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PLANTWIDE CONTROL STRUCTURES DESIGN FOR BUTYL ACETATE PROCESS

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A Thesis Submitted in Partial Fulfillment of the Requirements
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Department of Chemical Engineering
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อรชา รัตนนิพนธ์ : การออกแบบโครงสร้างการควบคุมแพลนท์ไวด์สำหรับกระบวนการบิวทิวอะซีเตท. (PLANTWIDE CONTROL STRUCTURES DESIGN FOR BUTYL ACETATE PROCESS) อ. ที่ปรึกษาวิทยานิพนธ์หลัก : ผศ.ดร.มนตรี วงศ์ศรี, 91 หน้า.

กระบวนการผลิตทางเคมี สิ่งสำคัญ คือการควบคุมกระบวนการเพื่อให้ระบบดำเนินงานไปตามเป้าหมายที่ต้องการ โดยให้เกิดความสูญเสียพลังงานและของเสียน้อยที่สุด โดยทั่วไป กระบวนการทางเคมีนั้นจะประกอบด้วยการหมุนเวียนมวลสารและการสะสมพลังงาน ซึ่งส่งผลทำให้ระบบการควบคุมมีความยุ่งยากมากขึ้น ดังนั้นจึงมีการนำหลักการควบคุมแพลนท์ไวด์เข้ามาช่วยในการพิจารณาการควบคุมกระบวนการที่ซับซ้อน โดยเน้นการมองภาพรวมของทั้งกระบวนการเพื่อให้ได้ระบบการควบคุมที่ดีขึ้น ในงานวิจัยนี้จึงได้ศึกษาการออกแบบโครงสร้างการควบคุมแพลนท์ไวด์ตามขั้นตอนของวงศ์ศรี ประยุกต์ใช้กับกระบวนการผลิตบิวทิวอะซีเตทโดยประกอบไปด้วย ถังปฏิกรณ์หนึ่งถัง หอกลั่นสามหอ และสารที่ใช้หมุนเวียนสองสาย บิวทิวอะซีเตทเป็นผลิตภัณฑ์ที่เกิดจากการทำปฏิกิริยากันระหว่างเมททิวอะซีเตทและบิวทานอลได้สารผลิตภัณฑ์สองสารคือบิวทิวอะซีเตทและเมทานอล โดยทำการออกแบบโครงสร้างการควบคุมและสร้างแบบจำลองกระบวนการในสภาวะคงตัวและสภาวะพลวัต จากนั้นทำการประเมินสมรรถนะโดยใช้ค่าปริพันธ์ของค่าความคลาดเคลื่อนสัมบูรณ์

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A structure of most industrial processes, including many different unit operations, several recycle streams and energy integration, is a complex flowsheet. Therefore plantwide control structure design is an important way to control processes which become more complex so that processes are designed and operated closer to constraints. This research is design of plantwide control structures for butyl acetate process, which consist of a reactor, three distillation columns and two recycle streams. It can be produced by the reaction of methyl acetate with butanol in a reversible, liquid-phase, mildly exothermic reaction. Methanol is the second product. The objective of this research is selection of controlled variables so that finding which variables that should be controlled system for quickly responding to disturbances and adjusting self to steady state while minimizing the deviation of the product quality. Plantwide control procedure of Wongsri(2012) is chosen for design the new control structures in order to develop control loops to achieve the required objectives. Steady state designs were performed in commercial process simulator and evaluate the performance using integrated absolute error (IAE) of the designed control structures.

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CHAPTER I

INTRODUCTIONS

1.1 Importance and Reasons for Research

The most important task in a chemical process is controlling the process consisting of a lot of measurements and control loops to achieve the required setpoint in such a way of minimizing energy loss and waste generation. A structure of most industrial processes, including several recycle streams, energy integration, and many different unit operations, is a complex flowsheet. Therefore industrial processes need a control system so that the plant can operate economically and safely. A plantwide control strategy was adapted for developing control loops to achieve the required objectives.

In the real operation, the process will not always operate at the design condition due to disturbance from the external factors and the internal factors. Thus, the plantwide control strategy is necessary to control the condition and compensate for any deviation occurred. The general problems of plantwide control structure design to generate a good controllability loop are selection appropriate of controlled variable and pairing of controlled variable to manipulated variable of process.

In this research, design control structure by using the “fixture point theorem” is applied to the butyl acetate process for selecting and paring controlled variables with manipulated variables

The most common use of normal butyl acetate is as a solvent in the production of lacquers and paints. Its other major use is in the creation of adhesives and hardened coatings. Normal butyl acetate is also used in the pharmaceutical industry as a solvent or an extraction agent. Its minor uses include cosmetic products, fragrance solvent in perfumes, as an anti-corrosive agent, in cleaning and car care products. It is also used in the synthetic fruit flouring industry. The main user end markets are the paints/lacquers, coatings, cosmetics, leather, cleaning and the pharmaceutical industries. It can be produced by the reaction of methyl acetate with butanol in a reversible, liquid-phase, mildly exothermic reaction. Methanol is the second product. The process consists of a reactor, three distillation columns and two recycle streams. The objective of this research is selection of controlled variables in order to finding which variables that should be controlled system for quickly responding to disturbances and adjusting self to steady state while minimizing the deviation of the product quality. Plantwide control procedure of Wongsri (2009) is chosen so that the objective can be achieved. Steady state design was performed in commercial process simulator and evaluate the performance using Integrated absolute error (IAE) of designed structures.

1.2 Research Objectives

To design and evaluate plantwide control structures of butyl acetate process using new design procedure of Wongsri (2012)

1.3 Scope of research

The scopes of this research can be listed as follows;

1. Simulation of the butyl acetate process is performed by using a commercial process simulator.
2. Description and data of butyl acetate process is obtained from William L. Luyben(2011).
3. New plantwide control structures for butyl acetate process are designed using new design procedure of Wongsri (2012).

1.4 Contribution of Research

The new plantwide control structures for butyl acetate process

1.5 Research Procedures

Procedure plans of this research are;

1. Study of plantwide control theory, the butyl acetate process and concerned information.
2. Simulations of the butyl acetate process both steady state and dynamic are performed by using commercial process simulator.
3. Simulate the reference control structure obtained from Luyben (2011)
4. Study the new design procedure (Wongsri 2012).
5. Design new plantwide control structures by using the new design procedure.

6. Simulate the dynamic of butyl acetate process with the new design control structures.
7. Evaluate the dynamic performance of the new design control structures.
8. Analyze of the design and simulate result
9. Conclude the thesis

1.6 Research Framework

The thesis matter is classified six chapters as follow;

Chapter I: is an introduction to this research. This chapter consists of importance and reasons for research, research objectives, scopes of research, contributions of research and research procedures.

Chapter II: presents literature review related to plantwide control structures design procedures, review of previous work on the butyl acetate process design.

Chapter III: covers some background information of plantwide and theory concerning with plantwide control fundamentals, new plantwide control design procedure, control issues for distillation column.

Chapter IV: describes process description and the design heat exchanger network for butyl acetate process.

Chapter V: describes the design of plantwide control structures and dynamic simulation results and compares with control structures of Luyben (2011).

Chapter IV: presents the conclusion of this research and makes the recommendation for future work.

CHAPTER II
LITERATURE REVIEW

2.1 Plantwide Control Structure Design

Luyben (1993) explored the challenging problems associated with the dynamics and control of recycle systems. Second-order kinetics are considered with two fresh-feed makeup streams. Two cases are considered: (1) instantaneous and complete one-pass conversion of one of the two components in the reactor so there is an excess of only one component that must be recycled and (2)incomplete conversion per pass so there are two recycle streams. It is shown that the generic liquid-recycle rule proposed by Luyben applies in both of these cases: “snowballing” is prevented by fixing the flow rate somewhere in the recycle system. An additional generic rule is proposed: fresh feed makeup of any component cannot be fixed unless the component undergoes complete single-pass conversion. In the complete one-pass conversion case, throughput can be set by fixing the flow rate of the limiting reactant. The makeup of the other reactant should be set by level control in the reflux drum of the distillation column. In the incomplete conversion case, two workable schemes were found: (1) Both recycle flow rates are fixed and both fresh-feed makeups are brought in on level control. Throughput is controlled by changing either the reactor temperature or the recycle flow rates. (2) One fresh-feed makeup controls reactor level and the other controls the composition in the reactor. Throughput is controlled by setting reactor temperature or reactor effluent flow rate.

Luyben et al. (1997) presented a general heuristic design procedure. The nine steps of the proposed procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental and safety constrain; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, the Eastman plantwide control process, and the HDA process. After that Luyben et al. (1998) prepared the plantwide control process’s book, which included introduction of plantwide control, plantwide control fundamentals, procedure of plantwide control design and industrial examples.

Jimenez and Costa-Lopez (2002) reported two papers. The second paper presented the production of butyl acetate and methanol by reacting methyl acetate and butanol in a reactive distillation column. The feed stream was a mixture of methyl acetate and methanol, which came from an upstream polyvinyl alcohol process. They proposed reacting methyl acetate with butanol to form butyl acetate and methanol. This liquid-phase reaction is reversible with an equilibrium constant of about unity. Kinetics are quite fast, and the heat effects are small. They studied a four-column process in which the key unit was a reactive distillation column. The presence of a minimum-boiling azeotrope between methyl acetate and methanol prevents the use of just a single reactive column because any unreacted methyl acetate that leaves the reaction zone will go out of the top of the column with methanol. Jimenez and Costa-Lopez1 claimed that an extractive agent (*o*-xylene) must be added to the reactive distillation column. Of course, this means the entrainer must be recovered in a subsequent column. In addition, there is the inevitable contamination of products with small amounts of the entrainer. In their first paper, the useful information used in this paper features the reaction equilibrium and kinetics.

$$\mathrm{MeAc} + \mathrm{BuOH} \leftrightarrow \mathrm{MeOH} + \mathrm{BuAc}$$

$$r = kc_{\mathrm{MeAc}}c_{\mathrm{BuOH}} - k'c_{\mathrm{BuAc}}c_{\mathrm{MeOH}}$$

$$k_{\mathrm{F}} = 2.018 \times 10^{8}\exp(-71960/RT)$$

$$k_{\mathrm{R}} = 2.839 \times 10^{8}\exp(-72670/RT)$$

Gangadwala et al. (2004) studied simulation and design for butyl acetate synthesis by reactive distillation. Butyl acetate (BuAc) can be produced by esterification of *n*-butanol (BuOH) with acetic acid (AcH) in the presence of a suitable acid catalyst. Classical processes make use of a homogeneous acid catalyst either in continuous reactive distillation or in batch reactive distillation. However, severe corrosion problems associated with homogeneous acid catalysts (e.g., sulfuric acid or *p*-toluenesulfonic acid) make these processes less attractive.

L. Luyben(2004) demonstrated that specification products can be economically produced without the use of an extraction agent, which simplifies the process. Two alternative processes are explored: (1) a conventional process with a reactor and three distillation columns, in which reactants leaving the reactor are recovered and recycled and methanol and butyl acetate products are produced at 99% purity, and (2) a process with a reactive distillation column and two conventional columns. In the latter process, the overhead of the reactive column is a methyl acetate/methanol mixture that is separated in a downstream column into a methanol bottoms product and a distillate with a composition close to the binary azeotrope (66.7 mol % methyl acetate at 15 psia), which is recycled back to the reactive distillation column. The bottoms of the reactive column is separated in another column into a butyl acetate bottoms product and a distillate that is about 90 mol % butanol, which is recycled back to the reactive column. Fresh butanol feed and the methyl acetate/methanol fresh feed streams are also fed to the reactive column.

Suntisrikomol (2008) used “Fixture Point Theorem” for HDA process to select appropriated the set of controlled variables from a large number of candidate output. The fixture point control theorem states that the most disturbed points must be satisfactory controlled by giving them consideration before other controlled variables. The maximum (scaled) gain is used to selecting and paring controlled variables with manipulated variables. In her study, the set of first rank of controlled variables are same as Luyben (1998). She selected three set of controlled variables (second and third rank from fixture point) and five control structures were designed and compared. In order to illustrate the dynamic behaviors of the control structures when economic disturbance load occur (such as change in methane composition in fresh feed gas and quencher outlet temperature), the performance of designed control structures were presented in IAE value and compared with reference structure. The designed structures are fast response and the most effective on compared with Araujo et al, 2006 and Luyben, 1998.

Detjareansri (2009) applied plantwide control procedure of Wongsri (2009) to alkylation process for design eight plantwide control structure then she evaluated the dynamic performance of the designed control structure compare with base case control structure (Luyben, 2002) by two types of disturbances: material and thermal disturbances. The designed control structure has a good performance because it can handle disturbances entering the process and can maintain product quality as compared by integral absolute error (IAE) and total energy use low.

In recent, Luyben (2011) studied production of butyl acetate consisting of reactor and three distillations. Rigorous economic analysis is used to determine the optimum flow rates of the two recycle streams. The conclusion is counterintuitive: the optimum methyl acetate recycle is larger than the butanol recycle.

CHAPTER III

PLANTWIDE CONTROL FUNDAMENTALS

3.1 Incentives for Chemical Process Control

A chemical plant is an arrangement of processing units (reactors, heat exchangers, pump, distillation columns, absorbers, evaporators, tanks, etc.), integrated with one another in a systematic and rational manner. The plant's overall objective is to convert certain raw materials into desired products using available sources of energy in the most economical way. There are three general classes of needs that a control system is called on to satisfy: suppressing the influence of external disturbances, ensuring the stability of a chemical process, and optimizing the performance of a chemical process (Stephanopoulos, 1984)

3.1.1. Suppressing the Influence of External disturbances.

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

3.1.2. Ensuring the Stability of a Chemical Process

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

3.1.3. Optimizing the Performance of Chemical Process

Safety and the satisfaction of product specifications are the two principal operational objectives for a chemical plant. Once these are achieved, the next goal is how to make the operation of the plant more profitable. It is clear that we would like to be able to change the operation of the plant (Flow rates, pressures, concentrations, temperatures) in such a way that an economic objective (profit) is always maximized.

3.2 Integrated Process

Tree 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 recycle.

(2) The effect of energy integration.

(3) The need to account for chemical component inventories.

If they did not have to worry about these issues, then they would not have to deal with a complex plantwide control problem. However, there are fundamental reasons why each of these exists in virtually all real processes.

3.2.1 Material recycles

Material is recycled for six basic and important reasons.

1. Increase conversion

For chemical processes involving reversible reactions, conversion of reactant s to products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.

2. Improve economics

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

3. Improve yields

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

4. Provide thermal sink

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

5. Prevent side reactions

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

6. Control properties

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

3.2.2 Energy Integration

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

3.2.3 Chemical component inventories

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

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

3.3 The plantwide control problem

3.3.1 Units in Series

If process units are arranged in a purely series configuration, where the products of each unit feed downstream units and there is no recycle of material or energy, the plantwide control problem is greatly simplified. We do not have to worry about the issues discussed in the previous section and we can simply configure the control scheme on each individual unit operation to handle load disturbances.

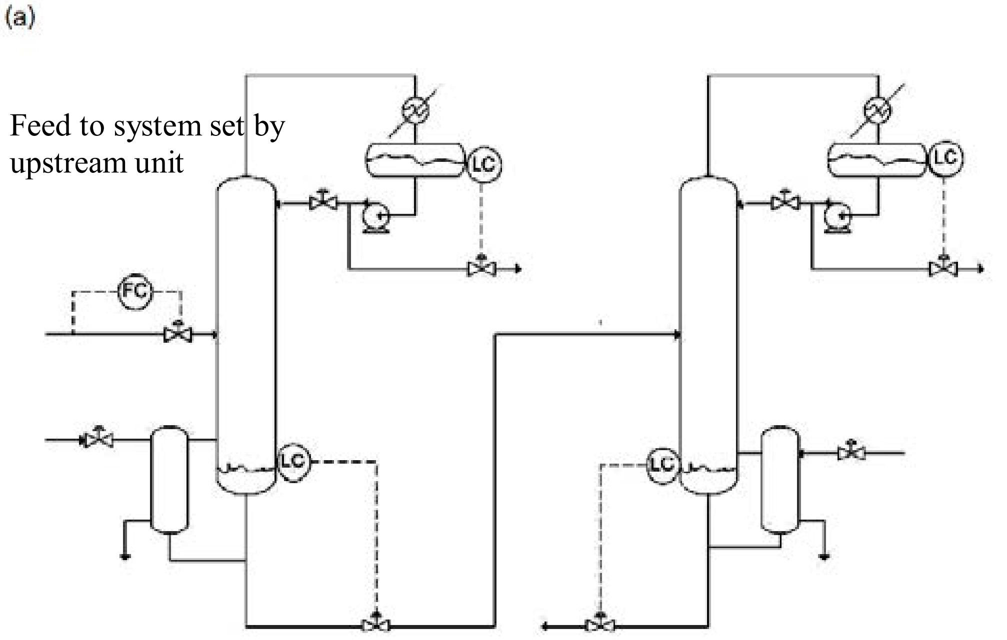
If production rate is set at the front end of the process, each unit will only see load disturbances coming from its upstream neighbor. If the plant is set up for "on-demand" production, changes in throughput will propagate back through the process. So any individual unit will see load disturbances coming from both its downstream neighbor (flow rate changes to achieve different throughputs) and its upstream neighbor (composition changes as the upstream units adjust to the load changes they see).

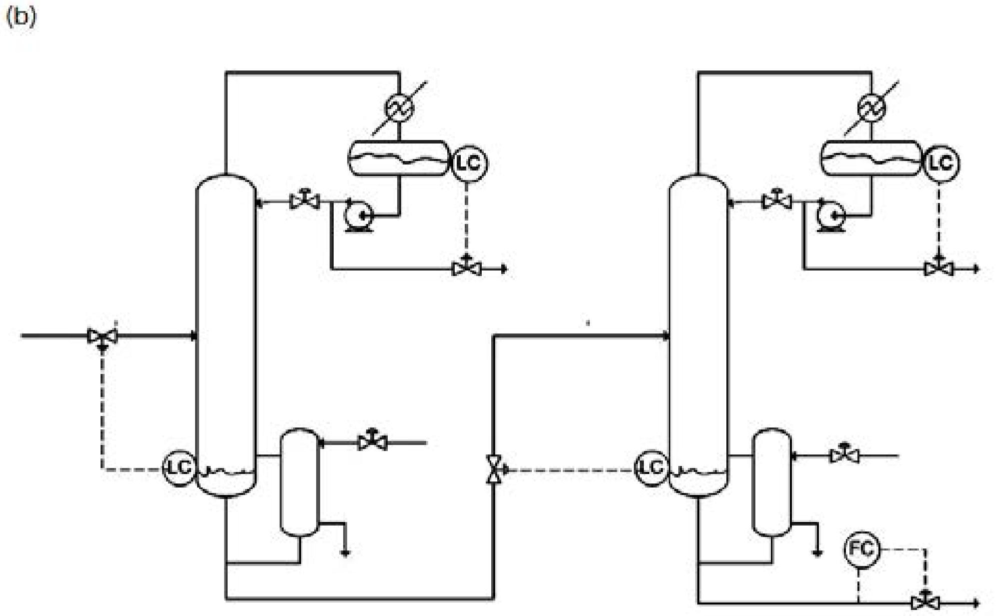
Figure 3.1 compares these two possible configurations for a simple plant. A fresh stream containing a mixture of chemical components A, B and C is fed into a two-column distillation train. The relative volatilities are $\alpha_A > \alpha_B > \alpha_C$**,** and we select the "direct" (or "light-out-first) separation sequence: A is taken out the top of the first column and B out the second column.

