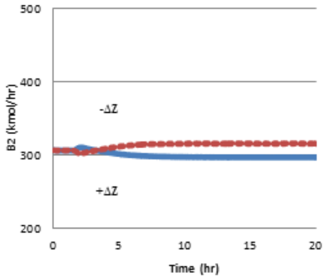
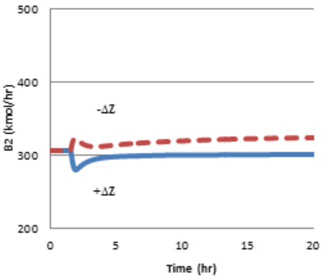
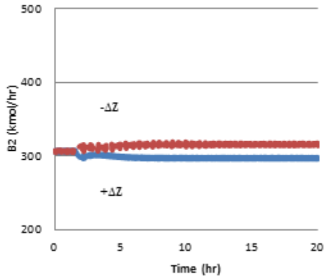
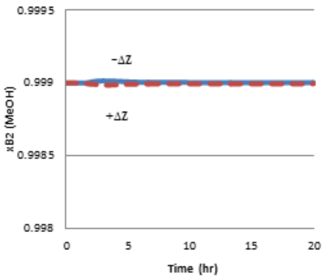
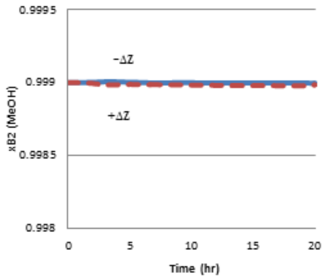
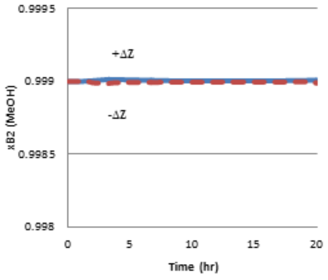
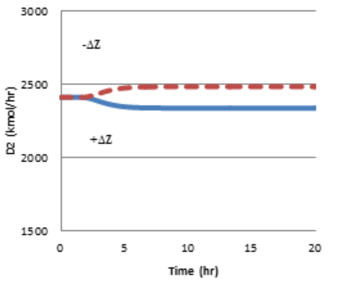
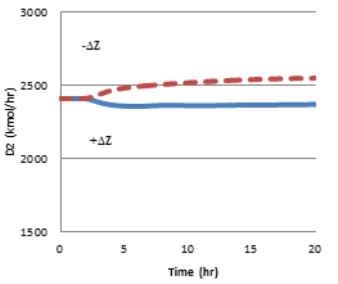
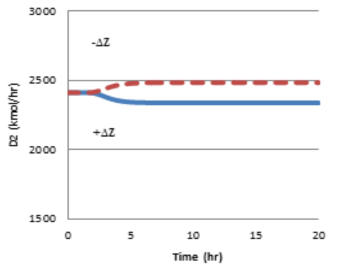
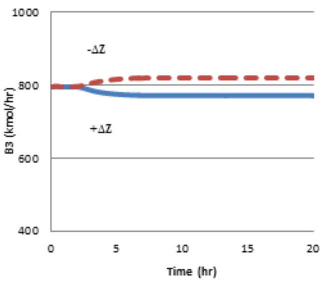
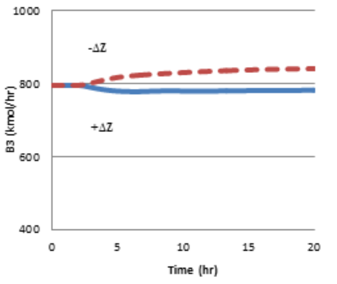
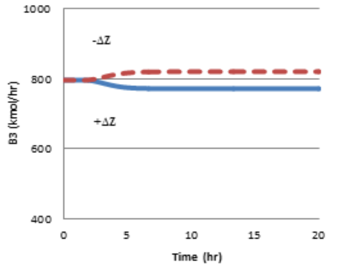
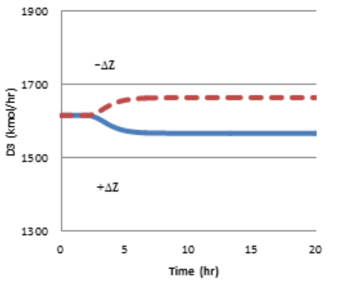
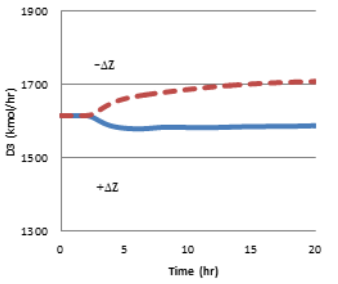
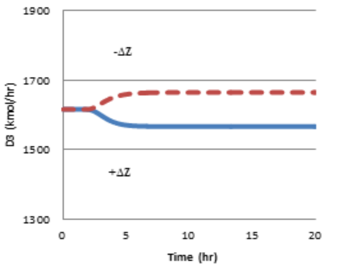
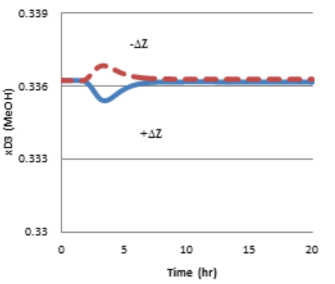
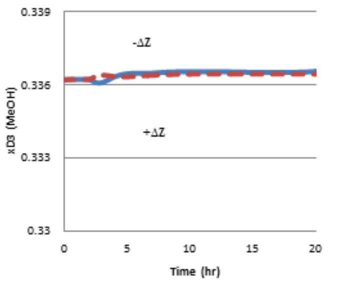
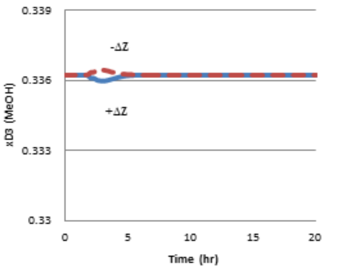
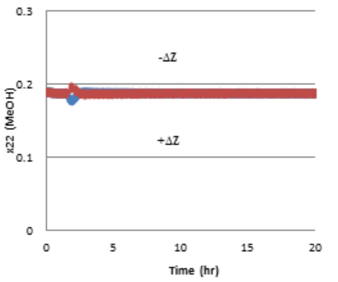
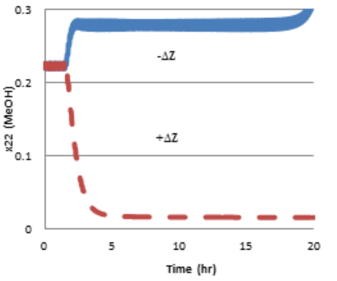
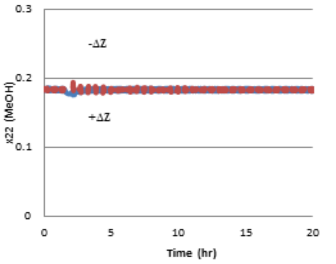
	Base Case	NCS1	NCS2
B1 (kmol/hr)			
xB1 (TAME)			
D1 (kmol/hr)			
B2 (kmol/hr)			
xB2 (MeOH)			

Table 5.28 (continue) The Dynamic responses of feed composition changed

	Base Case	NCS1	NCS2
D2 (kmol/hr)			
B3 (kmol/hr)			
D3 (kmol/hr)			
xD3 (MeOH)			
X22 (MeOH)			

3. Temperature of C5s fresh feed change.

In C5s fresh feed was tested by increasing temperature from 77 °C to 87 °C and decreasing from 77 °C to 67 °C. The dynamic response shows as Table 5.29. When, flowrate of all streams were considered, it shown that there was no difference in all control structure. Except methanol fresh feed and methanol feed to column C1 streams, NCS2 had little oscillation before went to set point at fifth hour. This behavior affected from composition control.

First and second reactors, the temperature of NCS2 converged to the desired target fastest. Temperature of column C1, base case had the deviation higher than another case. It effect of PI controller. But NCS1 had the oscillation all time between 109.8 °C to 109.85 °C because the reaction in the column not constant. For Column C2 and column C3, all case gave the same response.