Figure 3.1 shows the situation where the fresh feed stream is flow controlled into the process. The inventory loops (liquid levels) in each unit are controlled by manipulating flows leaving that unit. All disturbances propagate from unit to unit down the series configuration. The only disturbances that each unit sees are changes in its feed conditions.

Figure 3.1b shows the on-demand situation where the flow rate of product C leaving the bottom of the second column is set by the requirements of a downstream unit. Now some of the inventory loops the base of both columns) are controlled by manipulating the feed into each column.

When the units are arranged in series with no recycles, the plantwide control problem can be effectively broken up into the control of each individual unit operation. There is no recycle effect, no coupling, and no feedback of material from downstream to upstream units. The plant’s dynamic behavior is governed by the individual unit operations and the only path for disturbance propagation is linear along the process.





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.

3.3.2 Effects of recycle

Most real process contained recycle streams. The presence of recycle streams profoundly alters the plant's dynamic and steady state behavior. To gain an understanding of these effects, we look at some very simple recycle streams. The insight we obtain from these idealized, simplistic systems can be extended to the complex flowsheets of typical chemical processes. First the groundwork and have some feel for the complexities and phenomena that recycle streams produce in a plant.

Two basic effects of recycle:

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

(2) Recycle leads to the "snowball" effect. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flow rates. These disturbances can lead to even larger dynamic changes in flow, which propagate around the recycle loop. Both effects have implications for the inventory control of components.

3.3.3 Reaction/Separation Section Interaction

For the process considered in the previous section where the reaction is A → B, the overall reaction rate depends upon reactor holdup, temperature (rate constant), and reactant composition (mole fraction A) $R = V_Rkz$. The two control structures considered above produce fundamentally different behavior in handling disturbances. In the first, the separation section must absorb almost all of the changes. For example, to increase production rate of component B by 20 percent, the overall reaction rate must increase by 20 percent. Since both reactor temperature (and therefore k) and reactor holdup V_R are held constant, reactor composition z must increase 20 percent. This translates into a very significant change in the composition of the feed stream to the separation section. This means the load on the separation section changes significantly, producing large variations in recycle flow rates.

In the second structure, both reactor holdup V_R and reactor composition z can change, so the separation section sees a smaller load disturbance. This reduces the magnitude of the resulting change in recycle flow because the effects of the disturbance can be distributed between the reaction and separation sections.

If the tuning of the reactor level controller in the conventional structure (Fig. 3.2) is modified from normal PI to P only, then changes in production rate also produce changes in reactor holdup. This tends to compensate somewhat for the required changes in overall reaction rate and lessons the impact on the separation section. So both control system structure and the algorithm used in the inventory controller of the reactor affect the amount of this snowball phenomenon.

This example has a liquid-phase reactor, where volume can potentially be varied. If the reactor were vapor phase, reactor volume would be fixed. However, we now have an additional degree of freedom and can vary reactor pressure to affect reaction rate.

A very useful general conclusion from this simple binary system that is applicable to more complex processes: changes in production rate can be achieved only by changing conditions in the reactor. This means something that affects reaction rate in the reactor must vary: holdup in liquid-phase reactors, pressure in gas-phase reactors, temperature, concentrations of reactants (and products in reversible reactions), and catalyst activity or initiator addition rate. Some of these variables affect the conditions in the reactor more than others. Variables with a large effect are called *dominant*. By controlling the dominant variables in a process, we achieve what is called partial control. The term partial control arises because we typically have fewer available manipulators than variables we would like to control. The setpoints of the partial control loops are then manipulated to hold the important economic objectives in the desired ranges.

The plantwide control implication of this idea is that production rate changes should preferentially be achieve by modifying the setpoint of partial control loop in the reaction section. This means that the separation section will not be significantly disturbed. Using the control structure in Fig 3.2, changes in production rate require large changes in reactor composition, which disturb the column. Using the control structure shown in Fig.3.3,changes in production rate are achieved by altering the setpoint of a controlled dominant variable, reactor holdup, with only small changes in reactor composition. This means that the column is not disturbed as much as with the alternative control scheme.

Hence a goal of the plantwide control strategy is to handle variability in production rate and in fresh reactant feed compositions while minimizing changes in the feed stream to the separation section. This may not be physically possible or economically feasible. But if it is, the separation section will perform better to accommodate these changes and to maintain product quality, which is one of the vital objectives for plant operation. Reactor temperature, pressure, catalyst/initiator activity, and holdup are preferred dominant variables to control compared to direct or indirect manipulation of the recycle flows, which of course affect these separation section

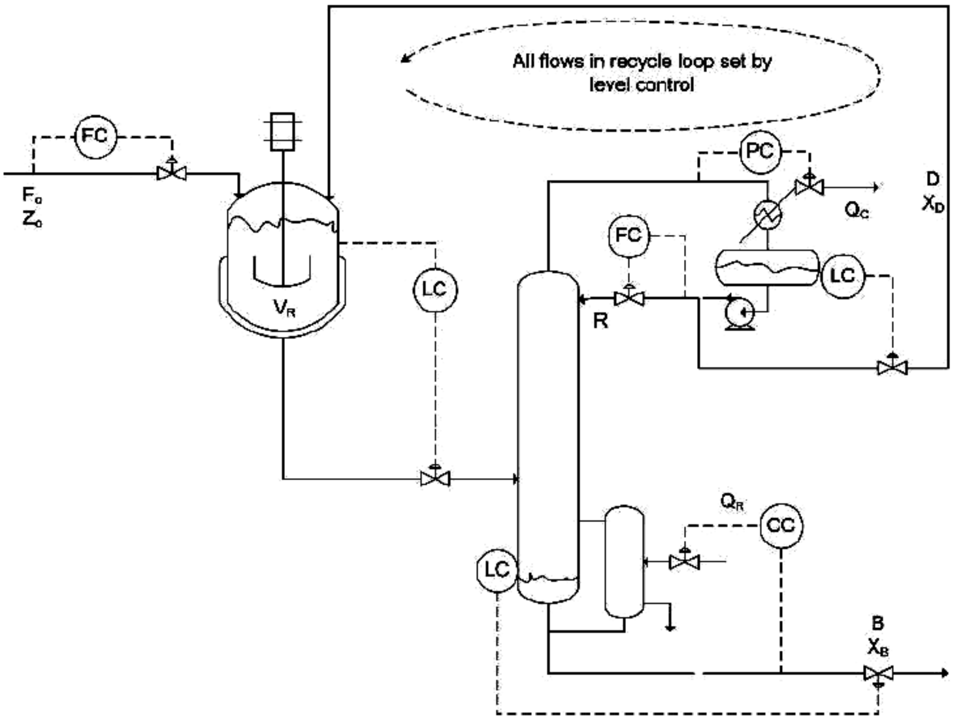


Figure 3.2 Conventional control structure with fixed reactor holdup

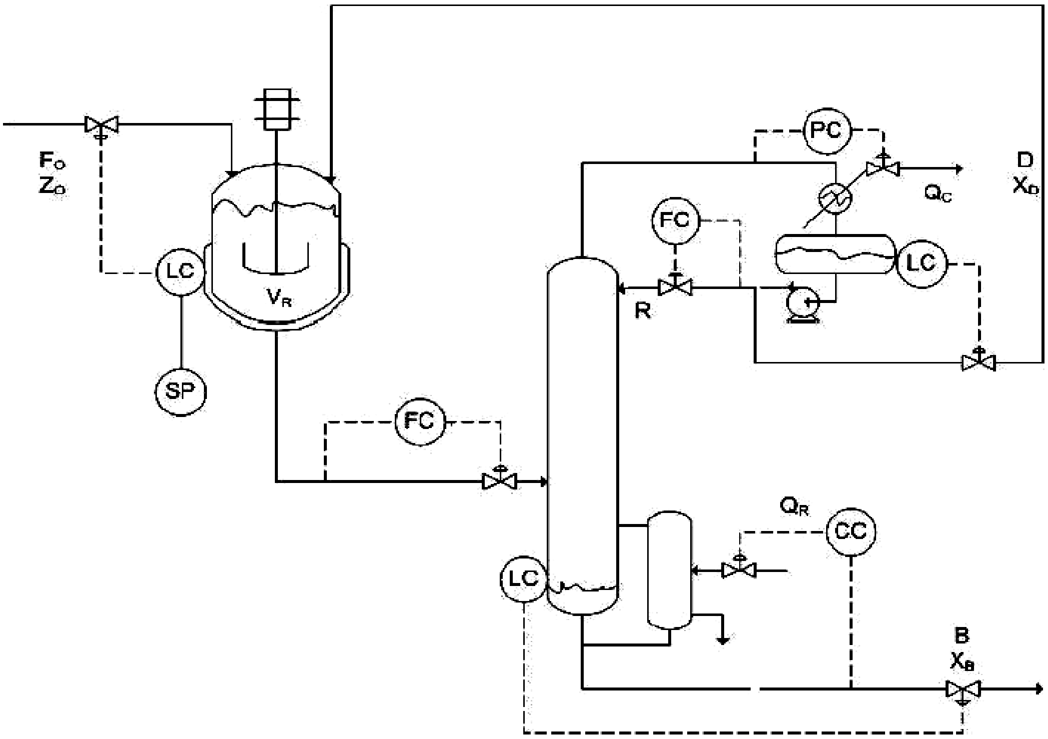


Figure 3.3 Control structure with variable reactor holdup.

3.4 Distillation Column Control Design Using Steady State Models: Usefulness and Limitations

3.4.1 Distillation Column Control Fundamentals

Figure 3.4 illustrates a schematic of a simple distillation column. This figure identifies the nomenclature used in this paper and points out the five valves available to control the column. There are five degrees of freedom represented by the feed valve, the steam valve, the reflux valve, the distillate valve, and the bottoms valve in a typical binary distillation column.

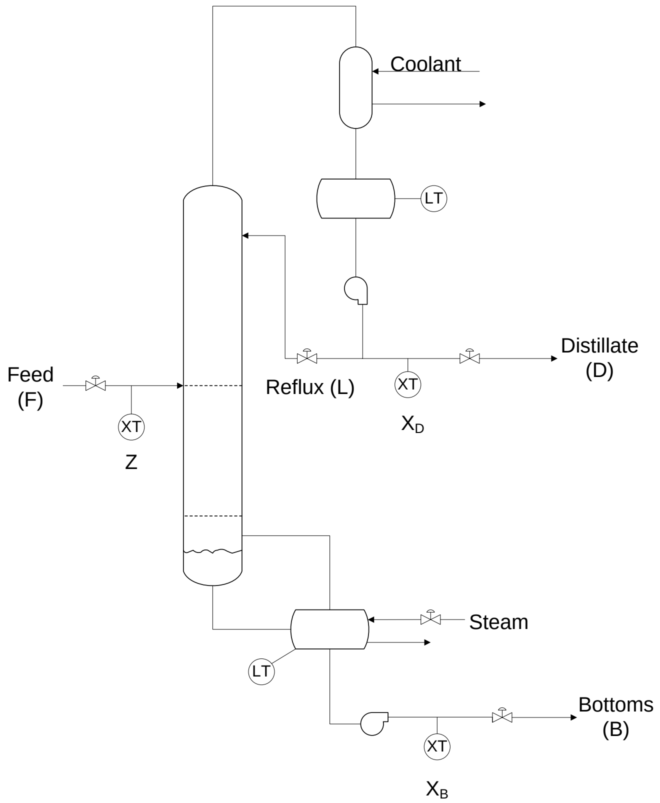
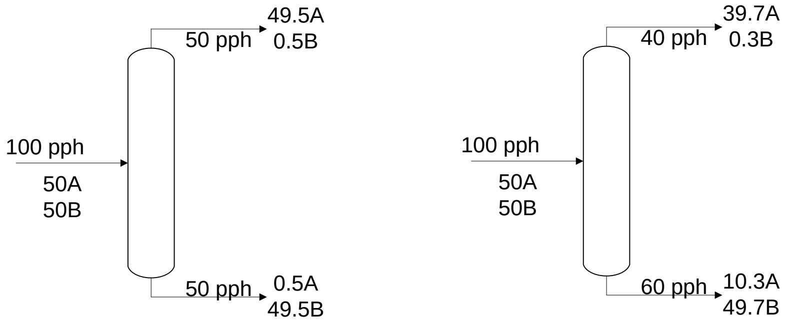
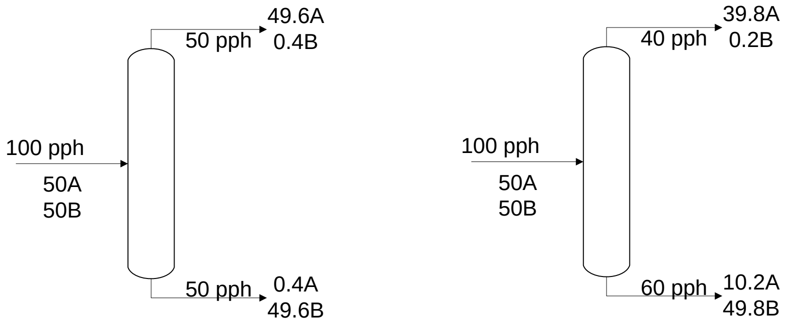


Figure 3.4 Schematic of simple distillation column

The five valves are used as follows. First, either of the feed, the bottoms and the distillate rate is set independently to define the production rate of the column, thereby eliminating one valve. We call this the demand stream. The reflux drum and the column bottoms level must be controlled, requiring two more valves. This leaves us with two compositions to be controlled with two valves. Traditionally, simple distillation is viewed as a 2x2 control problem because the remaining two composition control loops have strong interactions. No matter what valves we use for composition control or how we use them, fundamentally there are two things that we can manipulate: the feed split and the fractionation. An overall material balance for a column tells us that the distillate flow plus the bottoms flow must equal the feed flow. The feed split is simply the amount of feed that leaves as distillate versus the amount that leaves as bottoms. The other fundamental manipulative variable is the fractionation which is the amount of separation that occurs per stage. The overall fractionation in a column depends on the number of stages, the energy input, and the difficulty of the separation. In order to explain how we pick the single point control schemes it is necessary to show the relative effect of the feed split and fractionation on product compositions. The assumption is that the control objective is to produce high purity products in both ends of the column. This is the objective for the vast majority of cases that we work on. In Figure 3.5, we use some numerical examples to show the relative importance of the two manipulative variables.



Base Case **20% Feed Split Change**



20% Fractionation Change **20% Feed Split Change**
20% Fractionation Change

Figure 3.5 Numerical examples showing importance of feed split and fractionation

In the base case (top left), 100 pph is fed to the column made up of 50 pph of A and 50 pph of B. The feed split is such that 50 pph leaves as distillate and 50 pphleaves as bottoms. The column has sufficient heat input to produce enough fractionation to obtain 99% purity in the top and bottom of the column. In the second case (top right), the feed split is changed by 20% so that 40 pph leaves as distillate and 60 pph leaves as bottoms. The feed rate and composition are the same. In this case, we obtain 99.2% purity in the distillate but only 82.8% purity in the bottom. The explanation is that only 40 lb of the 50 lb of a fed to the column is being allowed to leave in the distillate stream. The remaining 10 pph of A has to leave the column and does so by forcing its way down the column and going out in the bottoms stream. This substantially reduces the bottoms purity. In the third case (bottom left), the feed conditions are the same, but now the fractionation is increased by 20%. In this case, we obtain slightly higher purities in both the top and the bottom of the column. In the last case (bottom right), a 20% feed split change is made simultaneously with a 200% fractionation increase. In this case, we obtain very high purity A in the overhead, but only 83% purity in the bottom. Again, the 50 lb of A fed to the column must leave the column and does so in part by forcing its way down the column and leaving in the bottoms stream, again drastically reducing the bottoms purity. This leads us to a very important concept in distillation column control. The feed split to the column is the most important variable to control; it must be right in order to achieve high purities in both the top and bottom of the column. While fractionation must be great enough to obtain the desired purity, it is only used to fine tune composition control. From this development it should be clear that adjusting feed split is equally important when feed composition and feed rate changes hit the column. When we select the manipulative variable for composition control, we must make sure that it is able to adjust the feed split. In this paper, we are not going to discuss pressure control. Pressure control is a subject in itself, and it is independent of our main topic of discussion. In almost all columns, we are able to achieve very tight and responsive pressure control so that it can be considered a constant. This is one way in which our approach differs from a popular academic approach which includes pressure control as one of the things to be controlled and coolant flow as one of the things to be manipulated. The academic approach always assumes the feed is the demand stream.

3.4.2 Specialized and Multicomponent Distillation Columns

We have applied this general procedure to many different types of specialized columns including homogeneous and heterogeneous azeotropes, extractive distillation, strippers and absorbers and multicomponent columns. We have also used this procedure for many different column configurations including columns with either liquid or vapor side draws, columns with partial condensers and with both packed and tray columns. Because we often encounter columns with multiple components in the feed, a little more should be said about these cases. In multicomponent columns, unlike binary columns, fixing temperature and pressure does not fix composition. In spite of this limitation, temperature control can still be used to meet many composition specifications. Often these results in larger yield losses or higher energy consumptions than if an on-line analyzer was available for control. This is where steady state models can be very helpful to us because we can use them to quantify the incremental benefit of on-line analyzers versus temperature control. In one case, we used this technique to document the yield improvement to be gained from the addition of an on-line analyzer. The savings was over two hundred thousand dollars a year.

3.4.3 Steady State Distillation Models

Steady state models are easily manipulated and provide robust solutions. In order to make a change to the solution conditions, only a few changes need to be made to the model input file. The model input file is then submitted to the software which finds a new solution. Generally, very little time is spent getting converged solutions, which allows us to efficiently generate the large number of case studies necessary for this design procedure.

3.5 Plantwide Control Design Procedures

Luyben et al., (1997) presented nine basic steps of plantwide control design procedure. They outline each step in general terms.

3.5.1 Establish control objectives

Assess the steady-state design and dynamic control objectives for the process.

This is probably the most important aspect of the problem because different control objectives lead to different control structures. There is an Old Persian saying “If you don’t know where you are going, any road will get you there!” This is certainly true in plantwide control. The “best” control structure for a plant depends upon the design and control criteria established.

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

3.5.2 Determine control degree of freedom

Count the number of control valves available.

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to setpoint. The valves must be legitimate (flow through a liquid-filled line can be regulated by only one control valve). The placement of these control valves can sometimes be made to improve dynamic performance, but often there is no choice in their location

3.5.3 Establish energy management system

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

They use the term energy management to describe two functions: (1) Must to provide a control system that removes exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used elsewhere in the process by other unit operations. This heat, however, must ultimately be dissipated to utilities. (2) If heat integration does occur between process streams, then this second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

3.5.4 Set production rate

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

Throughput changes can be achieved only by altering, either directly or indirectly, conditions in the reactor. To obtain higher production rate, they must increase overall reaction rates. This can be accomplished by raising temperature (higher specific reaction rate), increasing reactant concentrations, increasing reactor holdup (in liquid-phase reactors), or increasing reactor pressure (in gas-phase reactors).

3.5.5 Control product quality and handle safety, operational, and environmental constraints

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

They want tight control of these important quantities for economic and operational reasons. Hence they should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants, dead times and large steady-state gains. The former gives small closed-loop time constants and the latter prevents problems with the range ability of the manipulated variable (control valve saturation).

3.5.6 Fix a flow in every recycle loop and control inventories.

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

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flow in the recycle loop are controlled by levels. Gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields (Douglas doctrine). An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit (Richardson rule).

3.5.7 Check component balances.

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

They must identify the specific mechanism or control loop to guarantee that there will be no uncontrollable buildup of any chemical component within the process (Downs drill). What are the methods or loops to ensure that the overall component balances for all chemical species are satisfied at steady state? They don’t want reactant components to leave in the product streams because of the yield loss and the desired product purity specifications. Hence they are limited to the use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. Product and inert components all must have an exit path from the system. In many systems inerts are removed by purging off a small fraction of the recycle stream. The purge rate is adjusted to control the inert composition in the recycle stream so that an economic balance is maintained between capital and operating costs.

3.5.8 Control individual unit operations

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

Many effective control schemes have been established over the years for individual chemical units (Shinskey, 1988). For example, a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flow rate to a furnace supplying energy to the reactor. Crystallizers require manipulation of refrigeration load to control temperature. Oxygen concentration in the stack gas from a furnace is controlled to prevent excess fuel usage. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

3.5.9 Optimize economics or improve dynamic controllability

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

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

3.6 New Plantwide Control Structure Design Procedure

New design procedure of Wongsri (2012) presented plantwide control structure design procedure based on heuristics and mathematical analysis. In this procedure, the precedence of control variables is established. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method (Wongsri, 1990) to cover the material disturbances. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

Normally, plantwide control design procedures consider decision about plant control structures in perspective. The plantwide control structure design is complex: hierarchical, structural, having mixed objectives, containing many units and layers, and therefore confusing. One easy way to deal with this complexity is compartmentalizing it. However, the plant is not merely the units combined, it has it own properties. The whole is greater than the sun of its parts. There properties (or behavior) of a system as a whole emerge out of the interaction and the relationship of the components comprising the system. Therefore, a designer must deal with both parts and system.

New design procedures of Wongsri (2012) are:

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

List all control variables:

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

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

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

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

v. A flash separator has two degree of freedom.

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

How to select manipulated variables

i. A control variable and manipulated variable must have strong causal relationship (high gain)

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

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

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

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

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

3. Establish fixture plant

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

3.1 Keep the raw materials entered and reentered fixed

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

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

4. Handling the disturbances

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

4.1 Heat Disturbances

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

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

4.2 Material disturbances

4.2.1 Composition changed: At reactor, we adjust the reactor inlet temperature in order to keep the reactor outlet composition or the product component flow constant.

4.2.2 Total material flow in

4.2.3 Component flow

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

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

7. Optimize economics and improve control performance

8. Validate the designed control structures by rigorous dynamic simulation

CHAPTER IV

BUTYL ACETATE PROCESS

4.1 Introduction

The most common use of normal butyl acetate is as a solvent in the production of lacquers and paints.

4.2 Chemical Kinetics

Butyl Acetate can be produced by the reaction of methyl acetate with butanol. These is exothermic reactions are irreversible and occur in liquid phase. The overall process can be represented by

$$\mathrm{MeAc} + \mathrm{BuOH} \leftrightarrow \mathrm{MeOH} + \mathrm{BuAc}$$

The kinetics for the forward and reverse reactions are taken from information given by Jimenez and Costa-Lopez. The kinetic expressions used are given below with the overall reaction rate having first-order dependence on the two reactants and products. Concentrations are in molarity (kmol/m^3). Activation energies are in kJ/kmol and temperature is in K.

$$r = kc_{\mathrm{MeAc}}c_{\mathrm{BuOH}} - k'c_{\mathrm{BuAc}}c_{\mathrm{MeOH}}$$

$$k_{\mathrm{F}} = 2.018 \times 10^8 \exp(-71960/RT)$$

$$k_{\mathrm{R}} = 2.839 \times 10^8 \exp(-72670/RT)$$

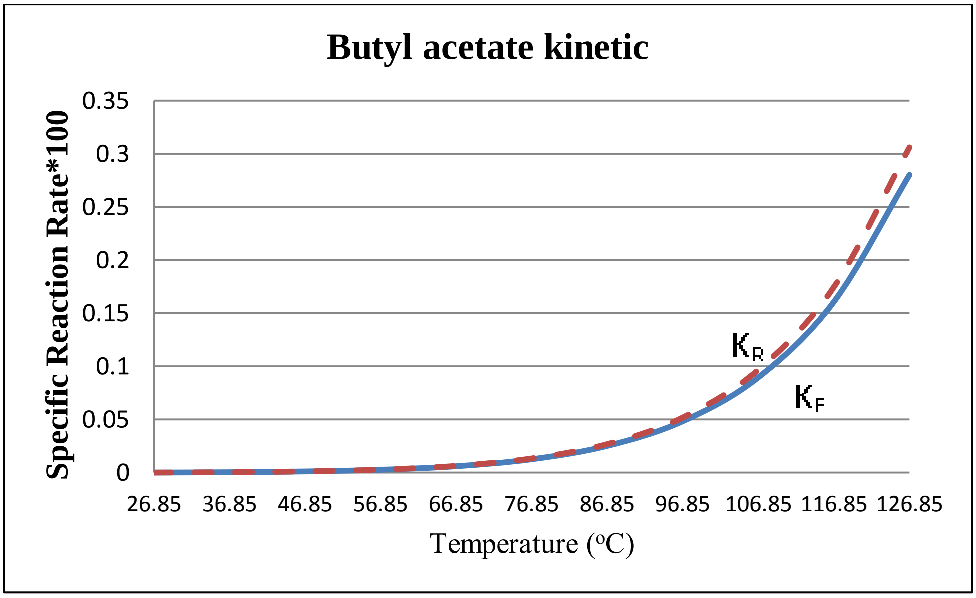


Figure4.1 Butyl acetate kinetic

Figure 4.1 showing relations between specific reaction rates and chemical equilibrium constant with temperature exhibits that specific reaction rates and chemical equilibrium constant depend on temperature. Therefore a reactor temperature about76.85 °C is appropriate temperature so that specific reaction rate high enough to drive the reaction to equilibrium in a small continuous stirred tank reactor (CSTR).

4.3 Phase Equilibrium

There are two binary azeotropes causing complexity of the phase equilibrium. The first azeotrope is mixture between methyl acetate and methanol with composition of 64% methyl acetate at 1.1 atm. Therefore separating in the second column which separates high-purity methnol in the bottom can only produce a distillate that has a composition near the azeotropic composition. The second azeotrope is mixture between butyl acetate and butanol at 4 atm. In the same way separating in the third column which separates high-purity butyl acetate in the bottom can only produce a distillate that has a composition near the azeotropic composition.

4.4 Process Description.

Butyl acetate process consists of a reactor, three distillation columns and two recycle streams. Fresh feed consisting of 60%mol methyl acetate, 40% mol methanol and flowrate107.5 kmol/h is combined with a methyl acetate/methanol recycle stream (153.8 kmol/h, 68%mol methyl acetate, 32%mol methanol). This combination form total methyl acetate/methanol stream (M_{tot}), which is fed into a 4 m^3 reactor operating at 76.85 ^oC and 5 atm. Fresh butanol (63.46 kmol/h) is combined with a butanol recycle stream (127.3 kmol/h, 90%mol butanol, 10%mol butyl acetate) total butanol stream (B_{tot}) , which is fed into the reactor. A small flow of inert gas (nitrogen) is used in reactor so that the pressure can be maintained while achieving the desired reactor temperature.

Reactor effluent is fed to column C1, which splits the two light components from the two heavy components. Methyl acetate and methanol go overhead while butyl acetate and butanol go out the bottom. The column has 37 stages and is fed on Stage 20 and operates at 1.2 atm. There is a small amount of nitrogen in the liquid fed to column C1 hence a partial condenser is used with a small flow (2 kmol/h) to remove any nitrogen.

The distillate stream from column C1 is fed to column C2, which produces high-purity methanol (97.8%mol) going out bottom and methyl acetate/methanol recycle stream (68%mol methyl acetate) going overhead. Because there is excessive nitrogen from column C1, a partial condenser is used with a small flow (1 kmol/h) to remove this excessive nitrogen. The distillate is recycled back to the reactor at a rate 153.8 kmol/h. The column has 27 stages and is fed on stage 18 and operates with a condenser pressure of 1.1 atm.

The bottom from column C1 is fed to column C3, which produces high-purity butyl acetate (99%mol) going out bottom and butyl acetate/butanol recycle stream (90%mol butanol) going overhead. The distillate is recycled back to the reactor at a rate 127.3 kmol/h. The column has 47 stages and is fed on Stage 27 and operates with a condenser pressure of 4 atm.

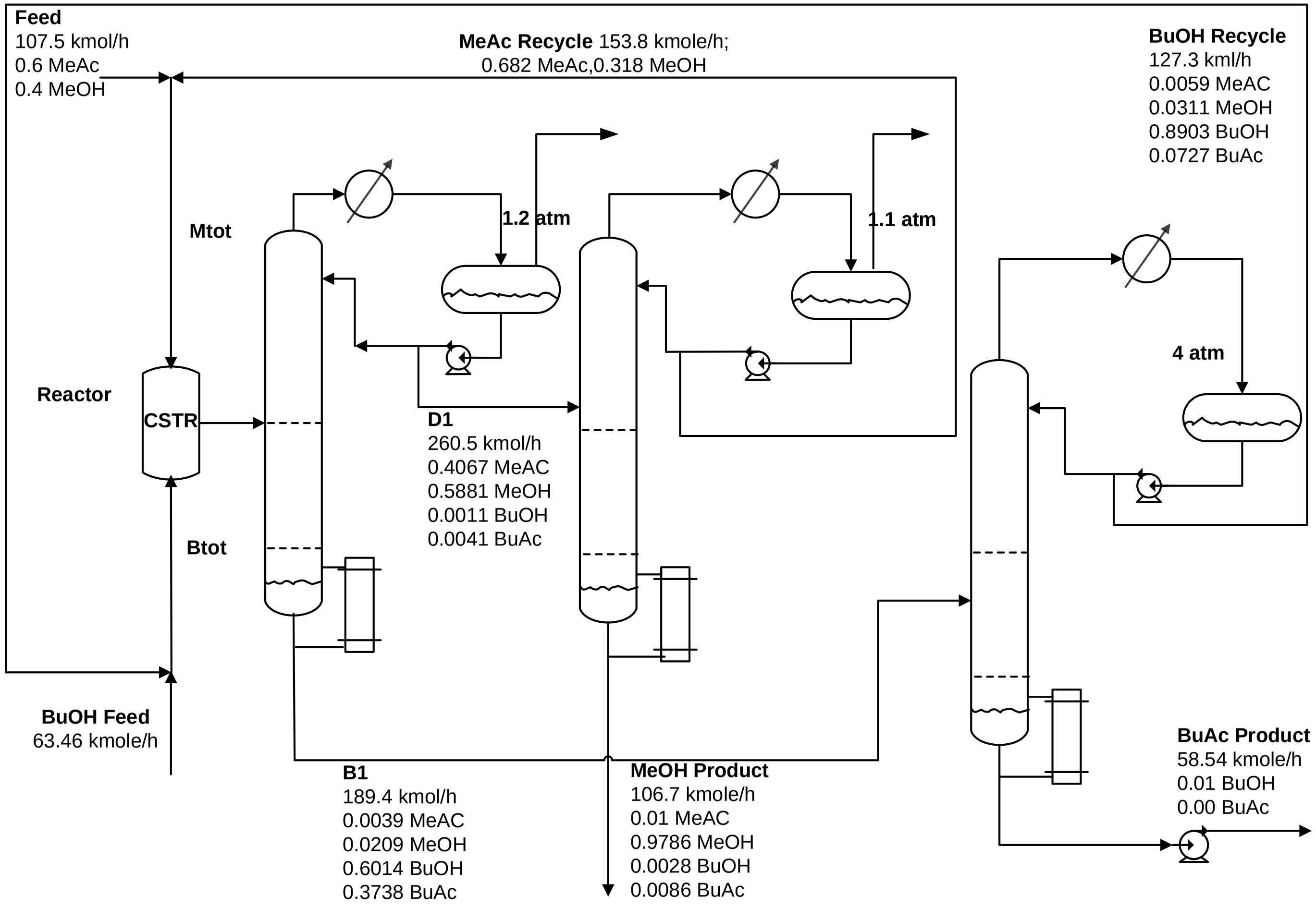


Figure 4.2 Flowsheet of butyl acetate process

CHAPTER V

CONTROL STRUCTURES DESIGN

The plant energy and mass balances are the essential task of plantwide for a complex plant consists of recycle streams and energy integration when the disturbance load come through the process. The control system is needed to reject loads and regulate an entire process into a design condition to achieve its objectives therefore our purpose of this chapter is to present the new control structures of butyl acetate process.

5.1 New Plantwide Control Strategies

In this research, the plantwide control structure design procedures in the butyl acetate process are designed based on the new design procedure given by Wongsri (2012) for all designed control structures and discussed below.

Step1: Gather plant information and control objectives. List all control variables and available manipulated variables (number of DOF)

Control objective

1. Product quality: butyl acetate composition about99 %mol and methanol composition about97.8% mol

2. Production capacity: more than 58.54 kmol/h of butyl acetate and 99 kmol/h of methanol

Table 5.1 Control variables of butyl acetate process

Unit	Control variables
Streams	- Flow rate
Reactor	- Temperature
	- Level
Distillation columns	- Condenser pressure
	- Reflux drum level
	Reboiler level
	- Tray temperature
	- Reflux flow or Reflux ratio

Table 5.2 Available manipulated variables of butyl acetate process

Unit	Manipulate variables	Number	DOF
Independent streams	Flow rate	2	2
CSTR reactor	Heat flow Effluent stream	1	3
Distillation columns	Distillate flow Bottom flow Reflux flow Condenser heat duty Reboiler heat duty Vent gas	3	17
Sum			22

Step2: Energy management via heat exchanger networks.

The energy for the butyl acetate process is not feasible enough to design any heat integrated networks. Somehow only possible heat integrated network that can possibly design is the heat integration of the temperatures of the C2 reboiler with the condenser temperature of the C3.However, heat integrated distillation can caused a complexity in controlling structure.

Step3: Establish fixture plant

3.1 Keep the raw materials entered and reentered fixed

There are two feed streams adding raw materials to the process therefore loops control used to keep material quantity are performed. First feed is mixture of methanol and methyl acetate which is kept quantity by controlling total methanol/methyl acetate flow rate (M_{tot}). Second feed is butanol fresh feed which is kept quantity by controlling total butanol flow rate (B_{tot}).

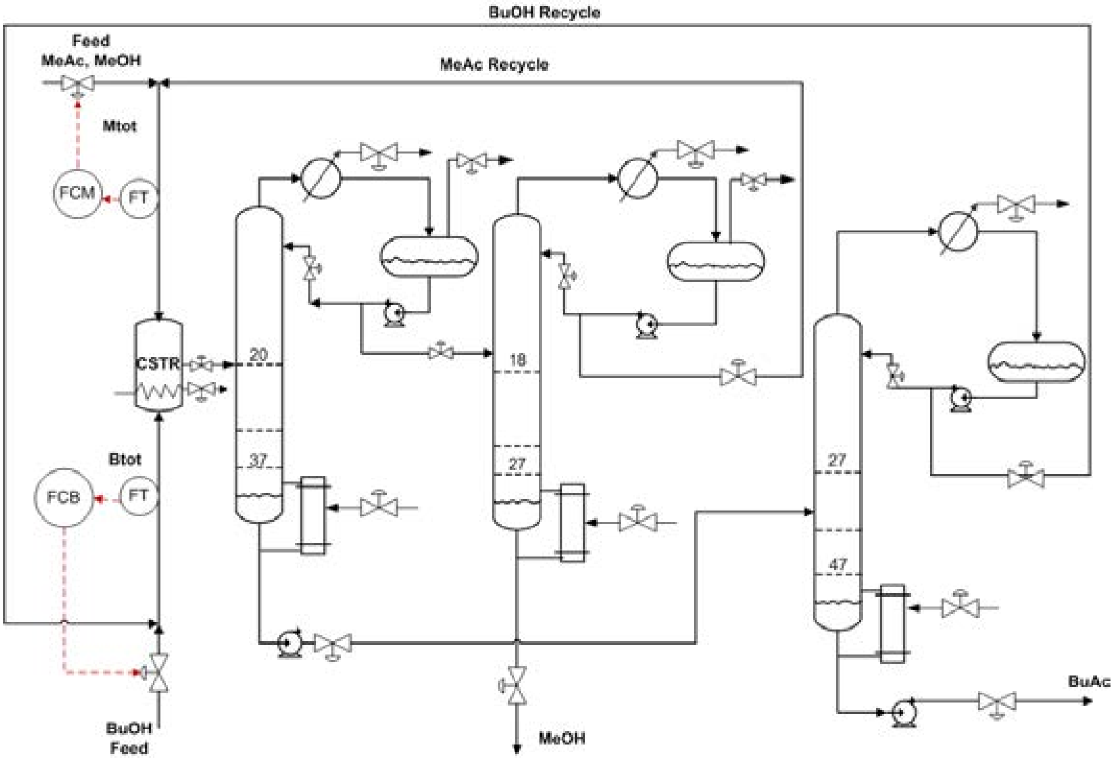


Figure 5.1 Keeping the raw materials entered and reentered fixed

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

There are two exit material streams including methanol and butyl acetate product stream. Methanol flow is adjusted to keep column C2 reboiler level and butanol flow is adjust to keep column C3 reboiler level.