Table 5.29 The Dynamic responses of feed Temperature changed

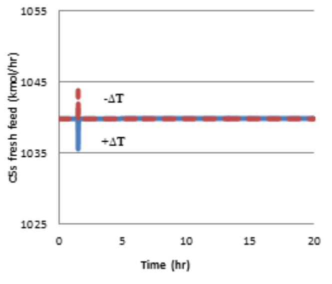
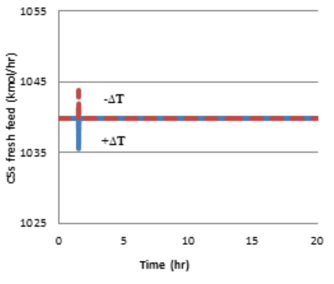
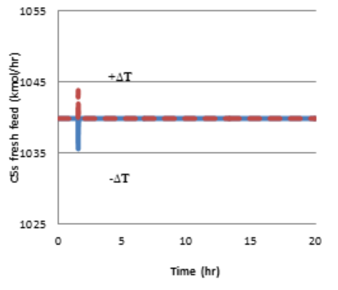
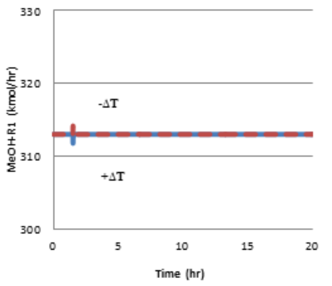
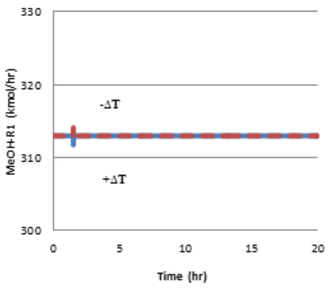
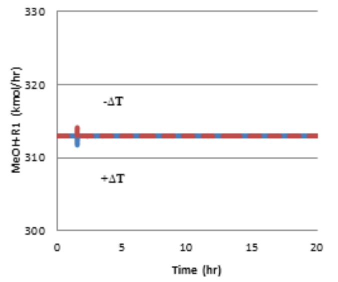
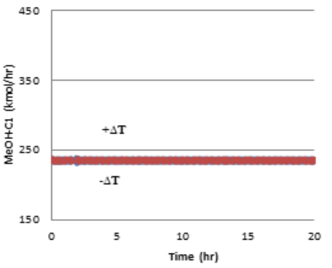
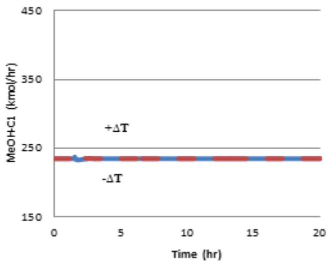
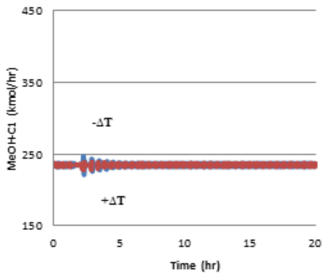
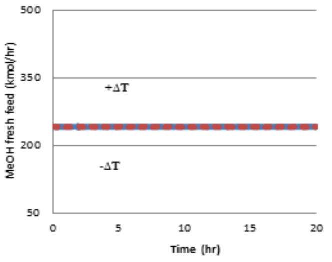
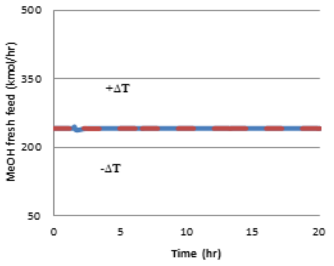
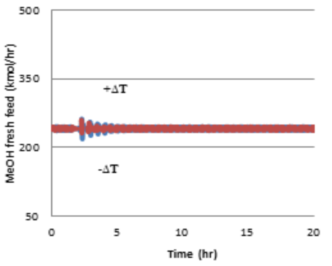
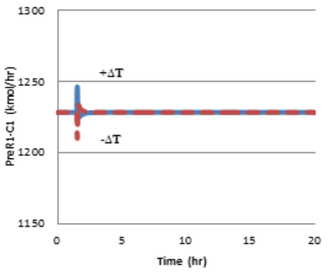
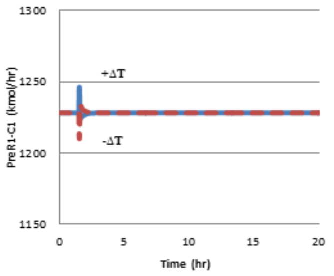
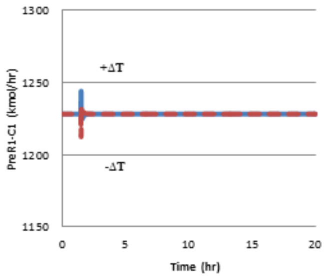
	Base Case	NCS1	NCS2
C5s fresh feed (kmol/hr)			
MeOH-R1 (kmol/hr)			
MeOH-C1 (kmol/hr)			
MeOH fresh feed (kmol/hr)			
PreR1-C1 (kmol/hr)			

Table 5.29 (continue) The Dynamic responses of feed Temperature changed

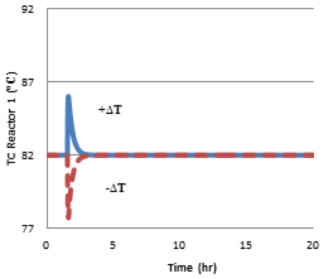
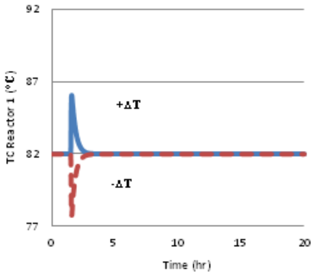
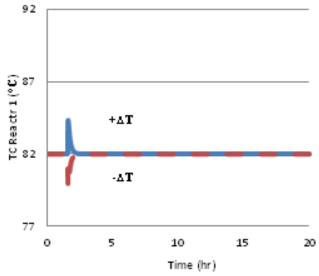
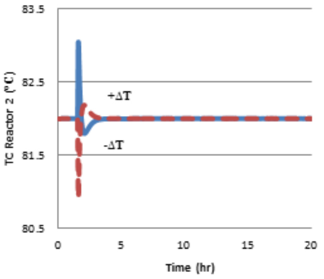
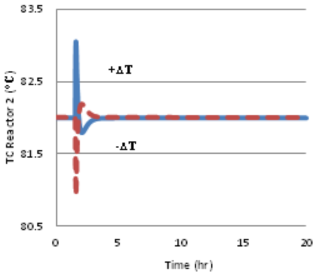
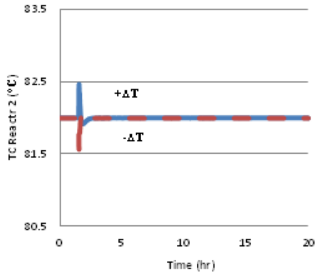
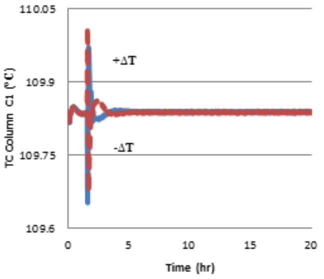
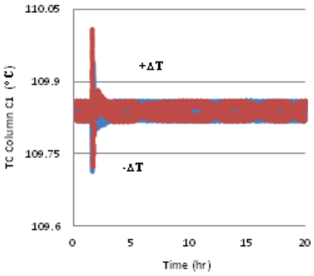
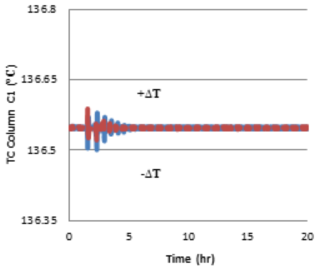
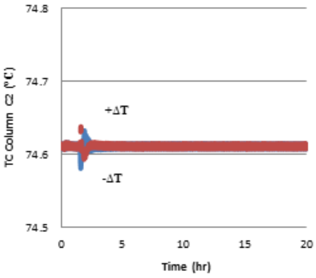
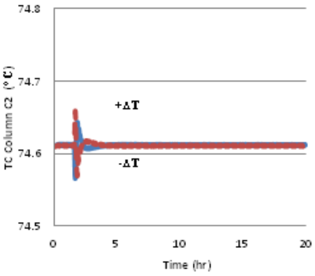
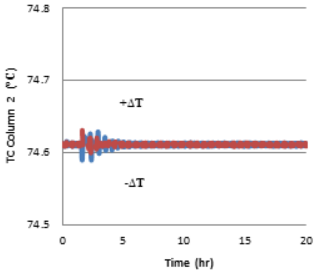
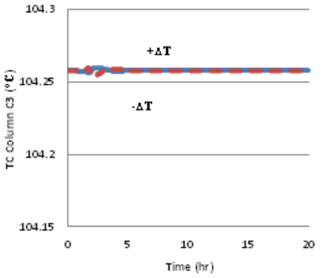
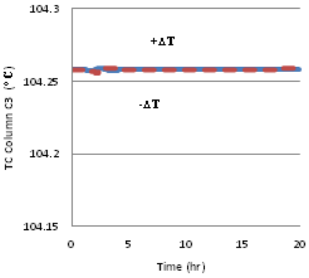
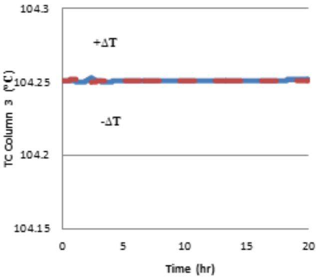
	Base Case	NCS1	NCS2
TC Reactor 1			
TC Reactor 2			
TC Column C1			
TC Column C2			
TC Column C3			