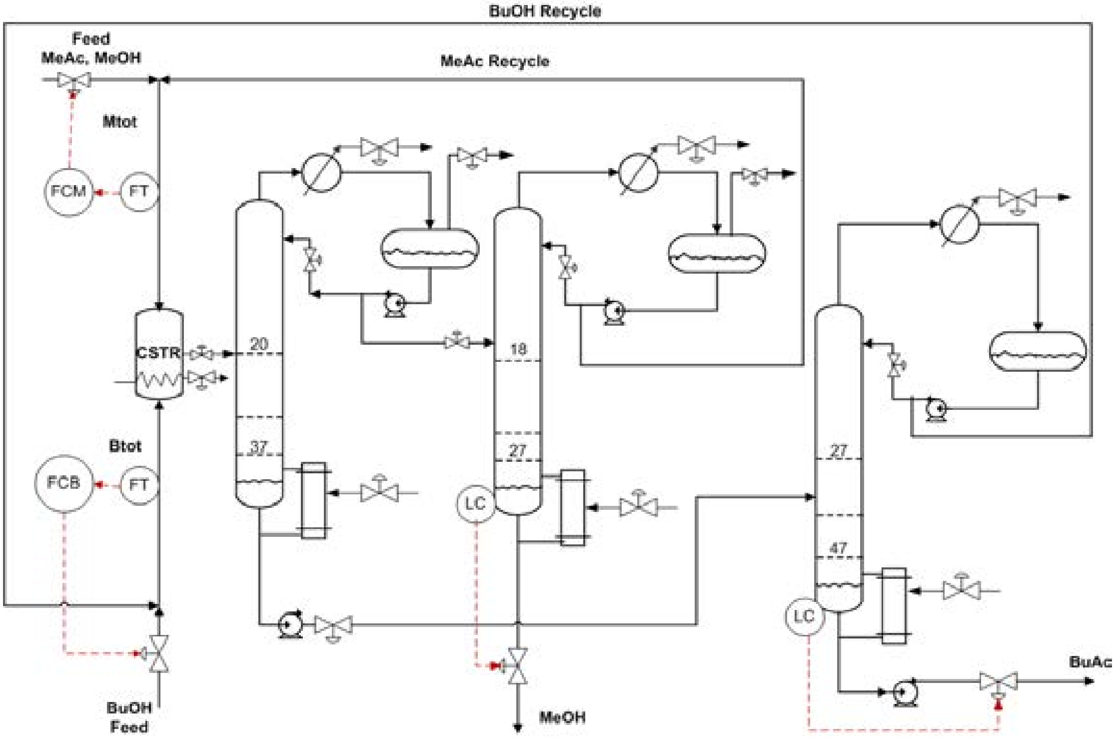


Figure 5.2 Adjusting the flow of exit material streams according to their accumulation

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

In this process has 4 components including methyl acetate, methanol, butanol and butyl acetate. Quantifiers of each component are different location. These and control loops are exhibited below.

- *Methyl acetate:* Quantifier of methyl acetate is at column C2 reflux drum.
- *Methanol:* Quantifier of methanol is at column C2 reboiler.
- *Butanol:* Quantifier of butanol is at column C3 reflux drum.
- *Butyl acetate:* Quantifier of butyl acetate is at column C2 reboiler.

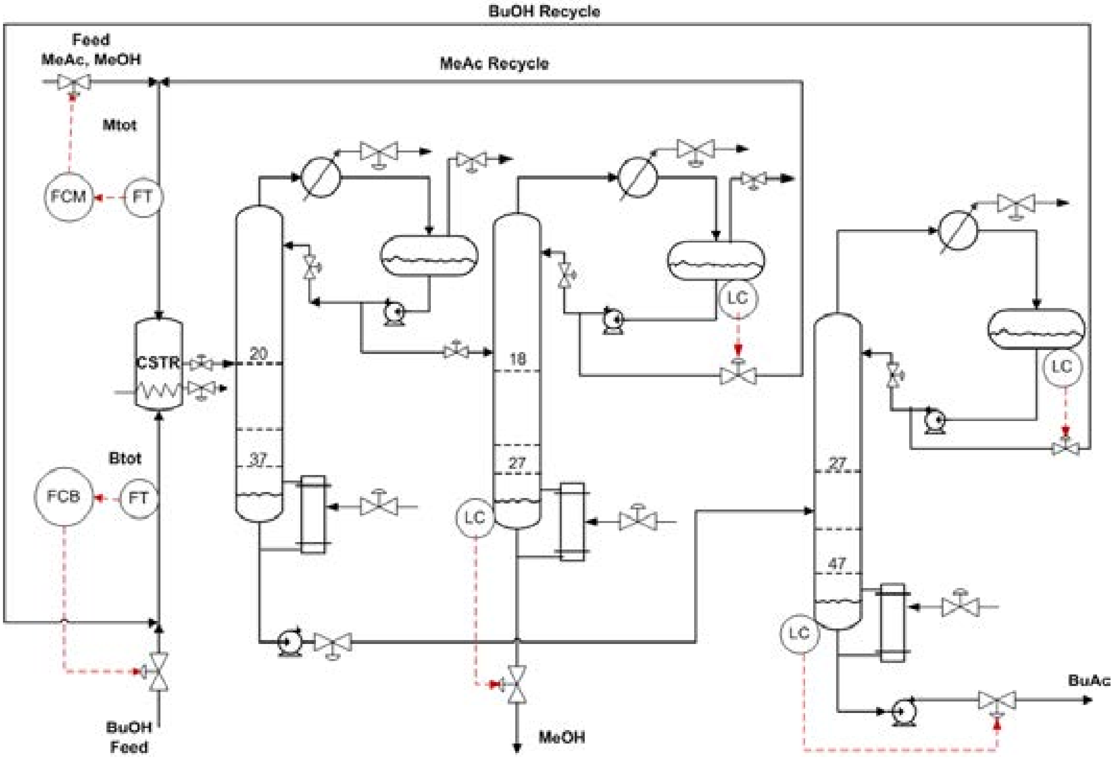


Figure 5.3 Locating the quantifiers for the rest of the components and design the control loops

Step4: Handling the disturbances

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

4.1 Heat Disturbances

Heat disturbance can be handled in four points. At reactor can handle heat disturbance by adjusting reactor heat duty. For all distillation columns can handle heat disturbance by adjusting reboilers heat input.

4.2 Material disturbances

There are path ways of any material showed in figure 5.4-7. The material path ways indicate the control structures to manage each material according to their path ways.

Methyl acetate is fed to react in reactor. Unconverted methyl acetate is fed to column C1 and taken overhead which is directed to distillate. Then it is fed to column

C2 and taken overhead which is directed to distillate also. Methyl acetate in distillate stream is recycled back to the reactor. In addition, there is controlling reflux flow to keep quantity of methyl acetate which is returned to the column to be constant.

Methanol is fed to reactor with methyl acetate and combined with methanol generated by reaction before it is fed to column C1 and taken overhead. Then it is fed to column C2, which produces high purity methanol out the bottom and a distillation stream with a methanol composition near azeotrope. The distillation stream is recycled back to the reactor.

Butanol is fed to react in the reactor. Unconverted butanol is fed to column C1 and leaves in the bottom which is directed to the bottom and then goes to column C3. In column C3, butanol is taken overhead which is directed to the distillate and recycled back to the reactor. Moreover, reflux flow of the column is fixed to keep quantity of butanol which is returned to the column to be constant.

For butyl acetate is generated in the reactor. Butyl acetate product is fed to column C1 and leaves in the bottom then goes to column C3, which produces high purity butyl acetate out the bottom and a distillate stream.

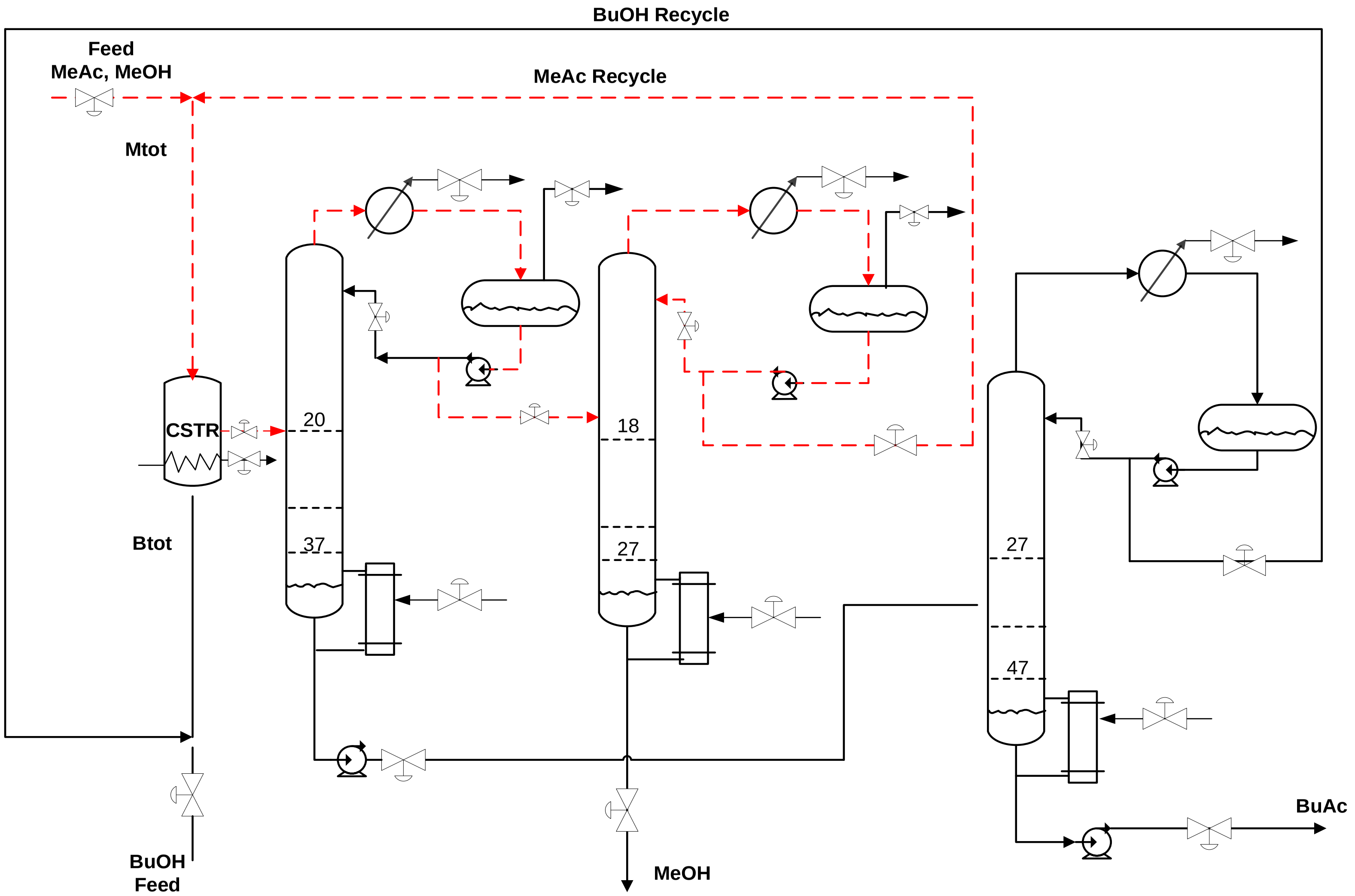


Figure 5.4 Path way of methyl acetate

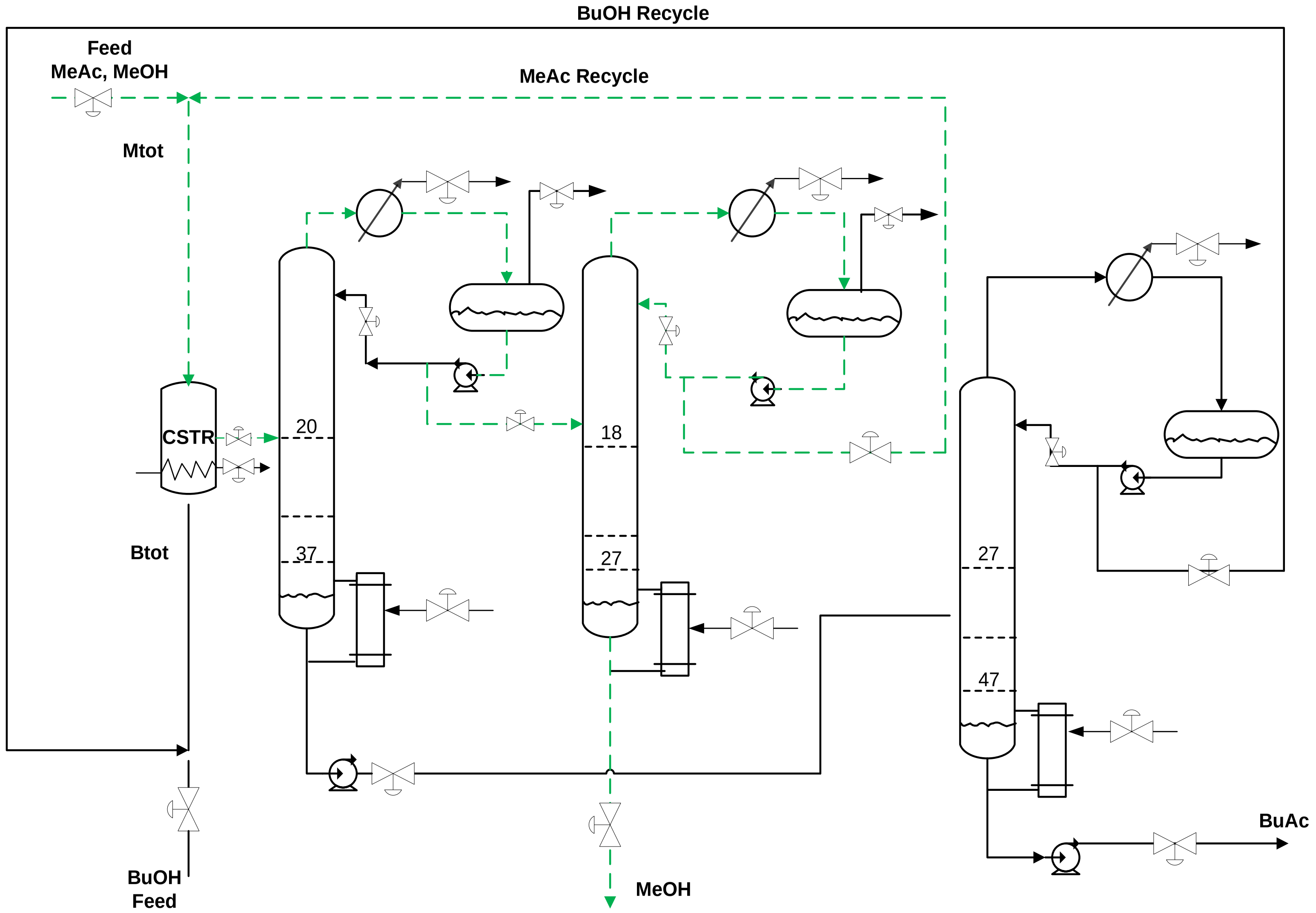


Figure 5.5 Path way of methanol

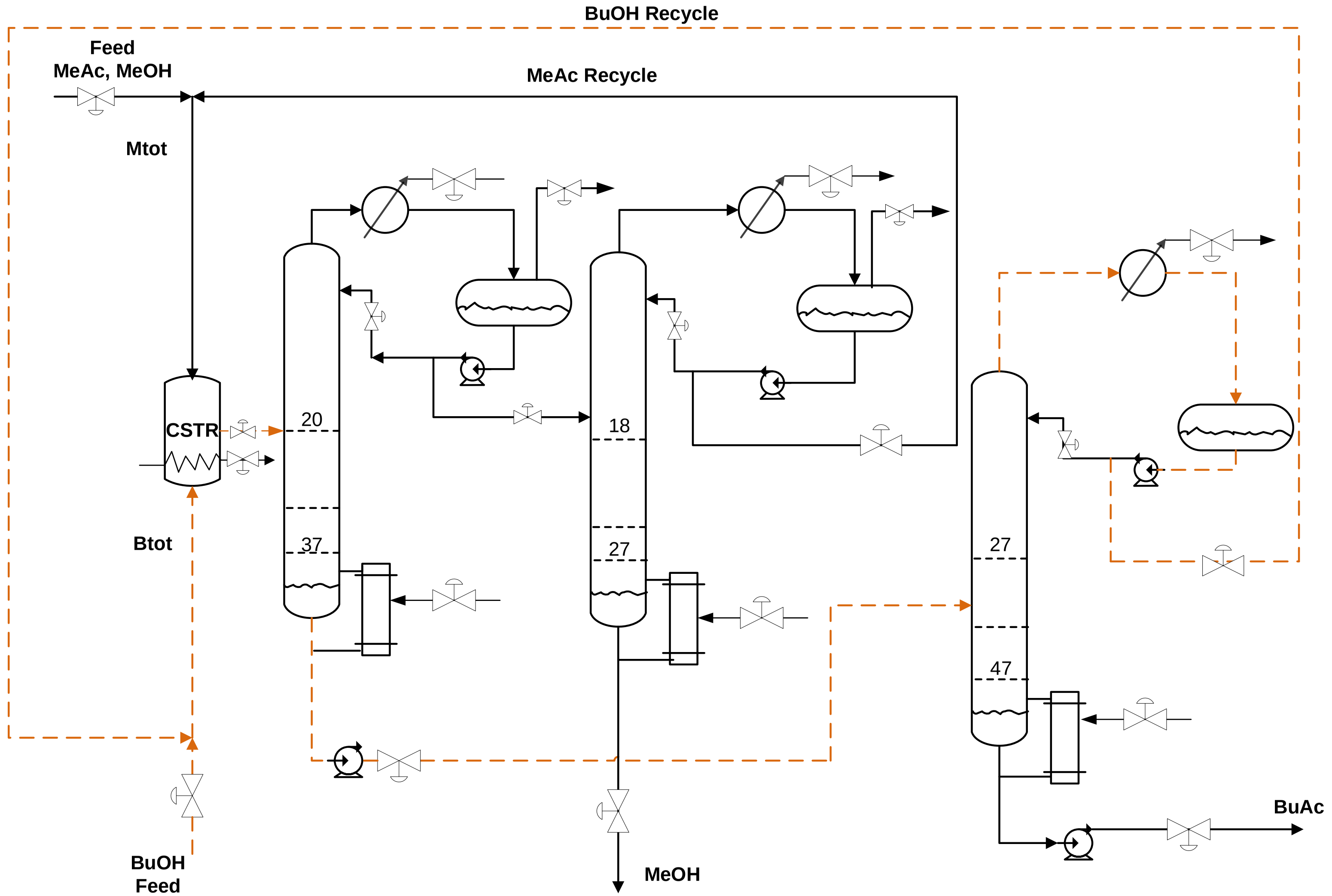


Figure 5.6 Path way of butanol

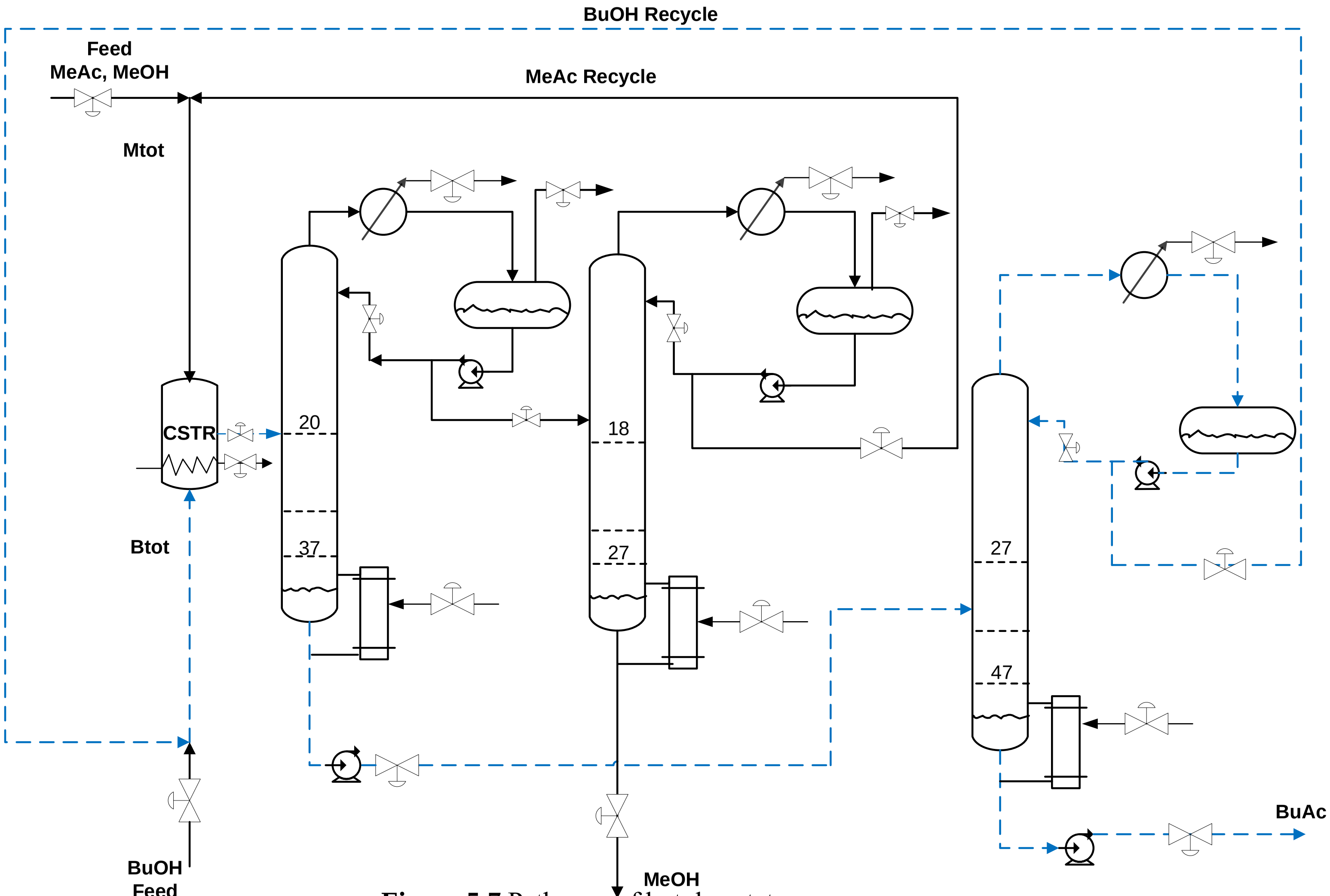


Figure 5.7 Path way of butyl acetate

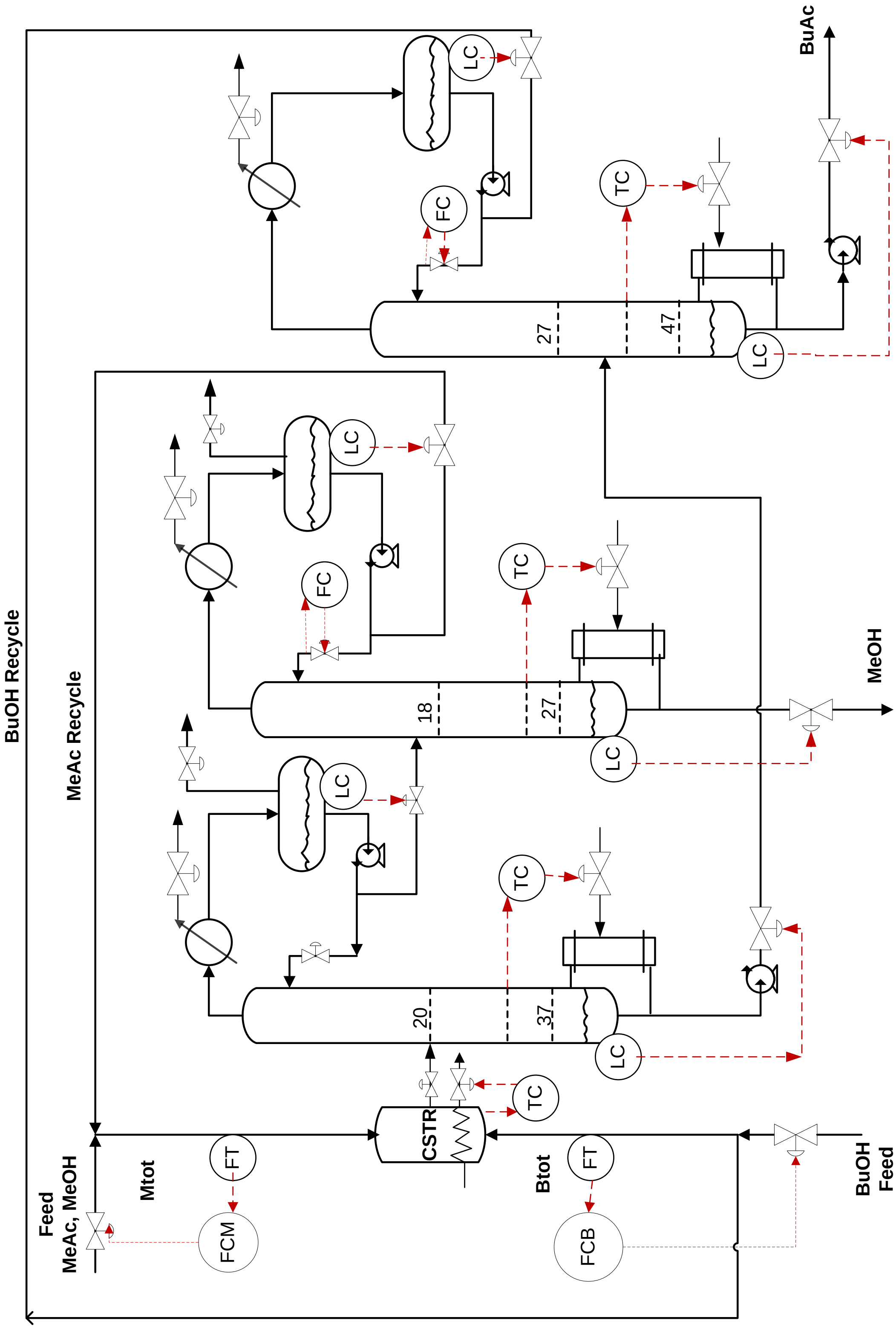


Figure 5.8 Control structure obtained from step 3-4

Step5: Find the most disturbed point and design the control loops to alleviate the effects of disturbances

1. Reactor

Control structure of reaction section is accomplished by testing disturbances and finding disturbed point for design control loop.

Table 5.3 Result of reactor obtained by testing heat disturbance (inlet temperature change)

Temperature change	Nominal	+10^{o}C	-10^{o}C
Temperature	76.85	76.85	76.85
Duty(kW)	94.29	131.8	57.63
Conversion	35.36	35.35	35.35
Butyl acetate composition	0.1587	0.1587	0.1587

Form the result of reactor obtained by changing of inlet temperature, which are increasing and decreasing 10 ^{o}C of the temperature, conversion of reaction and butyl acetate composition of effluence stream have a small deviation from nominal value when outlet temperature is fixed at 76.85 ^{o}C by adjust reactor duty.

Table 5.4 Results of reactor obtained by testing material disturbance (total flow change)

Total flow change	Nominal	5%	-5%
Temperature	76.85	76.85	76.85
Duty(kW)	94.29	99.72	88.89
Conversion	35.36	35.34	35.37
Butyl acetate composition	0.1587	0.1587	0.1588

The result obtained by changing of total flow shows a small effect on conversion of reaction and butyl acetate composition when the out temperature is fixed by adjust reactor duty. Therefore, temperature must be controlled by manipulating reactor duty in order to keep conversion and product composition.

2. Column C1

The typical procedure for selecting which tray to control is to look at steady-state temperature profile in the column at the base case condition. The temperature profile is found a location in the column where there are large temperature changes from tray to tray. In figure5.9, the slope of the temperature profile is the steepest on tray 35-37 and the location where there are large temperature changes from tray to tray is at tray 35 to 36. Tray 36 is selected to control by manipulating reboiler duty. The reflux ratio is controlled by measuring distillate flow rate and sanding this signal to a multiplier whose other input is the desired reflux ratio. The output signal from the multiplier is the set point of a reflux flow.

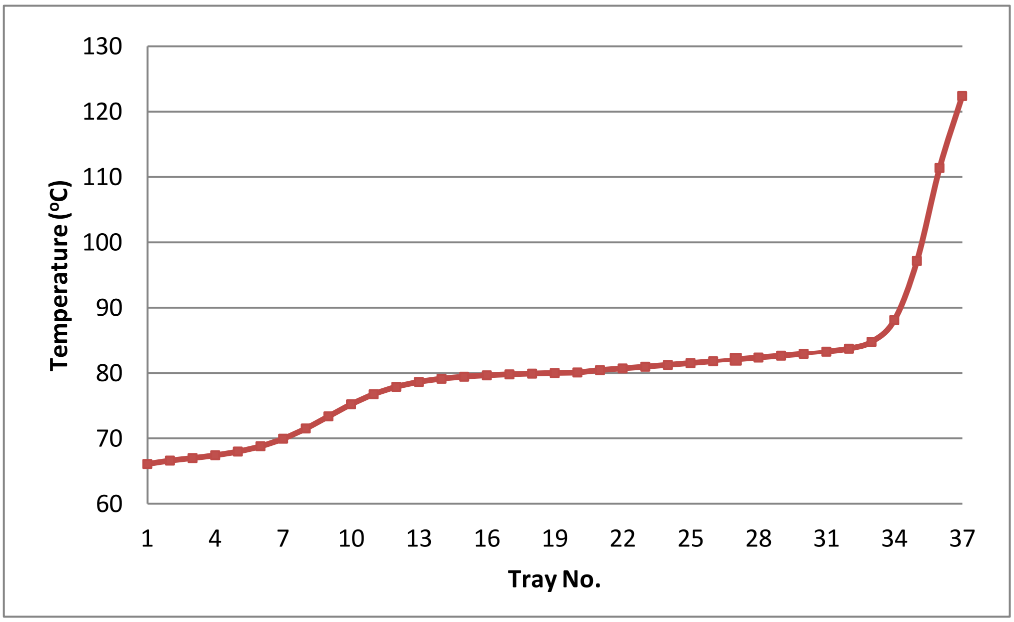


Figure 5.9 Temperature profile of column C1

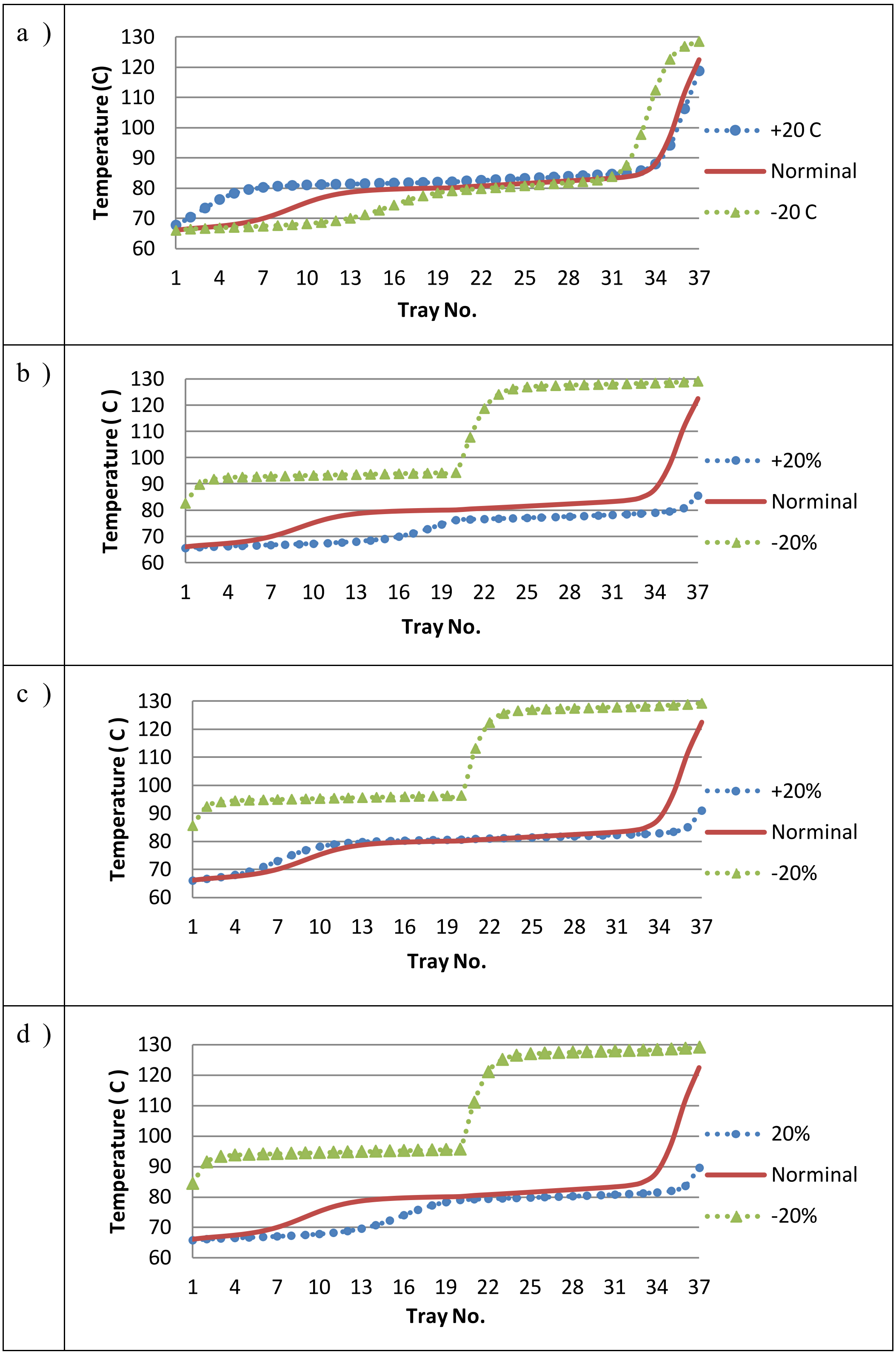
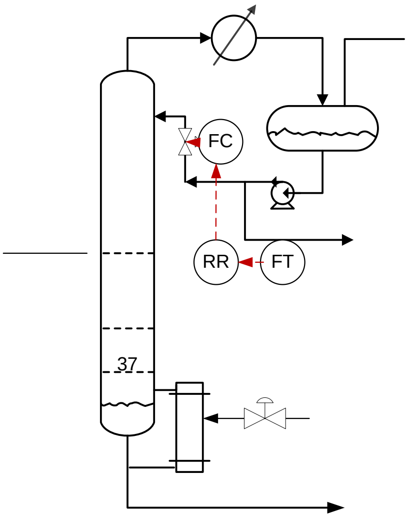


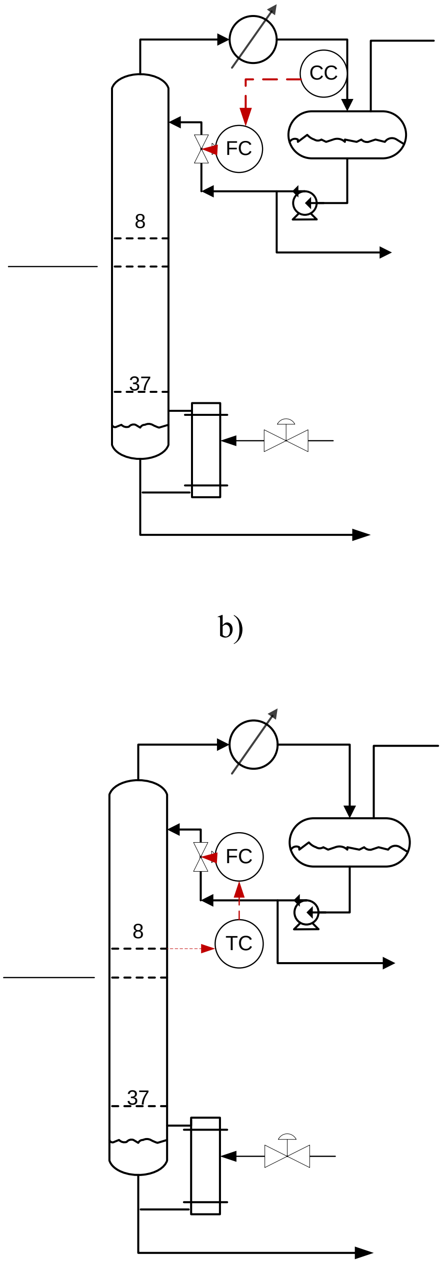
Figure 5.10 Temperature profile of column C1 when a) Inlet temperature change b) Inlet composition change c) Total flow change and d) Component flow change

According to figure 5.10, there are large effects around steep slope showing the strictly control must locate around here. Changing of inlet temperature causes an effect on temperature profile in the stripping and rectifying section. For changing of composition, total flow and component flow cause similar effect on temperature profile which increase when composition, total flow and component flow are decreased and decrease when they are increased.