Table 5.29 (continue) The Dynamic responses of feed Temperature changed

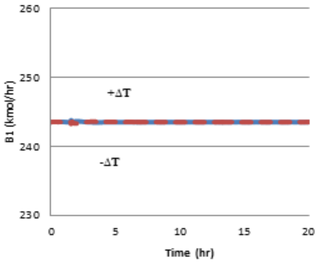
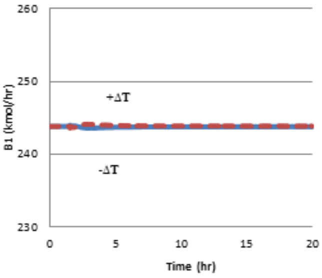
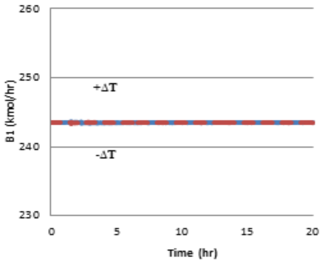
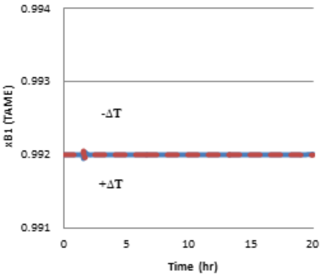
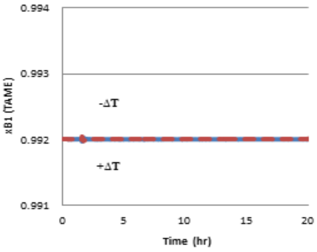
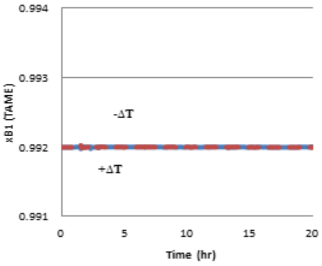
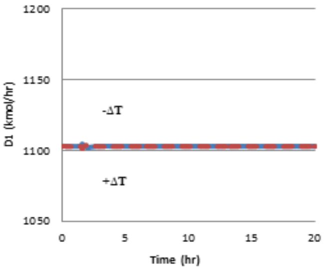
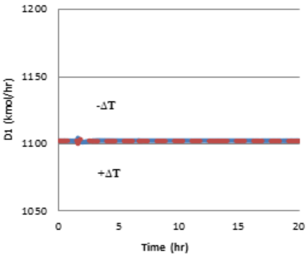
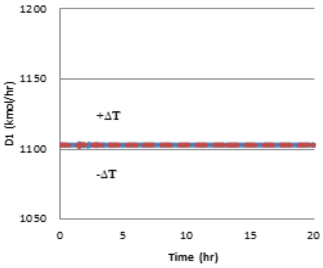
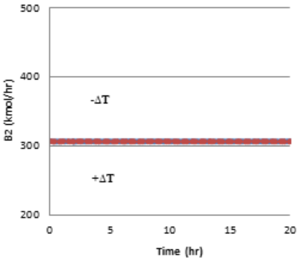
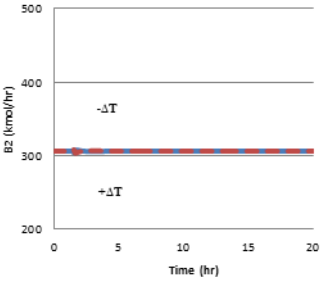
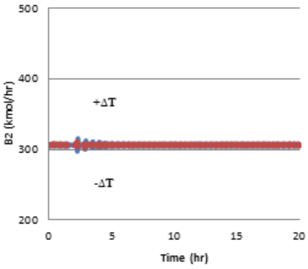
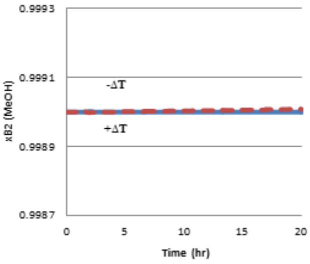
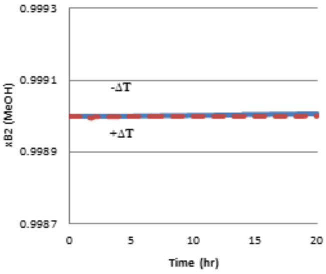
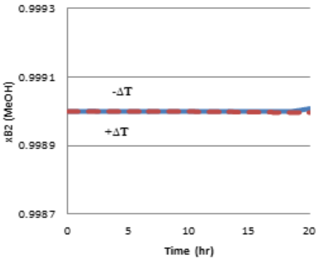
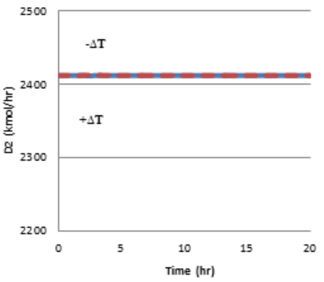
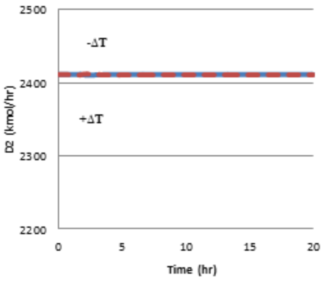
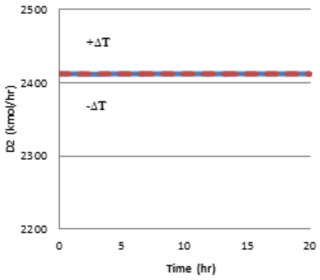
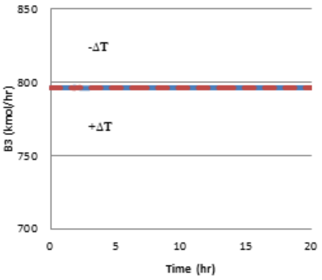
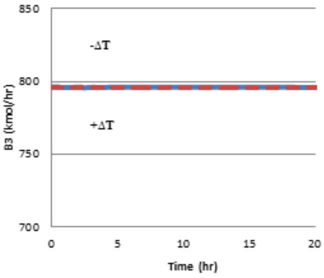
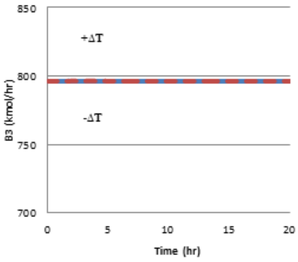
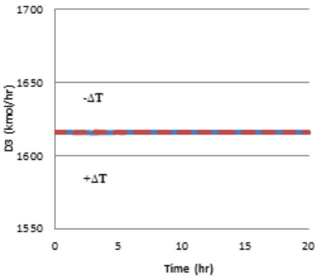
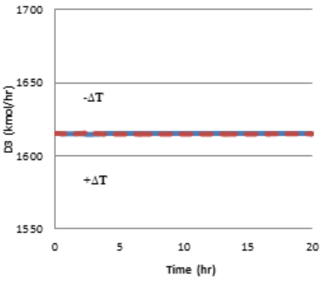
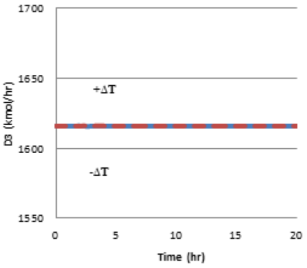
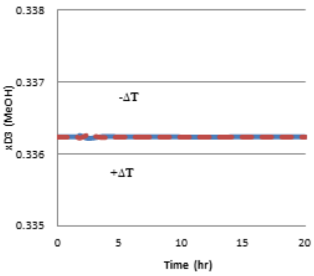
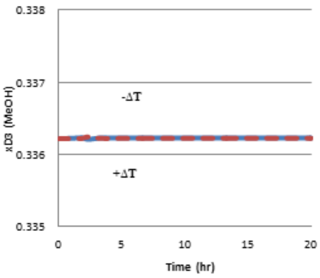
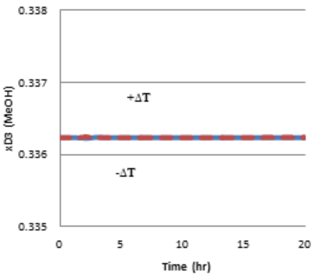
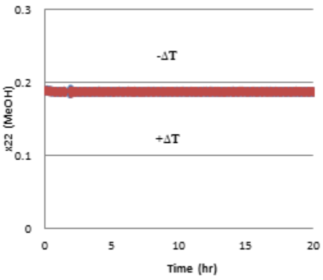
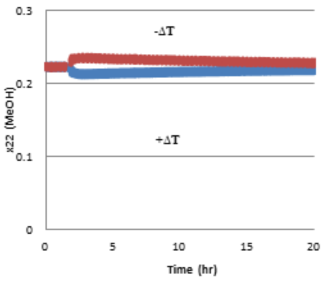
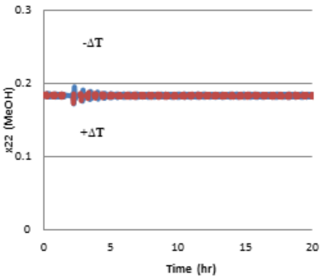
	Base Case	NCS1	NCS2
B1 (kmol/hr)			
xB1 (TAME)			
D1 (kmol/hr)			
B2 (kmol/hr)			
xB2 (MeOH)			