In addition, changes of several material disturbances effect on temperature in overhead of the column. Increasing of temperature at the rectifying section refers to butyl acetate going overhead. Therefore, reflux flow must be used as manipulated variable to maintain distillate and bottom purity affecting downstream in column C2 and C3. Three alternatives of column C1 are shown in figure 5.11.



a)



b)

c)

Figure 5.11 Alternatives for control the overhead product quality of column C1 a) Reflux ratio control b) Butyl acetate concentration control c) Temperature on tray 8 control

3. Column C2

In figure5.12, the slope of the temperature profile is the steepest on tray 21-25 and the location where there are large temperature changes from tray to tray is at tray 22 to 23. Tray 23 is selected to control by manipulating reboiler duty. Reflux flow is controlled.

According to figure 5.13, there are large effects around steep slope showing the strictly control must locate around here. Changing of inlet temperature causes a small on temperature profile. For changing of composition, total flow and component flow cause similar effect on temperature profile which increase when composition, total flow and component flow are decreased and decrease when they are increased.

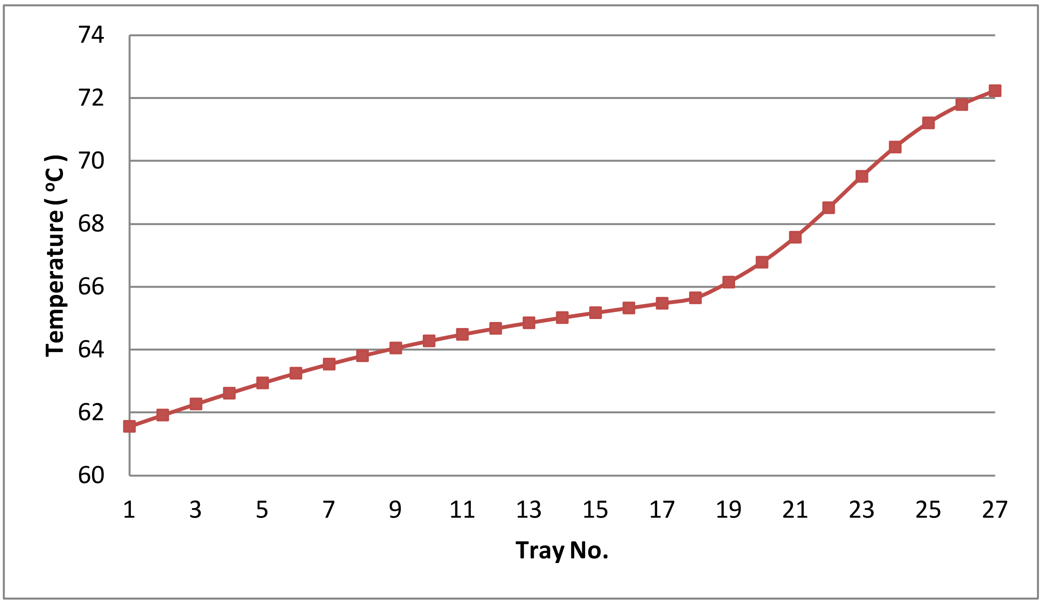


Figure 5.12 Temperature profile of column C2

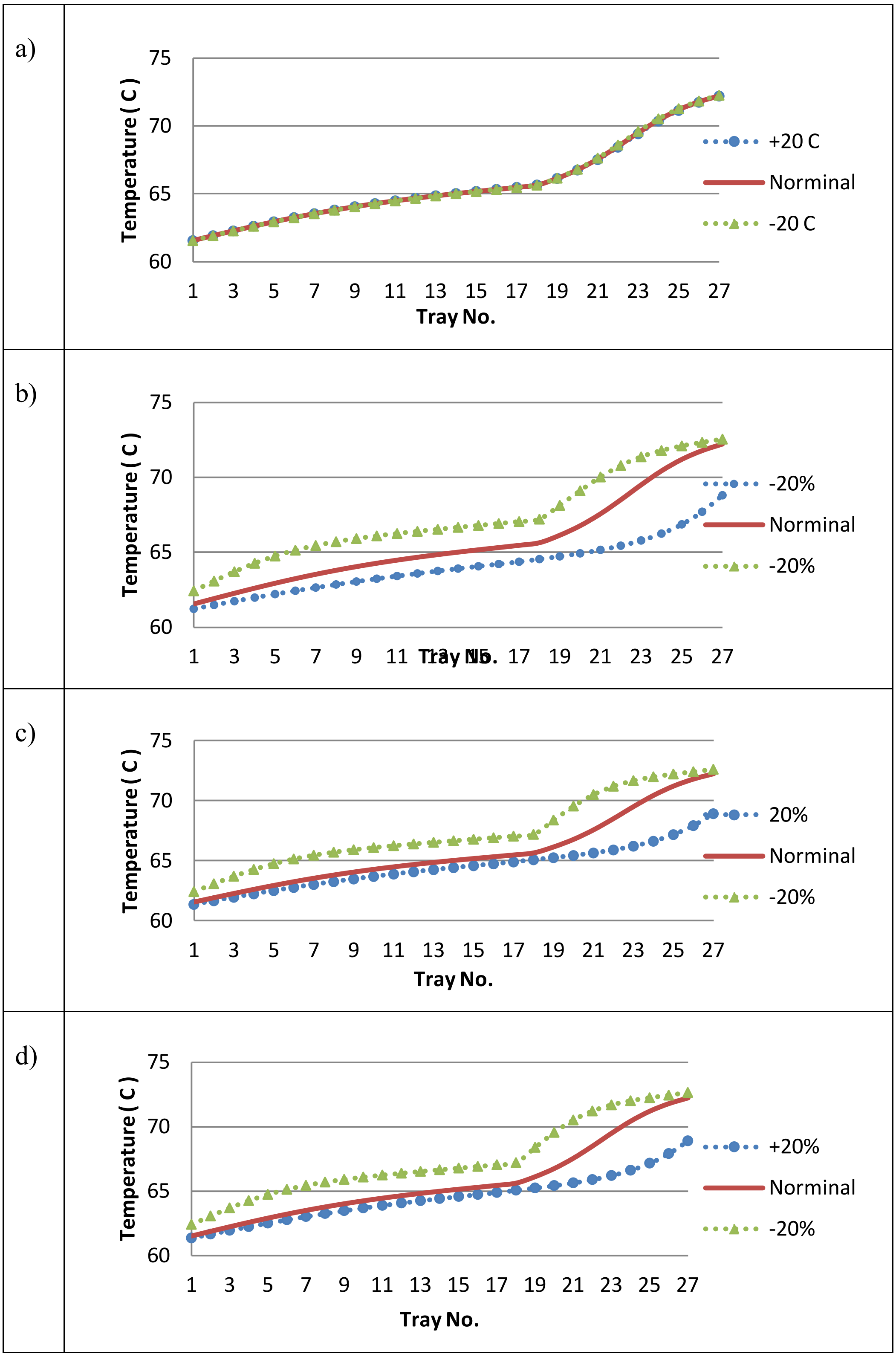


Figure 5.13 Temperature profile of column C2 when a) Inlet temperature change b) Inlet composition change c) Total flow change and d) Component flow change

4. Column C3

In figure5.14, the slope of the temperature profile is the steepest on tray 32-40 and the location where there are large temperature changes from tray to tray is at tray 37 to 38. Tray 38 is selected to control by manipulating reboiler duty. Reflux flow is controlled.

According to figure 5.15, there are large effects around steep slope showing the strictly control must locate around here. Changing of inlet temperature causes a small on temperature profile. For changing of composition, total flow and component flow cause similar effect on temperature profile which increase when composition, total flow and component flow are decreased and decrease when they are increased.

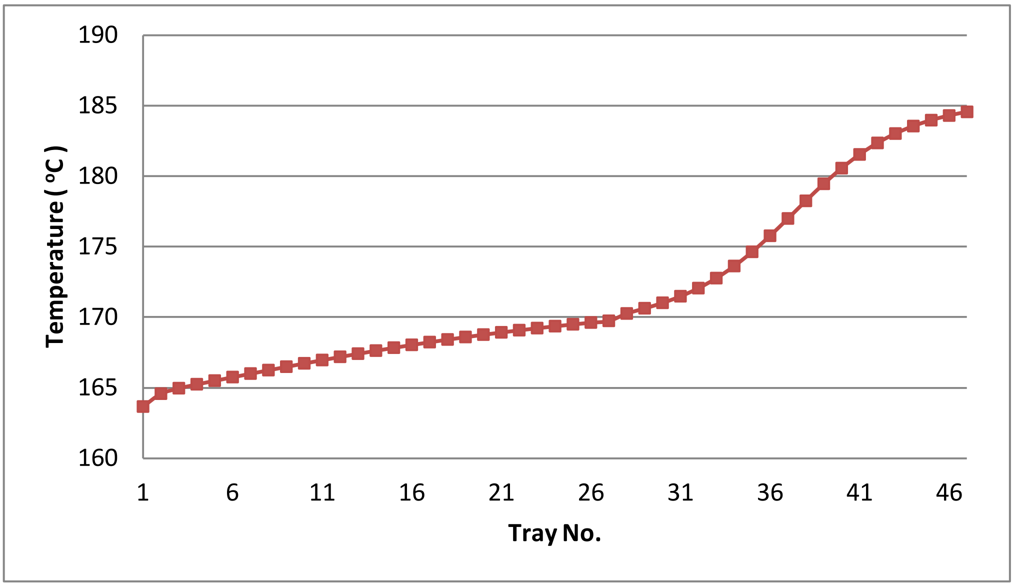


Figure 5.14 Temperature profile of column C3

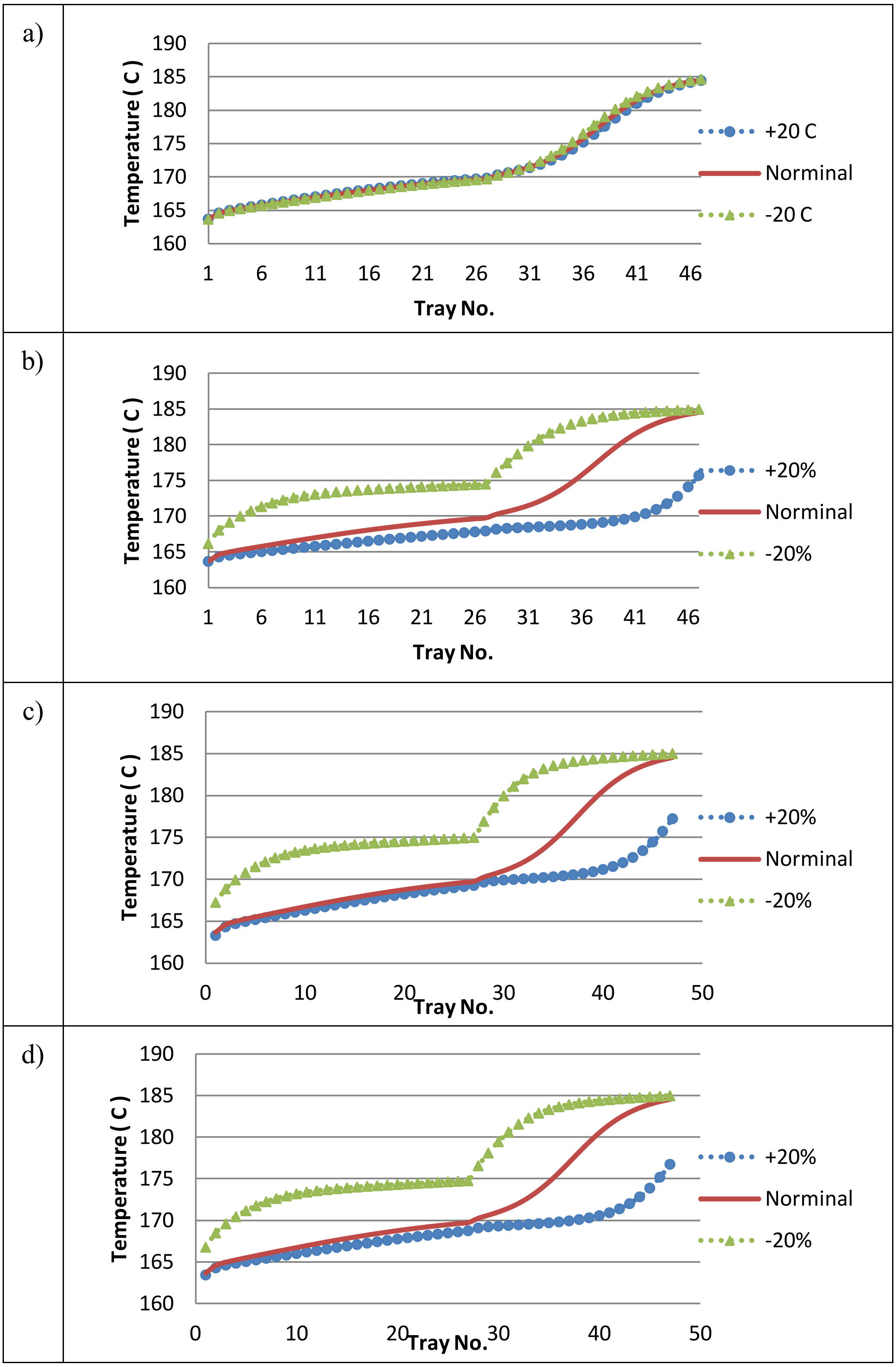


Figure 5.15 Temperature profile of column C3 when a) Inlet temperature change b) Inlet composition change c) Total flow change and d) Component flow change

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

The rest control loops are added in this step including pressure controls and level controls of the vessels.

The total butanol flow rate is ratioed to the total methyl acetate flow rate to keep in correct stoichiometric ratio. Base case control structure and design control structures are shown in figure 5.16-19.

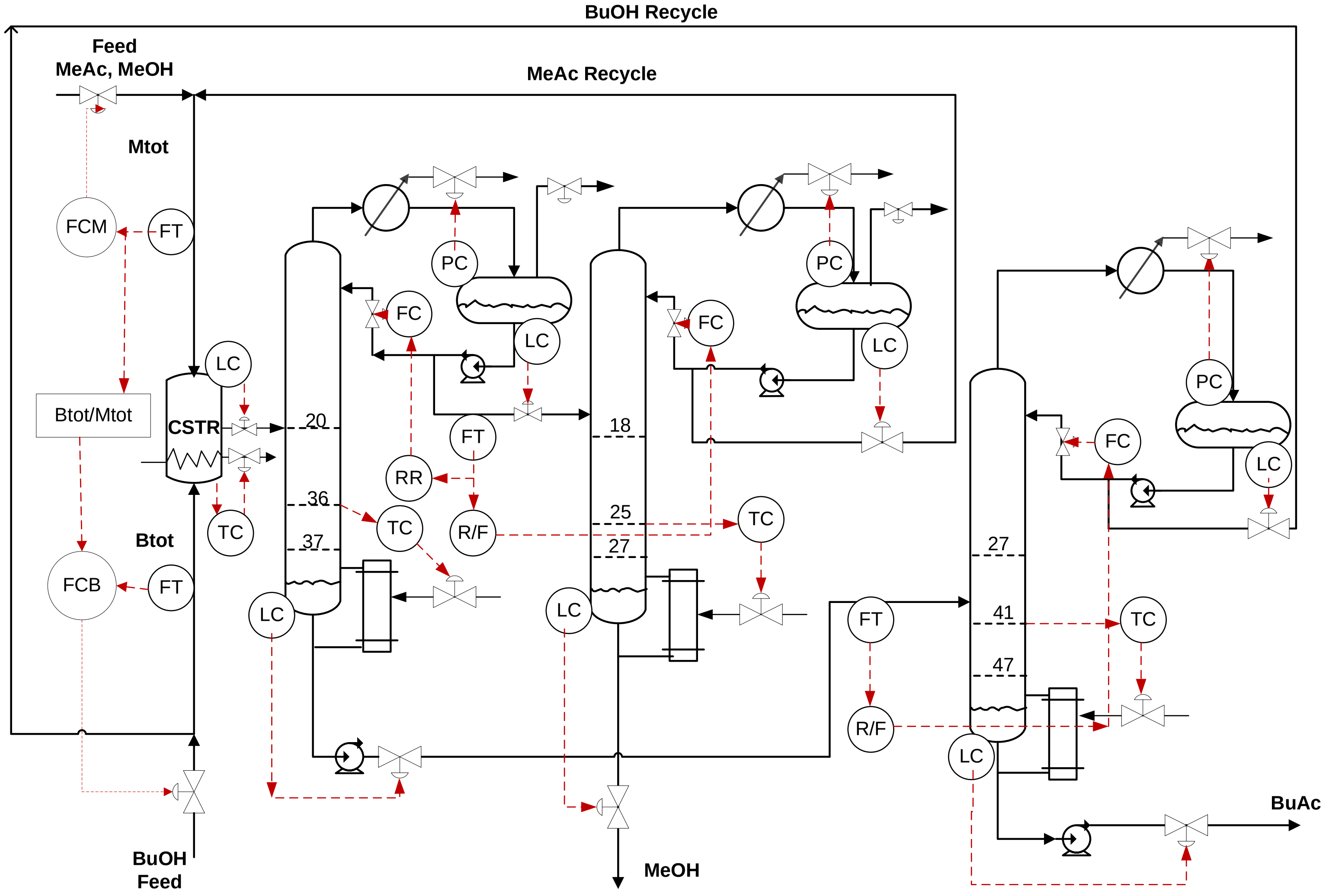


Figure 5.16 Base case control structure

Table 5.5 Control structure lists of base case

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE
MeAc/MeOH feed	FCM	Total flow rate	Feed flow rate	PI	Reverse	√	
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	√	
CSTR reactor	TC	Temperature	Reactor duty	PI	Direct	√	√
	LC	Liquid level	Effluence flow rate	P	Direct		
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 36	Reboiler duty	PI	Reverse	√	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 25	Reboiler duty	PI	Reverse	√	√
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 41	Reboiler duty	PI	Reverse	√	√