Table 5.29 (continue) The Dynamic responses of feed Temperature changed

	Base Case	NCS1	NCS2
D2 (kmol/hr)			
B3 (kmol/hr)			
D3 (kmol/hr)			
xD3 (MeOH)			
X22 (MeOH)			

4. Component of C5s fresh fees change.

The flowrate of isoamylene in C5s fresh feed was changed ±10% from nominal case. The response shows as Table 5.30. When the component of the limiting reactant in C5s feed flowrate was increased, it affected to increase all methanol streams and the product rate. On the other hand, if the component of the limiting reactant was decreased, methanol streams and product rate was reduced too. The methanol fresh feed flowrate in base case gradually increased but the fresh feed of NCS1 and NCS2 rapidly changes because of the differential location to control. In base case the methanol fresh feed was adjusted from the liquid level in bottom of column C2 but in NCS1 and NCS2 were adjusted from the flowrate of methanol feed to column C1 and the methanol composition on tray 22 in column C1, respectively.

All control structures, the temperature controllers gave the same responses of the temperature in all units. The small deviation of reactors temperature of new control structures affected from PID controller.

Composition of TAME at bottom flowrate in column C1, all cases studied went to the new steady state. NCS2 gave the closest to the set point.

Table 5.30 The Dynamic responses of feed component flow changed

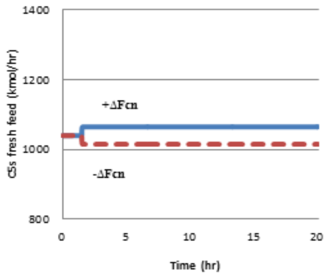
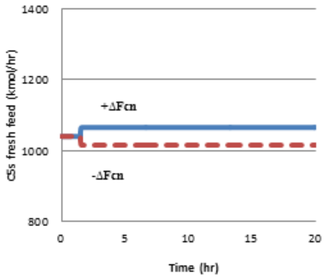
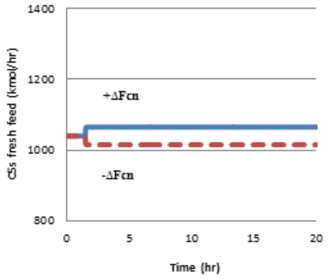
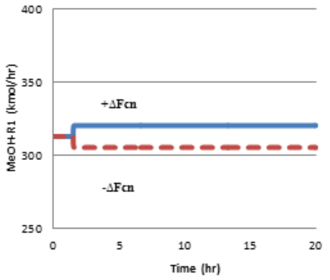
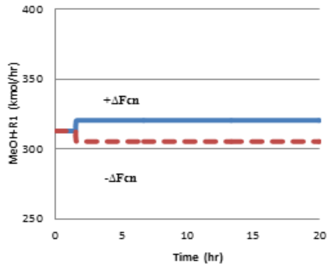
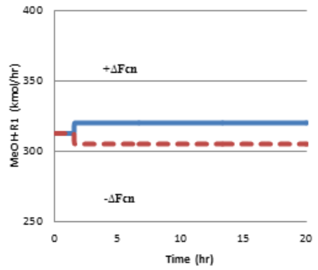
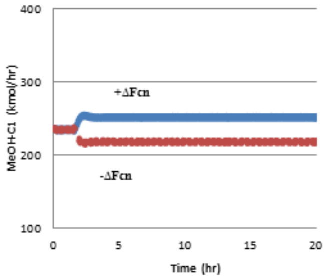
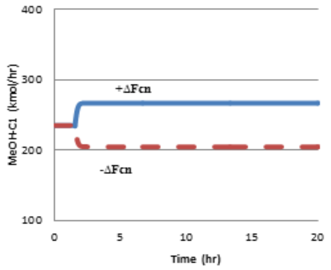
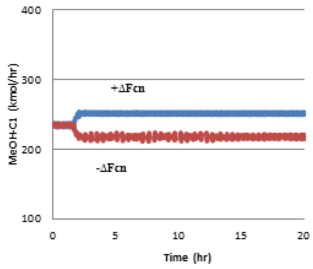
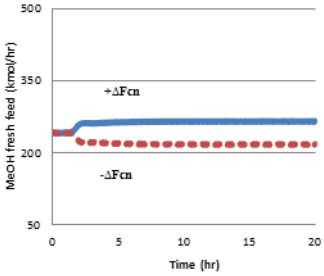
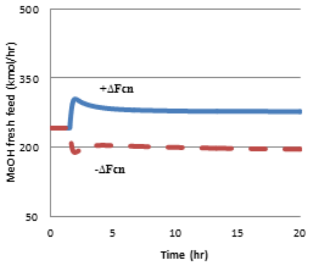
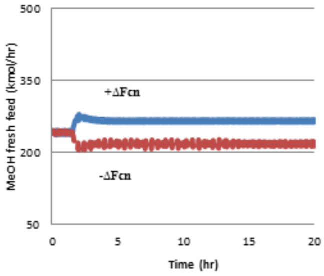
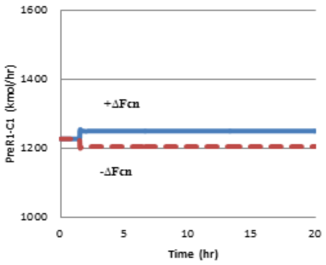
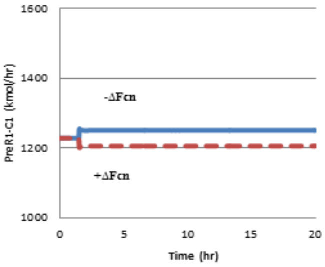
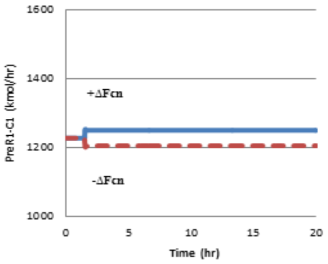
	Base Case	NCS1	NCS2
C5s fresh feed (kmol/hr)			
MeOH-R1 (kmol/hr)			
MeOH-C1 (kmol/hr)			
MeOH fresh feed (kmol/hr)			
PreR1-C1 (kmol/hr)			

Table 5.30 (continue) The Dynamic responses of feed component flow changed

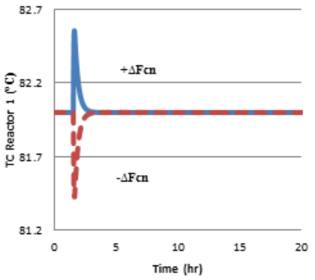
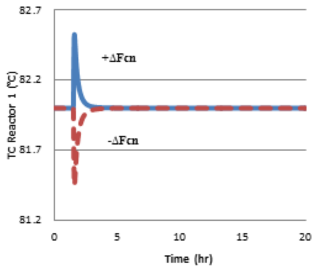
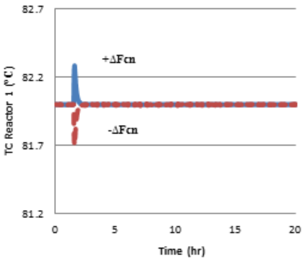
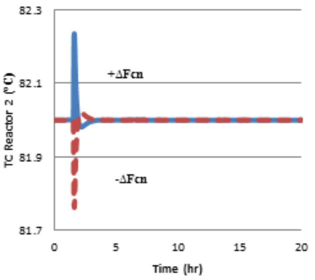
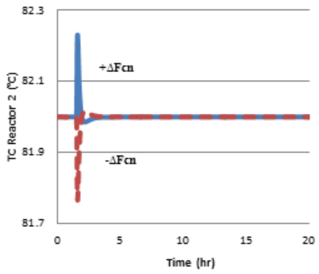
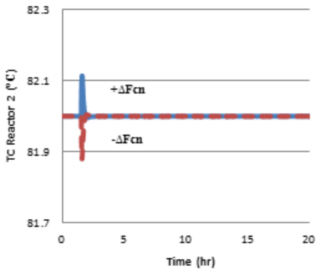
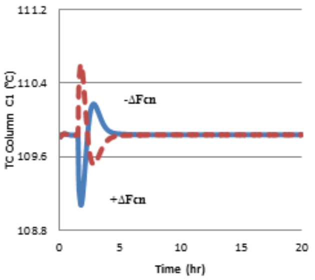
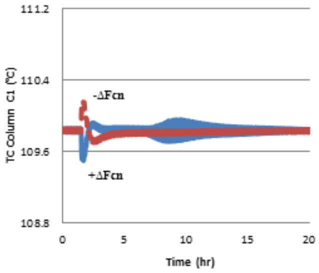
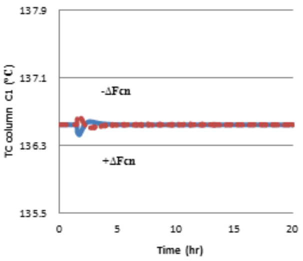
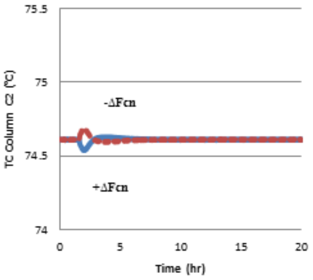
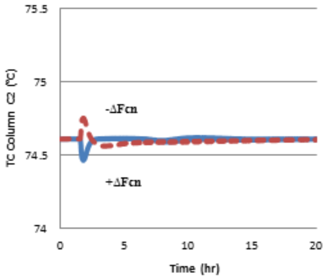
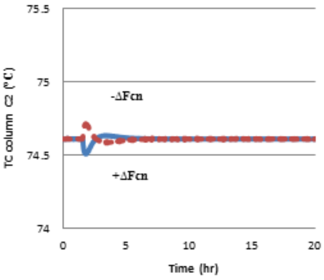
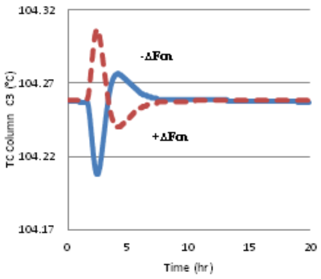
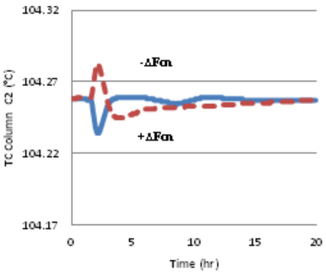
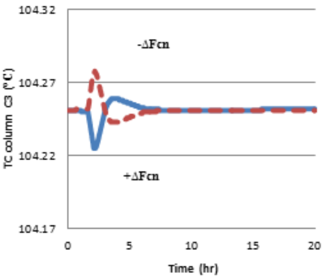
	Base Case	NCS1	NCS2
TC Reactor 1 (°C)			
TC Reactor 2 (°C)			
TC Column C1(°C)			
TC Column C2 (°C)			
TC Column C3 (°C)			