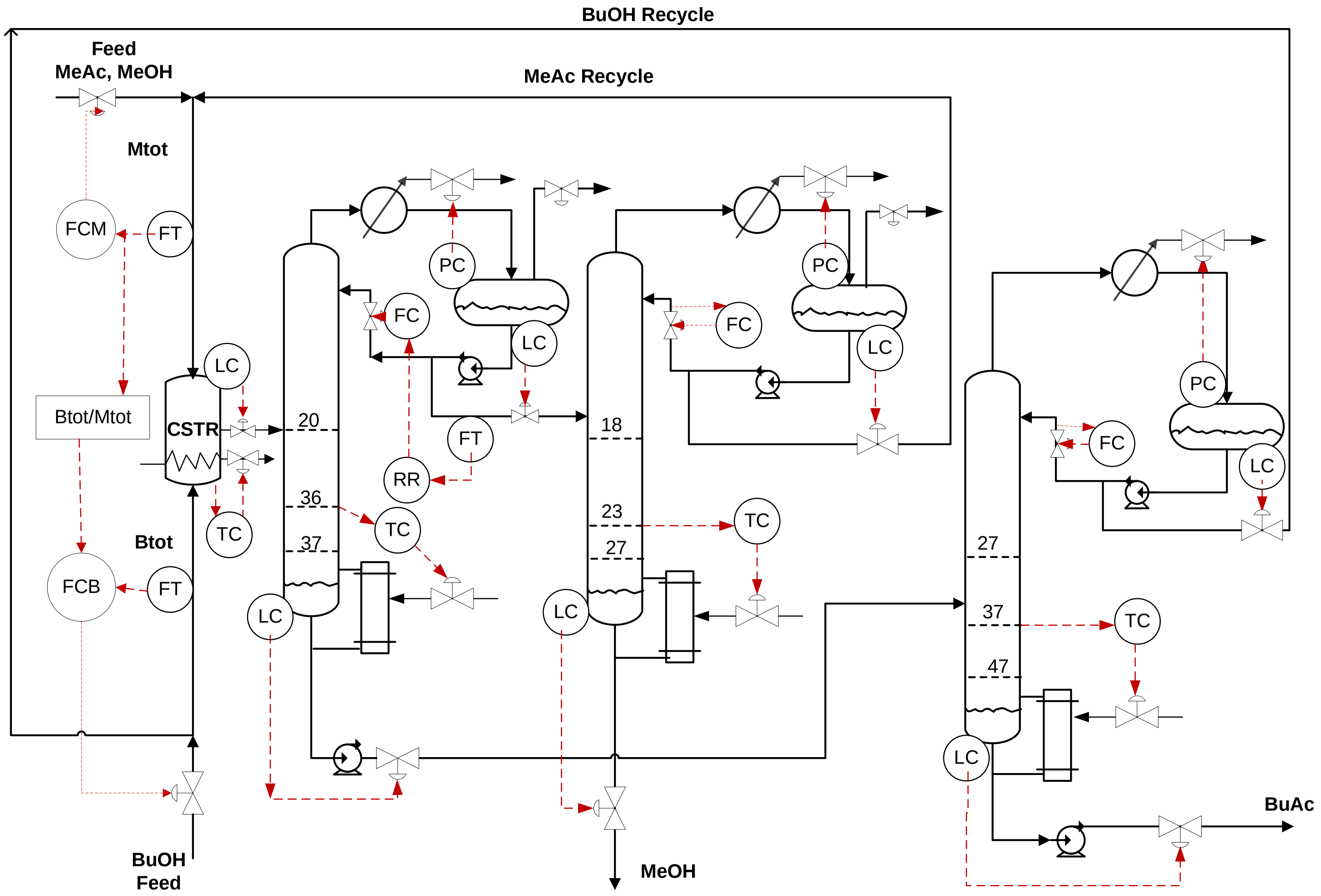


Figure 5.17 Design control structure I (CS1)

Table 5.6 Control structure lists of design control structure I (CS1)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	√	
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	√	
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	√	√
	LC	Liquid level	Effluence flow rate	P	Direct		
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	√	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	√	√
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	√	√

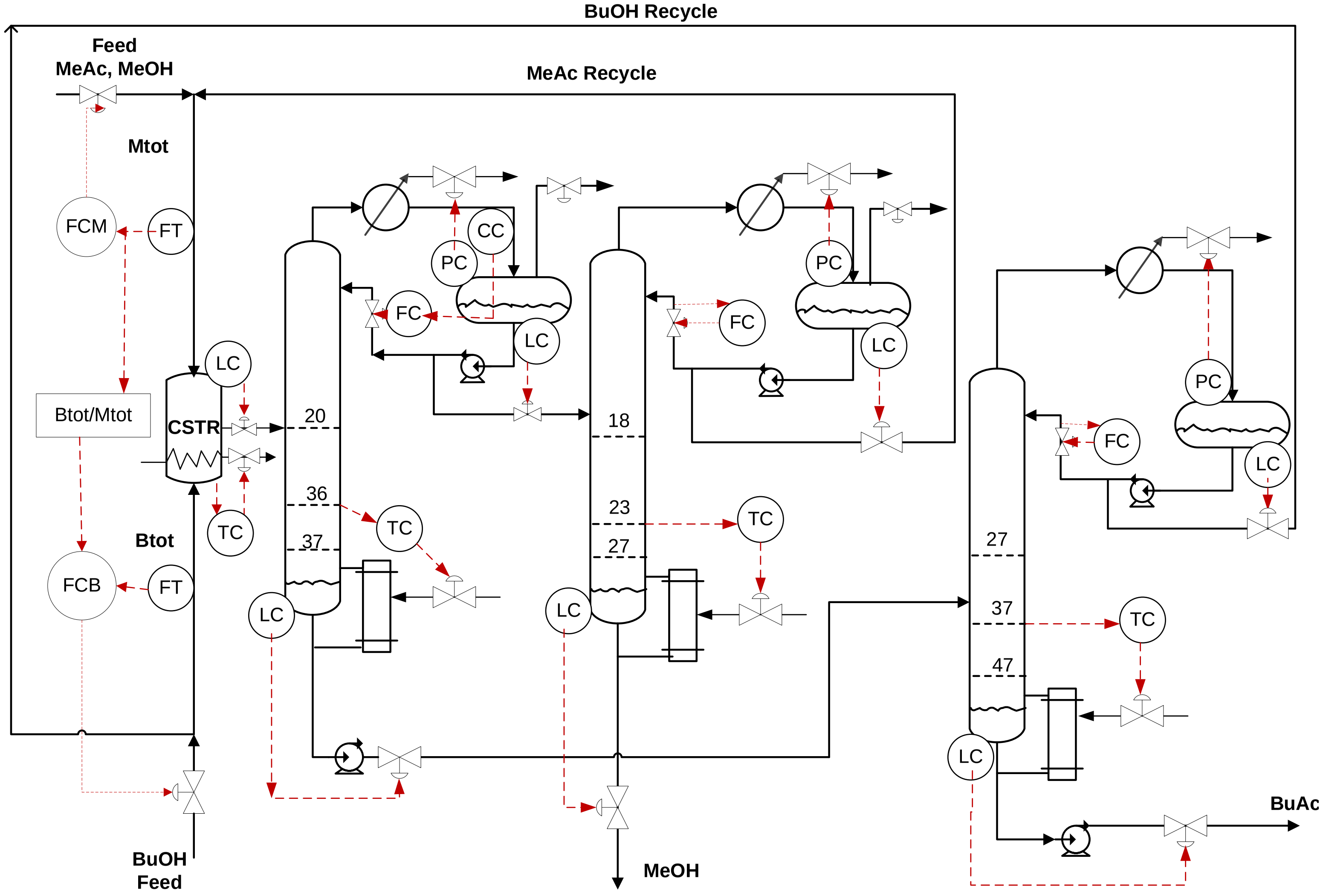


Figure 5.18 Design control structure II (CS2)

Table 5.7 Control structure lists of design control structure II (CS2)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	√	
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	√	
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	√	√
	LC	Liquid level	Effluence flow rate	P	Direct		
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	CC	Butyl acetate mole fraction	Reflux flow rate	PID	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	√	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	√	√
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	√	√

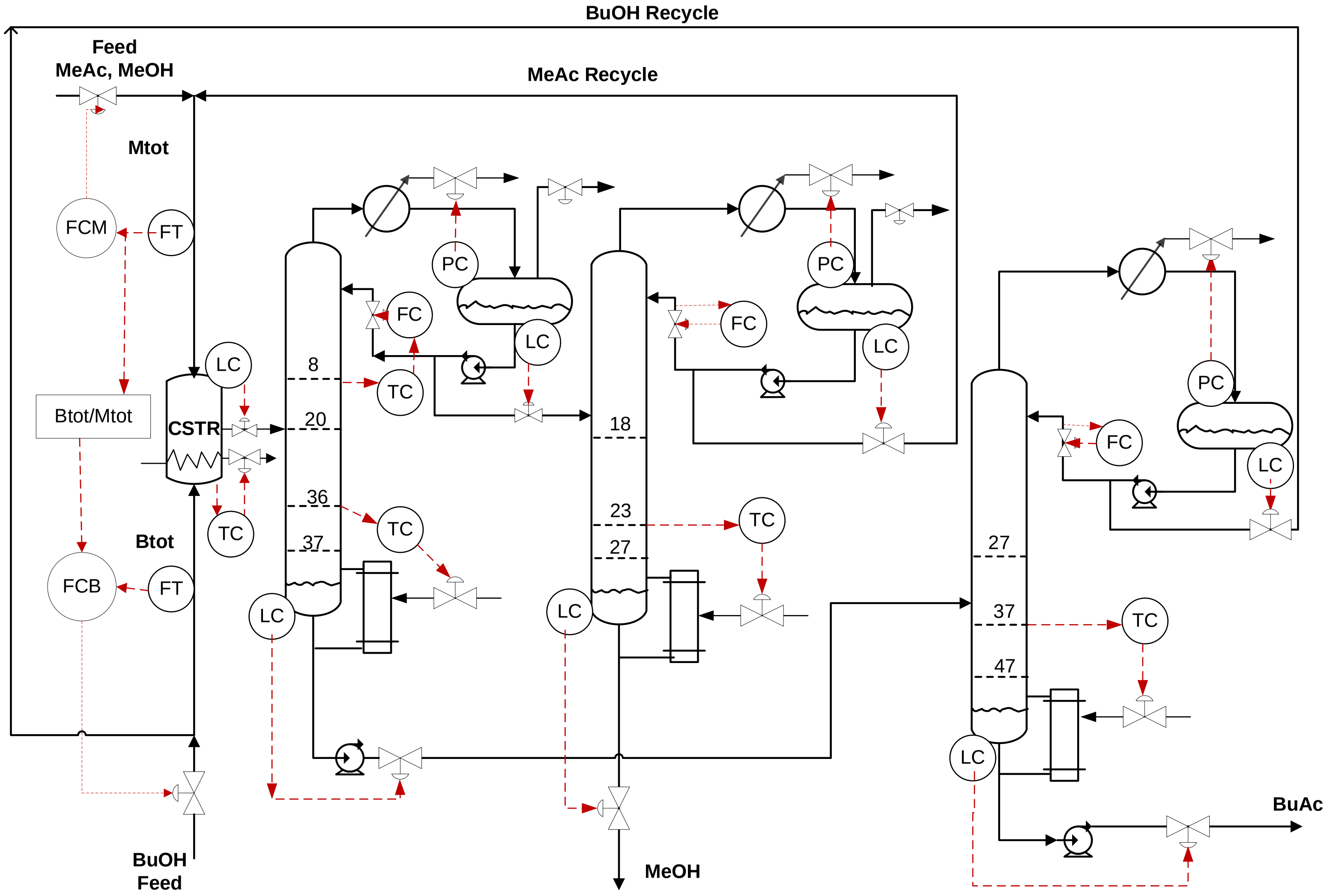


Figure 5.19 Design control structure III (CS3)

Table 5.8 Control structure lists of design control structure III (CS3)

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	√	
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	√	
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	√	√
	LC	Liquid level	Effluence flow rate	P	Direct		
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	TC	Temperature tray 8	Reflux flow rate	PID	Reverse	√	
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	√	√
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboilerlevel	Bottom flow rate	P	Direct		
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	√	√
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	√	√
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	LC	Reboiler level	Bottom flow rate	P	Direct		
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	√	√

Step 7: Optimize economics and improve control performance

Economic optimum design is performed by varying reactor size and reactor temperature for finding the most feasible reactor size and reactor temperature. The total number of trays is varied in each column to find the minimum TAC. The feed tray location that minimizes reboiler heat input is found for each value of total stage.

In addition, PID controls are used to control temperature and concentration of the new control structures.

Step8: Validate the designed control structures by rigorous dynamic simulation

Dynamic simulation results are evaluated by changing total methyl acetate flow, feed composition and feed temperature.

1. Total methyl acetate flow change

Total methyl acetate is varied by change set point of total flow controller. The set point increases by step change from261 kgmole/hr to 274 kgmole/hr and decreases by step change from 261 kgmole/hr to248 kgmole/hr.

Table 5.9 shows responses of variable disturbed by total methyl acetate changing. Reactor temperature controller can control temperature in all of control structures. In base case control structure, the temperature deviation of reactor is about 0.35˚C which is returned to the set point (76.85˚C) in about 7 hours. For three design control structures, changes of the reactor temperature are in the same direction. Their temperature deviations are only about 0.1˚C and returned to the set point in about 4 hours. The smaller deviation is effect of PID controller.

Deviations of column C1, C2 and C3 tray temperature and time used for return to the set point in design control structures are smaller than base case because controlling tray temperature in design control structures use PID controller effecting smaller deviation.

Change of distillate of column C1 in base case is similar to change in case CS1 because reflux ratios of column C1 in both structures are fixed. Butyl acetate mole fraction in distillate of column C1in case of base case and CS1 changes according to methyl acetate change. In case of CS2 butyl acetate mole fraction is controlled by manipulating reflux flow. In case of CS3 butyl acetate mole fraction changes according to not only methyl acetate change but according to top temperature fixed also. In case of CS2 and CS3 can manage butyl acetate going to overhead which effect on downstream in column C2.

Column C1 bottom flow rate of all control structures change in the same direction which change according to butyl acetate inlet quantity. In base case control structure, change of methyl acetate mole fraction in column C1 bottom flow is largest because of large methyl acetate recycle flow rate (D2).

Column C2 feed is from distillate stream of column C1 hence its distillate flow rate and bottom flow rate depend on column C1 distillate stream. Purity of bottom product (methanol) can be maintained close to specification.

Column C3 feed is from bottom stream of column C1 hence distillate and bottom flow rate of this column depend on column C1bottom stream. Purity of bottom product (butyl acetate) can be maintained close to specification.

Table 5.9 Dynamic responses with total methyl acetate change

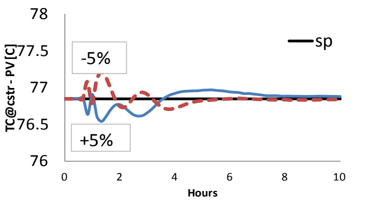
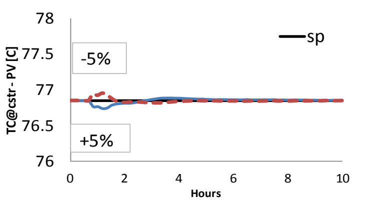
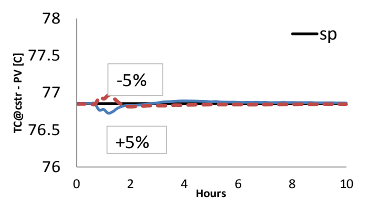
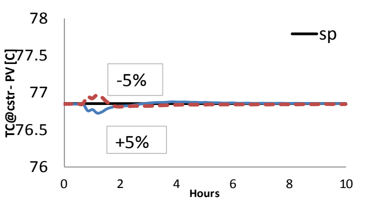
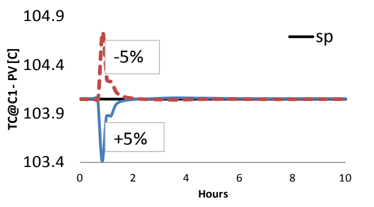
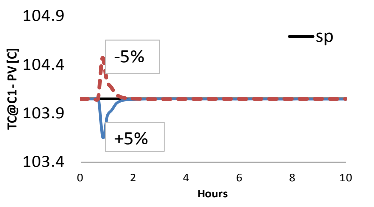
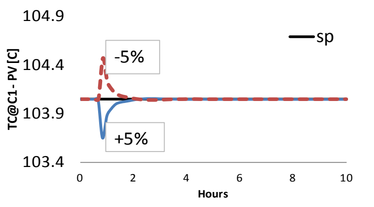
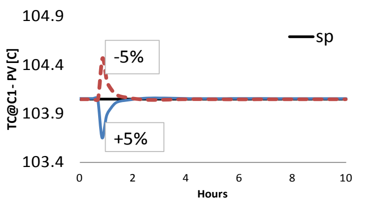
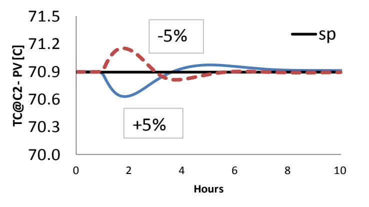
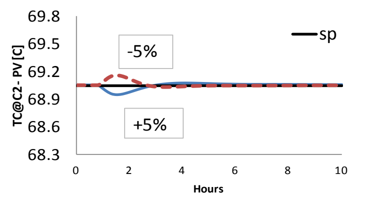
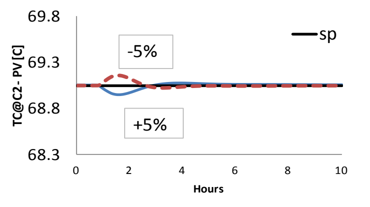
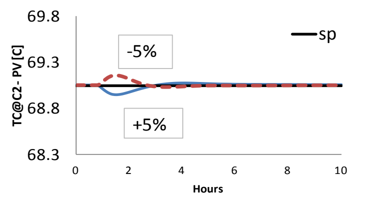
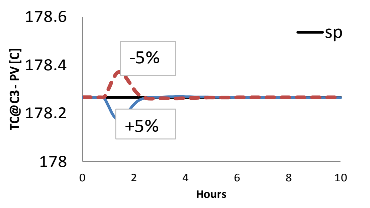
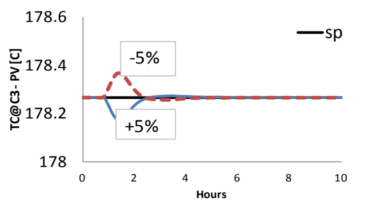
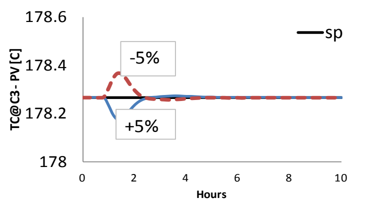
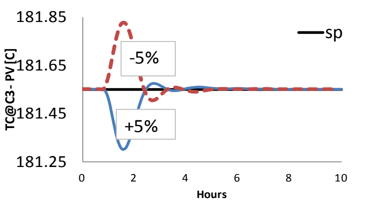
	BC	CS1	CS2	CS3
a.TC@CSTR				
b.TC@C1				
c.TC@C2				
d.TC@C3				