Table 5.30 (continue) The Dynamic responses of feed component flow changed

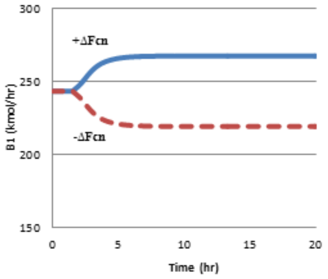
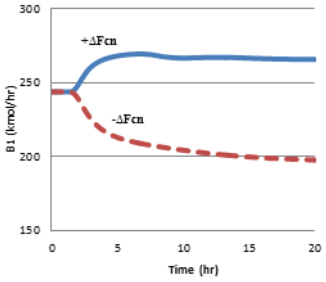
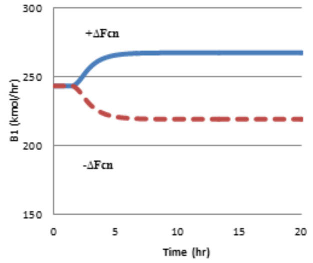
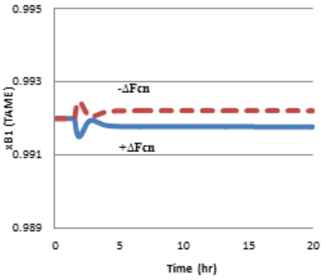
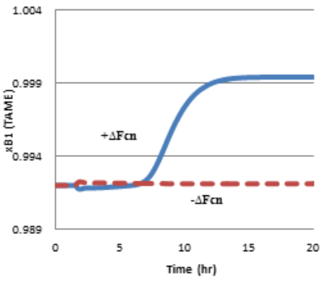
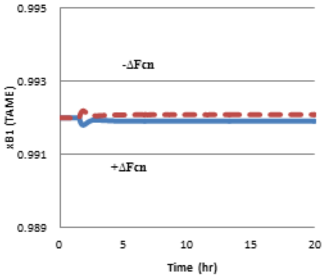
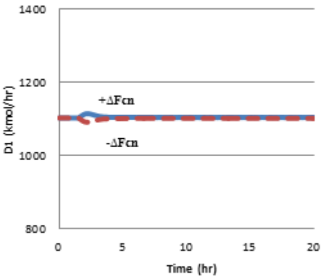
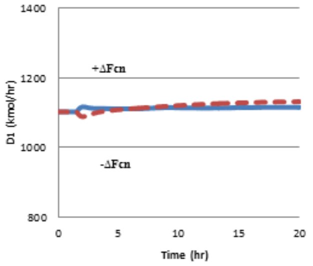
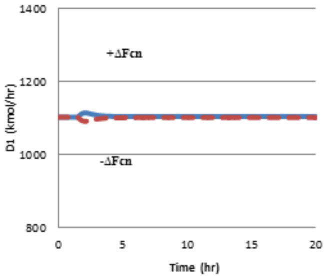
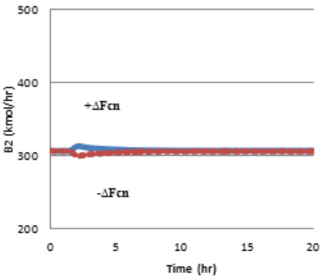
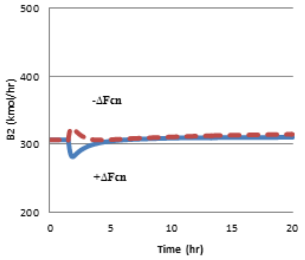
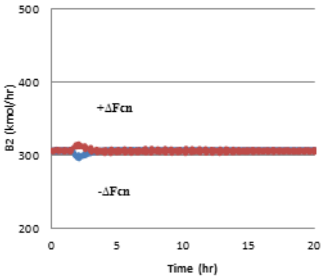
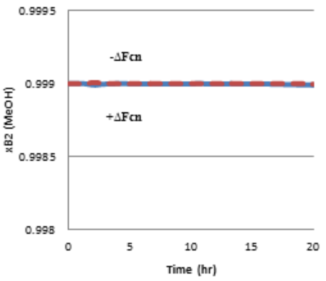
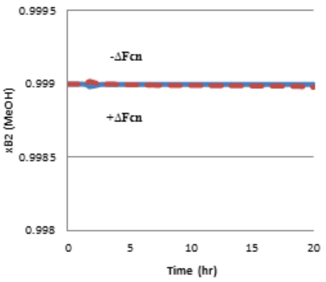
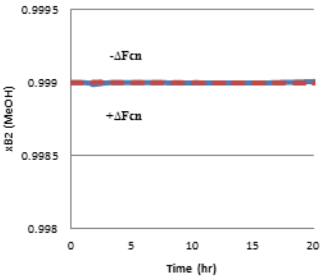
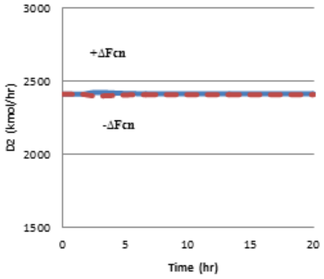
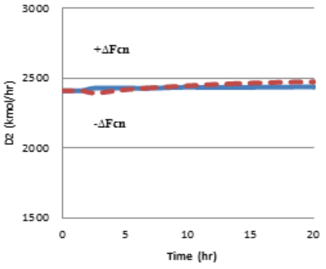
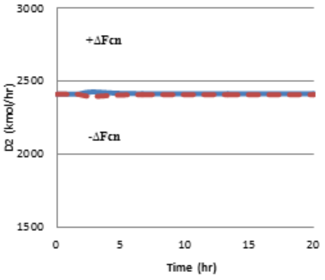
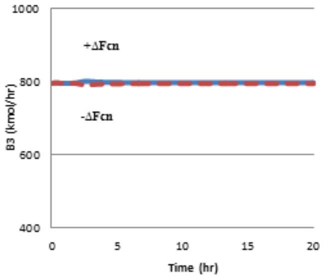
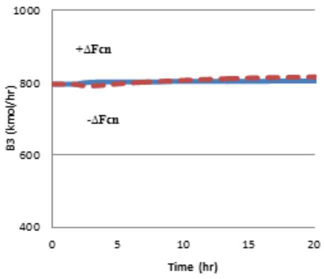
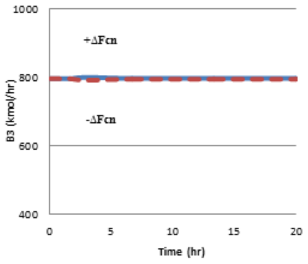
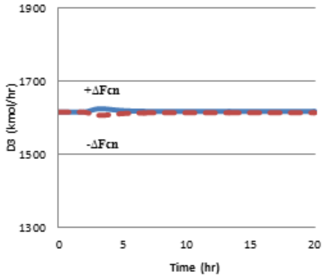
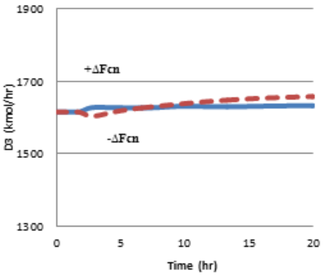
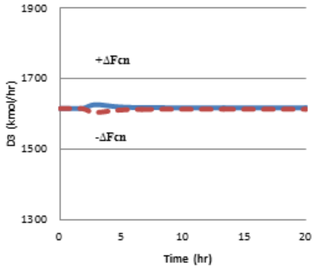
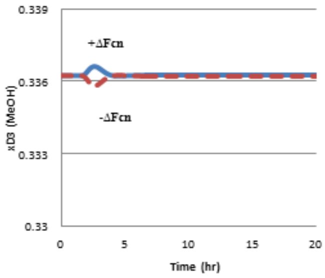
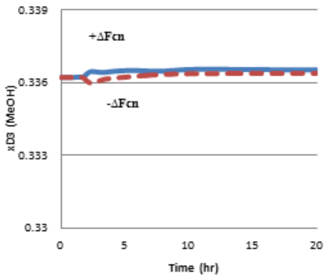
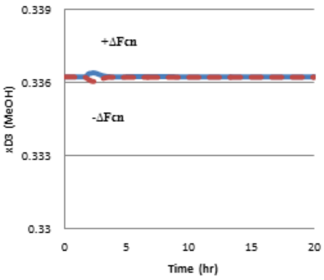
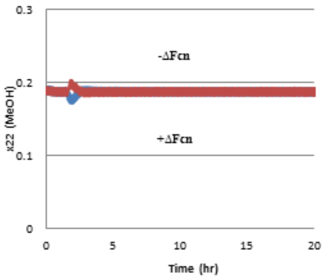
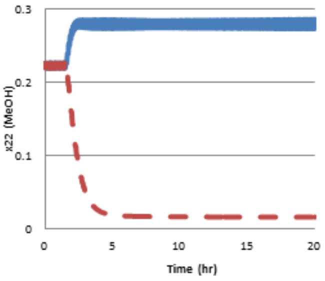
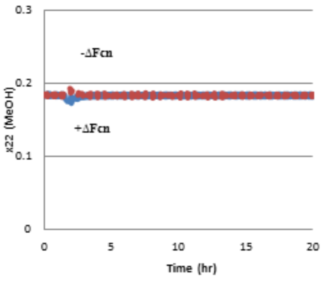
	Base Case	NCS1	NCS2
B1 (kmol/hr)			
xB1 (TAME)			
D1 (kmol/hr)			
B2 (kmol/hr)			
xB2 (MeOH)			

Table 5.30 (continue) The Dynamic responses of feed component flow changed

	Base Case	NCS1	NCS2
D2 (kmol/hr)			
B3 (kmol/hr)			
D3 (kmol/hr)			
xD3 (MeOH)			
X22 (MeOH)			

5.2 Evaluation of the Dynamic Performance

The integral of the absolute errors (IAE) were focused for evaluation the dynamic performance of the control structures. The IAE was determined from the loop control of temperature, pressure, composition, level, and flow control loops.

The temperature and pressure control loops were considered for the safety. The quality loop control was analyzed from composition loops. The safety and the quality control loops in the process operation causes the operation smoothly and security. The IAE value was determined after control structures were tested by the disturbances.

The IAE criterion was defined as

$$IAE = \int_{0}^{time} |\, e(t)|\, dt$$

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

The IAE were evaluated to select the best control structure. The minimum IAE value means the best control structure that operating smoothly and safety and keeping the product quality in commercial requirement. The IAE value for all disturbances tested shows in Table 5.31-5.34.

From the obtaining IAE value of pressure control loops for all tested fell in a satisfying range in all control structures. In the part of the temperature and composition control loop, new control structure design 2 (NCS2) gave the smallest IAE value than other case in all disturbances tested. Therefore, the best results of the new plantwide control structure design 2 (NCS2) affected to the good operation and the good controlling of the product purity.

Table 5.31 IAE of control loops total feed flow change

Control loop	Base case	NCS1	NCS2
Composition	0.0616	0.0868	**0.0462**
Temperature	11.9391	5.2877	**3.6627**
Pressure	**0.0312**	0.0349	0.0335

Table 5.32 IAE of control loops feed composition change

Control loop	Base case	NCS1	NCS2
Composition	0.0459	0.3302	**0.0404**
Temperature	4.3435	3.0422	**1.3580**
Pressure	0.0097	0.0155	**0.0079**

Table 5.33 IAE of control loops feed temperature change

Control loop	Base case	NCS1	NCS2
Composition	0.0004	0.0036	**0.0002**
Temperature	3.8684	4.2127	**1.2268**
Pressure	0.0016	**0.0012**	0.0018

Table 5.34 IAE of control loops feed component flow change

Control loop	Base case	NCS1	NCS2
Composition	0.0400	0.2896	**0.0352**
Temperature	2.5068	2.5434	**0.7885**
Pressure	**0.0040**	0.0301	0.0065

5.3 Utility cost

The duties used in cooling and heating and the works used in pumps were applied to calculated Utilities costs· The cost of cooling water and the steam used in the process is 0.354$/GJ. The low pressure steam in the process is 4.7$/GJ. The electric cost is $16.8/GJ.

Table 5.35-5.38 show the utilities cost of all disturbances tested. The Utilities cost of NCS1 was highest cost but in the base case and NCS2 were the most closely. Utilities cost of base case less than new control structure for all disturbances tested. Sum of utility cost in all disturbances tested for two control structure is shown in Figure 5.27.

Table 5.35 Utilities cost with total feed flowrate change

Utilities	Base case	NCS1	NCS2
Energy (GJ/h)	600.64	600.49	600.70
Cost (m$/year)	13.3732	13.4375	13.3742
Work (kW)	390.48	391.03	395.87
Cost (m$/year)	0.2018	0.2021	0.2046
Utilities Cost (m$/year)	13.5750	13.6396	13.5787

Table 5.36 Utilities cost with feed composition change

Utilities	Base case	NCS1	NCS2
Energy (GJ/h)	600.74	612.77	600.72
Cost (m$/year)	13.3725	13.6468	13.3711
Work (kW)	392.59	394.18	397.99
Cost (m$/year)	0.2029	0.2037	0.2057
Utilities Cost (m$/year)	13.5754	13.8505	13.5768

Table 5.37 Utilities cost with feed temperature change

Utilities	Base case	NCS1	NCS2
Energy (GJ/h)	602.32	601.97	602.33
Cost (m$/year)	13.3775	13.3698	13.3779
Work (kW)	392.92	392.87	398.31
Cost (m$/year)	0.2030	0.2030	0.2058
Utilities Cost (m$/year)	13.5805	13.5728	13.5837

Table 5.38 Utilities cost with feed component flow change

Utilities	Base case	NCS1	NCS2
Energy (GJ/h)	600.76	611.41	600.73
Cost (m$/year)	13.3726	13.6158	13.3725
Work (kW)	392.92	394.63	398.34
Cost (m$/year)	0.2030	0.2039	0.2058
Utilities Cost (m$/year)	13.5756	13.8197	13.5783

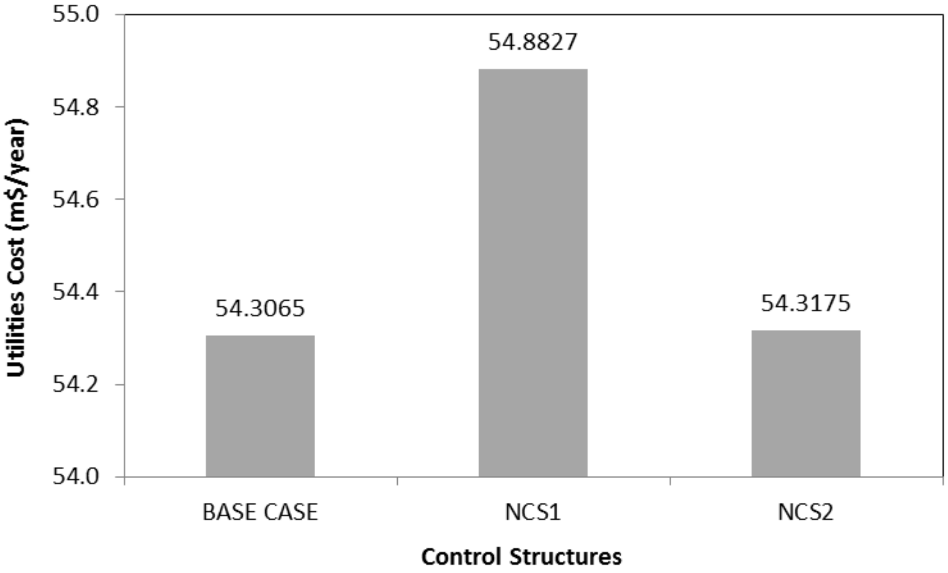


Figure 5.27 The total utility costs of each control structures

CHAPTER VI

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

The new design procedure of Wongsri is designed in plantwide level and based on heuristics analysis. It has the systematic steps and specific guidelines are apparent. This procedure designs for emphasis on maintaining the plant operating conditions and selection the best set of control structure.

This research, the plantwide control structure design by Wongsri is applied to *tert*-amyl methyl ether process. The efficiency of new control structure designed is evaluated by the IAE value is the disturbances tests (total feed, feed composition, feed temperature, and feed component change).

From all cases studies, the NCS2 give the best performance dynamic behavior of the control structure which could management the process safety and smoothly operation by the utility cost fall in a satisfying range.

6.2 Recommendation

The performances of the control structure 1 (NCS1) can be designed for more effectively control by adding the enhanced controllers can also improve the performances of control structure. Furthermore, the plantwide control structure design procedure by Wongsri could be applied to the other process control.

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APPENDICES

APPENDIX A

EQUIPMENT DATA AND STREAM INFORMATION

Table A.1 Equipment data

Units operation	Properties	Size
Reactor R1	Diameter (m) Total volume (m^3)	1.85 10
Reactor R2	Diameter (m) Total volume (m^3)	1.85 10
Reflux drum column C1	Diameter (m) Length (m)	3.88 7.77
Reflux drum column C2	Diameter (m) Length (m)	3.3 6.62
Reflux drum column C3	Diameter (m) Length (m)	3.3 6.58
Reboiler column C1	Diameter (m) Height (m)	4.5 9
Reboiler column C2	Diameter (m) Height (m)	2.25 4.5
Reboiler column C3	Diameter (m) Height (m)	4.5 9

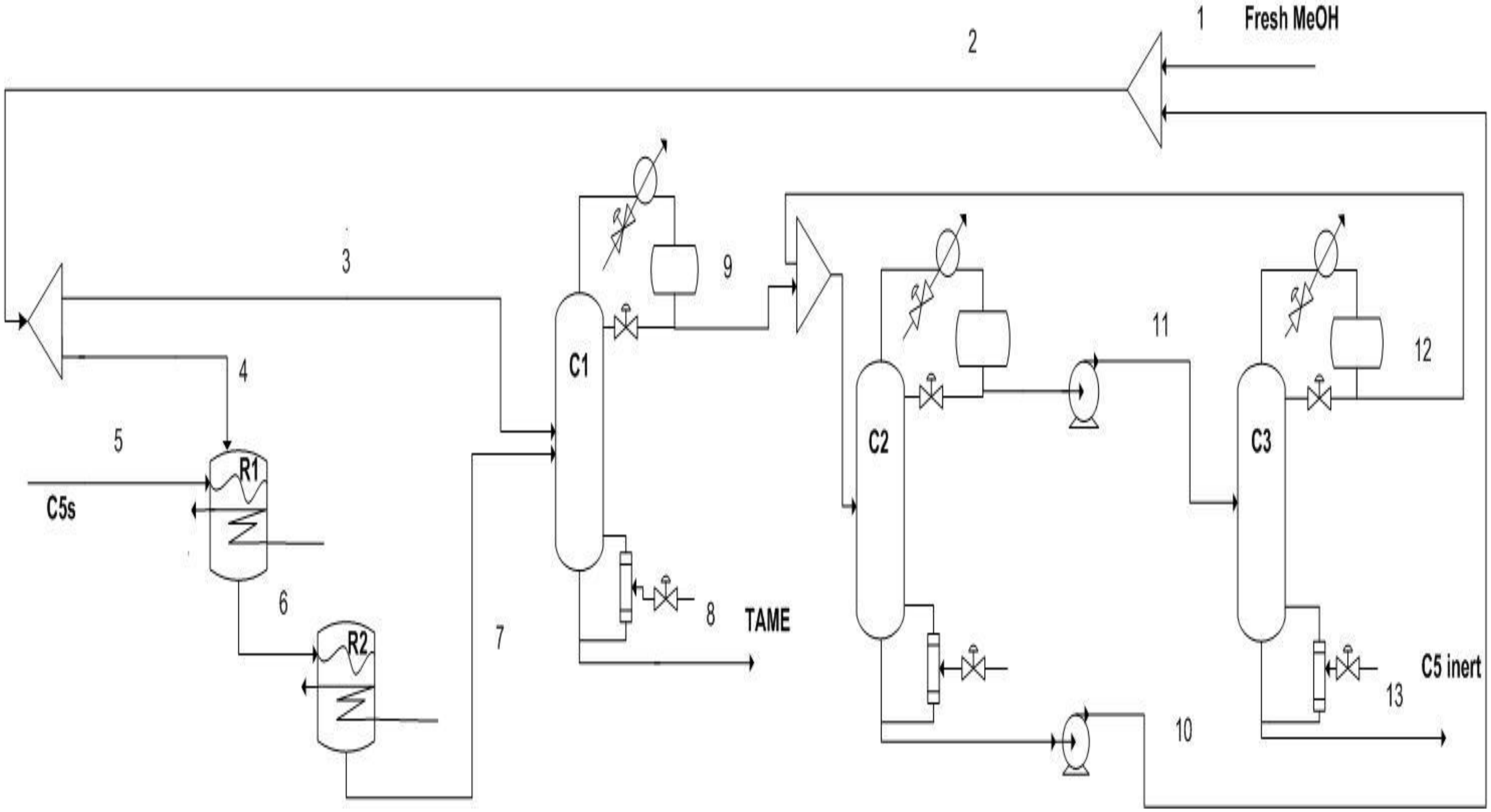

Figure A.1 Process flow sheet

Table A.2 Stream information

Stream	1	2	3	4	5	6	7
Flowrate (kmol/hr)	241.456	548.084622	235.084506	313	1039.864	1252.15059	1228.31148
Temperature (C)	70	78	78.0673306	78.0260012	78	82.0076969	74.4853491
Pressure (bar)	10.5	8.5	4.21371429	6.5	8.5	6	4.26228571
Mole fraction							
2M1B	-	2.8501e-06	2.8499e-06	2.8499e-06	0.08231845	0.03575969	0.02707359
2M2B	-	9.7811e-06	9.7803e-06	9.7803e-06	0.15848226	0.08378706	0.07538530
Methanol	1	0.99944055	0.99944055	0.99944055	0	0.16939774	0.15327738
TAME	-	8.1124e-08	8.1112e-08	8.1112e-08	0.00010001	0.08051542	0.1014861
N-Pentane	-	7.6443e-05	7.6443e-05	7.6443e-05	0.08501111	0.07061764	0.07198819
Isopentane	-	0.00015116	0.00015117	0.00015117	0.48198611	0.40030913	0.40807835
1-Pentene	-	2.9906e-05	2.9906e-05	2.9906e-05	0.03660094	0.03040318	0.03099324
2-Pentene	-	0.00028922	0.00028922	0.00028922	0.1555011	0.12921012	0.13171783

Table A.2 (continue) Stream information

Stream	8	9	10	11	12	13
Flowrate (kmol/hr)	243.49683	1103.00682	306.628622	2412.37748	1615.99929	796.377483
Temperature (C)	116.412694	46.2568109	84.1561744	45.7487903	45.2171919	118.758914
Pressure (bar)	2.34	2.04	8.5	10.04	2.04	10.09
Mole fraction						
2M1B	0.00010575	0.00321716	5.0943e-06	0.00378177	0.00345054	0.00445428
2M2B	0.00230486	0.00437579	1.7483e-05	0.00330634	0.00195233	0.00605393
Methanol	1.3673e-08	0.27772541	0.999	0.22524226	0.33623674	1.2918e-05
TAME	0.992	4.0635e-08	1.4501e-07	1.4912e-10	1.4936e-12	4.4868e-10
N-Pentane	0.00119578	0.07991857	0.00013663	0.06347414	0.04023192	0.110637
Isopentane	0.00075214	0.45430336	0.00027020	0.54235432	0.49959582	0.62911952
1-Pentene	0.00010588	0.03449716	5.3455e-05	0.04281769	0.04038257	0.04775900
2-Pentene	0.00353554	0.14596249	0.00051697	0.11902347	0.07815005	0.20196334

APPENDIX B

TUNING PARAMETERS

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	T_i
Methanol feed	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	312.999 kmol/hr	0-626	0.5	0.3
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	1039.864 kmol/hr	0-2079.7	0.5	0.3
Reactor R1	TC	Temperature	Reactor duty	PI	Reverse	82°C	32-132	0.35	12
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999
Reactor R2	TC	Temperature	Reactor duty	PI	Reverse	82°C	32-132	1.2	9.24
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	4 bar	0-8	20	12
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.855 m	0-9.71	2	99999
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	4	0-8	0.7	0.05
	TC	Temperature tray 32	Reboiler duty	PI	Reverse	109.8°C	0-219.6	0.43	9
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624 m	0-11.248	2	99999
	CC	Composition tray 22	Methanol feed flow rate to C1	PI	Reverse	0.18767	0-0.5848	1.2	15

Table B.1 (continue) Type of controllers and tuning parameters of base case

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	T_i
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	2	0-4	20	12
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.139 m	0-8.278	2	99999
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	0.4	0-0.8	0.5	0.3
	TC	Temperature tray 9	Reboiler duty	PI	Reverse	74.6°C	0-100	0.41	11
	LC	Reboiler level	Bottom flowrate	PI	Direct	2.823m	0-5.637	2	99999
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	10	0-20	20	12
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.114	0-8.229	2	99999
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	1	0-2	0.5	0.3
	TC	Temperature tray 4	Reboiler duty	PI	Reverse	104.2	0-228.5	1.8	8.4
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624	0-11.248	2	99999

Table B.2 Type of controllers and tuning parameters of NCS1

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	T_i	T_d
Methanol feed	FC	Total flowrate	Feed flowrate	PI	Reverse	548.3 kmol/hr	0-1096.6	2.9	0.02	-
	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	312.999 kmol/hr	0-626	3.5	0.03	-
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	1040 kmol/hr	0-2079.7	0.5	0.3	-
Reactor R1	TC	Temperature	Reactor duty	PI	Reverse	82°C	32-132	0.34	12	-
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999	-
Reactor R2	TC	Temperature	Reactor duty	PI	Reverse	82°C	32-132	1.2	9.24	-
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	4 bar	0-8	25	20	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.855 m	0-9.71	2	99999	-
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	4	0-8	0.7	0.05	-
	TC	Temperature tray 34	Reboiler duty	PID	Reverse	109.8 °C	0-219.6	1.43	7.9	0.6
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624 m	0-11.248	2	99999	-
	FC	Flowrate of 2M1B in PreR1-C1 Stream	Methanol feed flowrate to C1	PI	Reverse	235.3 kmol/hr	0-470.6	0.5	2	-

Table B.2 (continue) Type of controllers and tuning parameters of NCS1

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	T_i	T_d
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	2	0-4	20	12	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.139 m	0-8.278	2	99999	-
	FC	Reflux flow	Reflux flowrate	PI	Reverse	60548.96 kg/hr	0-121098	0.5	0.3	-
	TC	Temperature tray 9	Reboiler duty	PID	Reverse	74.6°C	0-100	0.23	9.2	0.7
	LC	Reboiler level	Bottom flowrate	PI	Direct	2.824 m	0-5.637	2	99999	-
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	10	0-20	20	12	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.115 m	0-8.229	2	99999	-
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	1	0-2	0.5	0.3	-
	TC	Temperature tray 4	Reboiler duty	PID	Reverse	104.2°C	0-228.5	5.81	7.9	0.6
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624 m	0-11.248	2	99999	-

Table B.3 Type of controllers and tuning parameters of NCS2

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	T_i	T_d
Methanol feed	FC	Total flowrate	Feed flowrate	PI	Reverse	535.84 kmol/hr	0-1096.17	0.5	0.3	-
	FC	Flowrate to reactor	Feed flowrate to reactor	PI	Reverse	312.999 kmol/hr	0-626	0.5	0.3	-
C5s feed	FC	Total feed flowrate	Feed flowrate	PI	Reverse	1039.864 kmol/hr	0-2079.7	0.5	0.3	-
Reactor R1	TC	Temperature	Reactor duty	PID	Reverse	82°C	32-132	0.83	7.9	0.6
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999	-
Reactor R2	TC	Temperature	Reactor duty	PID	Reverse	82°C	32-132	1.94	7.9	0.6
	LC	Liquid level	Effluence flowrate	P	Direct	5.1776 m	0-7.72	10	99999	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Reverse	4 bar	0-8	20	12	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.855 m	0-9.71	2	99999	-
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	4	0-8	0.5	0.3	-
	TC	Temperature tray 34	Reboiler duty	PID	Reverse	136.5°C	0-273	4.27	9.2	0.7
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624 m	0-11.248	2	99999	-
	CC	Composition tray 22	Methanol feed flowrate to C1	PID	Reverse	0.184	0-0.368	0.72	34.3	2.5

Table B.3 (continue) Type of controllers and tuning parameters of NCS2

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	T_i	T_d
Column C2	PC	Condenser pressure	Condenser duty	PI	Reverse	2 bar	0-4	20	12	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.139 m	0-8.278	2	99999	-
	FC	Reflux flux	Reflux flowrate	PI	Reverse	60575.46 kg/hr	0-121150.9	0.5	0.3	-
	TC	Temperature tray 9	Reboiler duty	PID	Reverse	74.6	0-100	0.57	9.2	0.7
	LC	Reboiler level	Bottom flowrate	PI	Direct	2.8186 m	0-5.637	2	99999	-
Column C3	PC	Condenser pressure	Condenser duty	PI	Reverse	10 bar	0-20	20	12	-
	LC	Reflux drum level	Distillate flowrate	P	Direct	4.1147 m	0-8.229	2	99999	-
	FC	Reflux ratio	Reflux flowrate	PI	Reverse	1	0-2	0.5	0.3	-
	TC	Temperature tray 4	Reboiler duty	PID	Reverse	104.2°C	0-208.5	5.14	9.2	0.7
	LC	Reboiler level	Bottom flowrate	P	Direct	5.624 m	0-11.248	2	99999	-

VITA

Miss Thitima Tapaneeyapong was born in Songkhla, Thailand on August 2, 1989. She received the Bachelor Degree of Engineering, field of Chemical Engineering from Prince of Songkla University in 2010. After that she entered the Graduate School of Chulalongkorn University to pursue the Master of Engineering in Chemical Engineering and completed in 2012.