Table 5.9 (Continue) Dynamic responses with total methyl acetate change

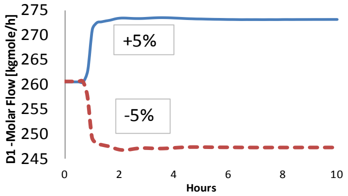
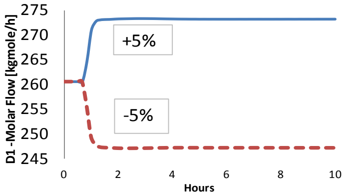
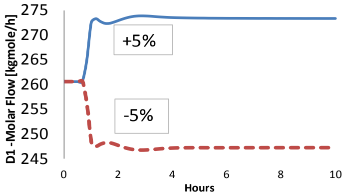
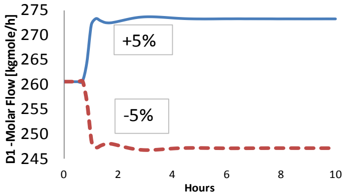
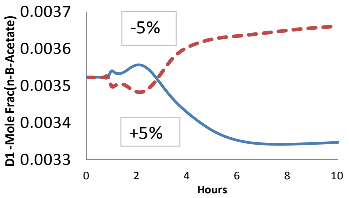
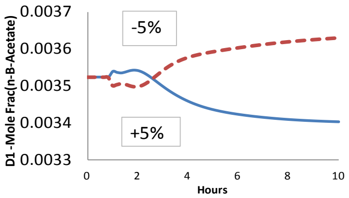
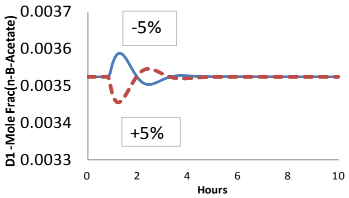
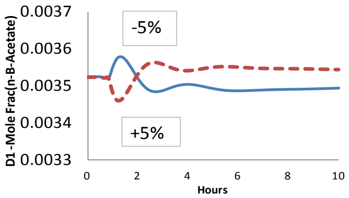
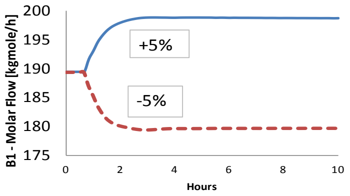
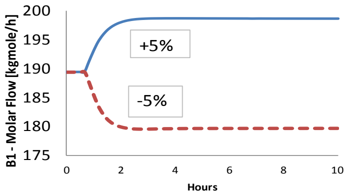
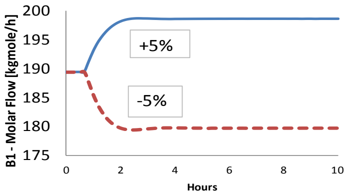
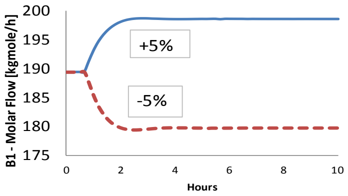
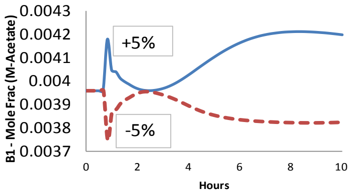
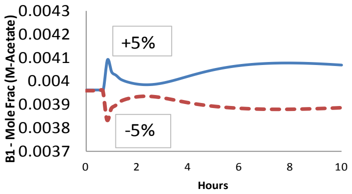
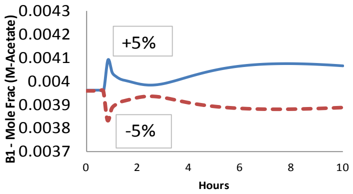
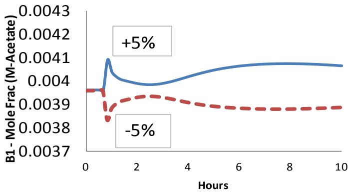
	BC	CS1	CS2	CS3
e.D1 Molar flow				
f.D1 BuAc mole fraction				
g.B1 Molar flow				
h.B1Methyl acetate mole fraction				

Table 5.9 (Continue) Dynamic responses with total methyl acetate change

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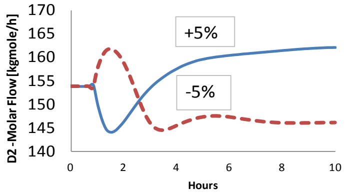
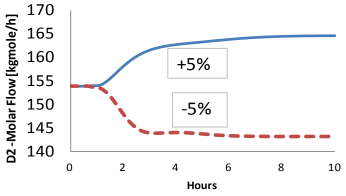
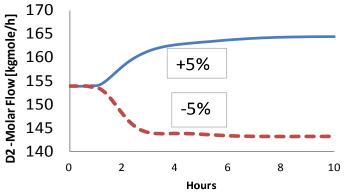
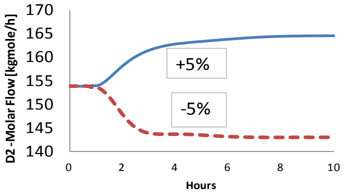
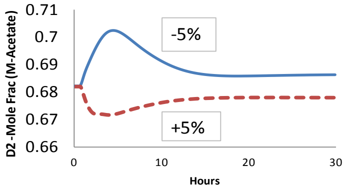
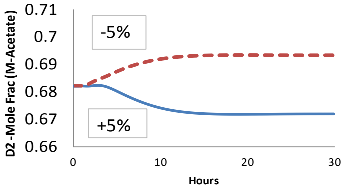
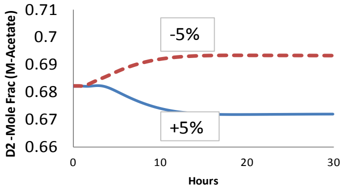
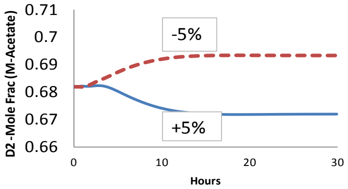
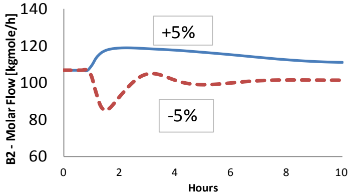
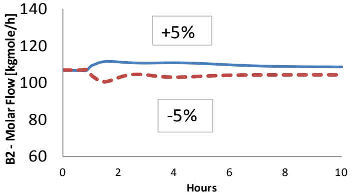
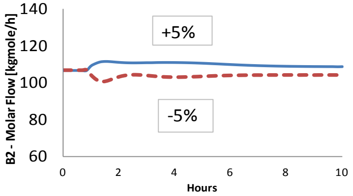
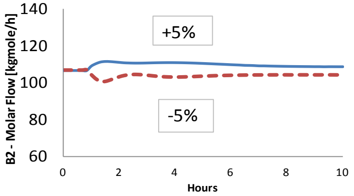
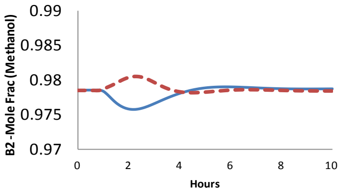
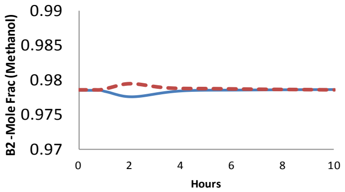
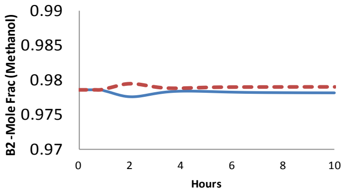
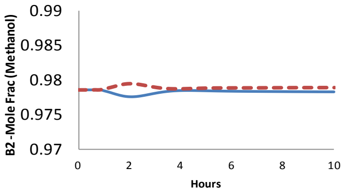
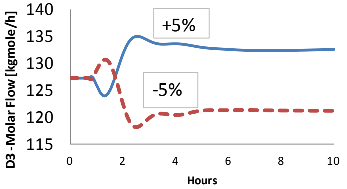
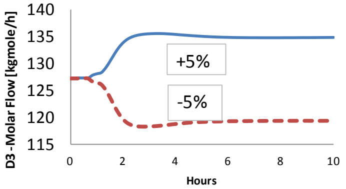
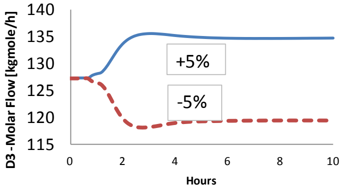
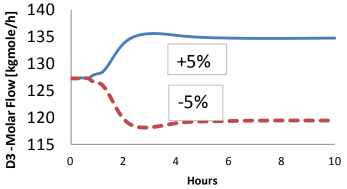
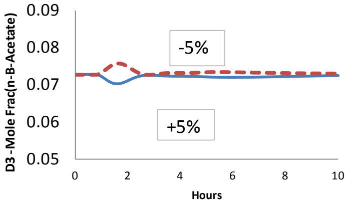
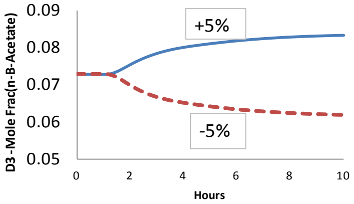
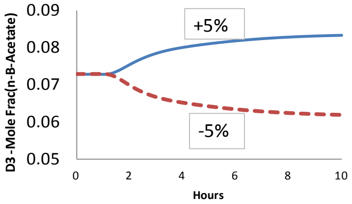
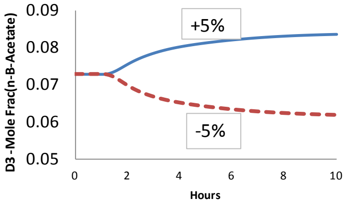
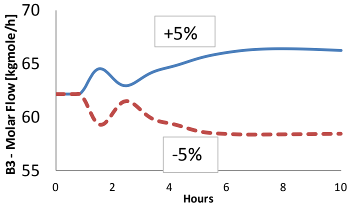
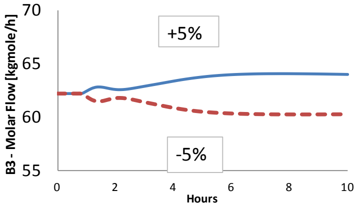
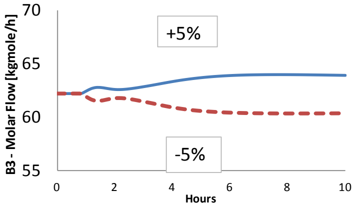
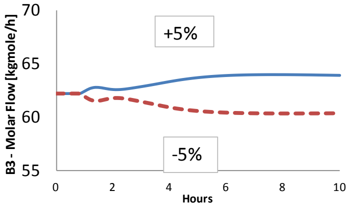
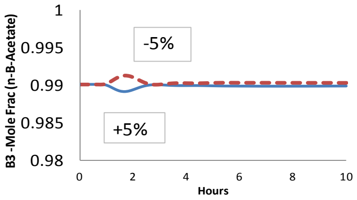
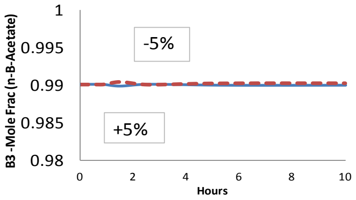
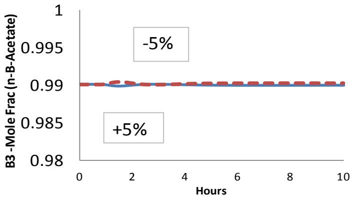
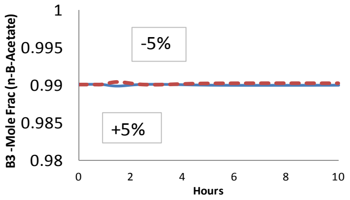
i.D2 Molar flow				
j.D2 MeAc mole fraction				
k.B2 Molar flow				
l.B2Methanol mole fraction				

Table 5.9 (Continue) Dynamic responses with total methyl acetate change

	BC	CS1	CS2	CS3
m.D3 Molar flow				
n.D3 BuAc mole fraction				
o.B3 Molar flow				
p.B3 BuAc mole fraction				

2. Feed composition change

Composition of feed is changed by increasing composition of methyl acetate from 0.6 to 0.66 and decreasing methyl acetate composition from 0.6 to 0.54.

Table 5.10 shows responses of variable disturbed by feed composition changing. Reactor temperature controller can control temperature in all of control structures. In base case control structure, the temperature deviation of reactor is larger than design control structures because in case of design control structures use PID controller.

Deviations of column C1, C2 and C3 tray temperature and time used for return to the set point in design control structures are smaller than base case because controlling tray temperature in design control structures use PID controller effecting smaller deviation.

Changing of feed composition has no effect on column C1 distillate and bottom flow rate. However, it affects purity of distillate flow. In case of base case and CS1 change of impurity are similar. In case CS2 butyl acetate impurity is controlled and CS3 butyl acetate impurity depends on top temperature controlled. Methyl acetate impurity in bottom flow direct variation with methyl acetate composition changed.

Distillate flow rate of column C2 change depends on methyl acetate composition changed. When methyl acetate composition increases methyl acetate purity of the distillate decreases which is affected by reflux ratio changed. Change of methyl acetate composition reverse variation with methanol composition therefore bottom flow rate which is methanol product flow reverse variation with methyl acetate composition changed. Methanol product purity in case CS3 is closest to specification because of controlling of top tray temperature in column C1.

Distillate stream of column C3 is butanol rich distillate. Butanol decreases because it is used for converts to product in reactor. In bottom flow is butyl acetate product which direct variation with reactance changed. In all of control structure can maintain product purity.

Table 5.10 Dynamic responses with feed composition change

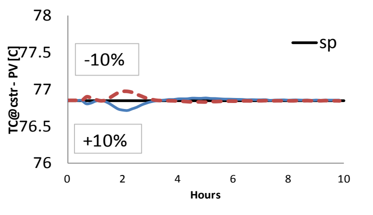
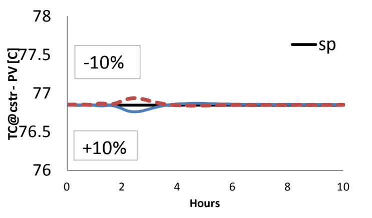
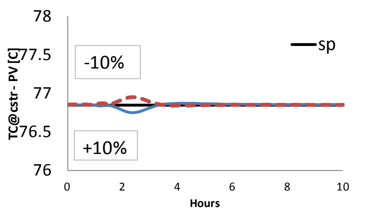
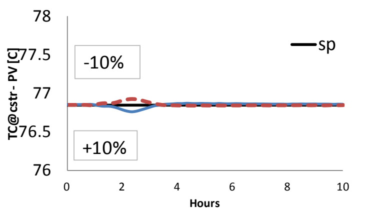
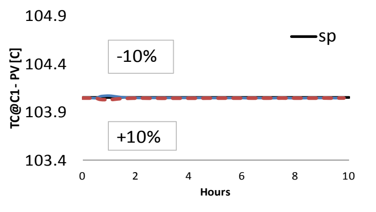
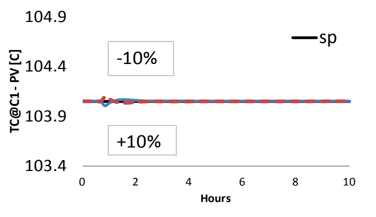
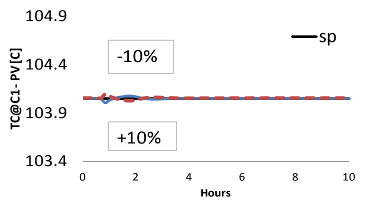
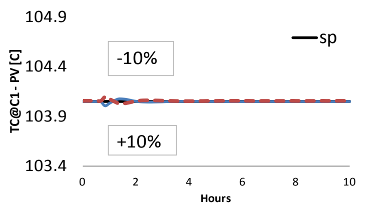
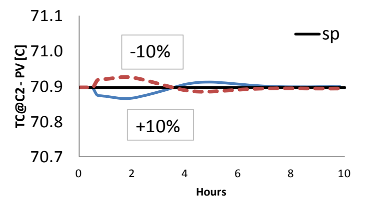
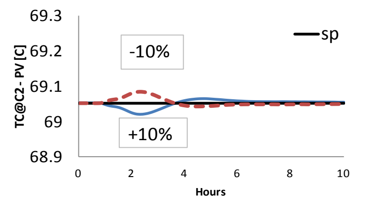
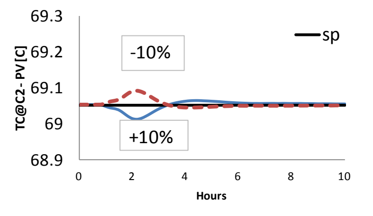
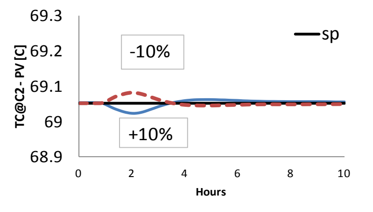
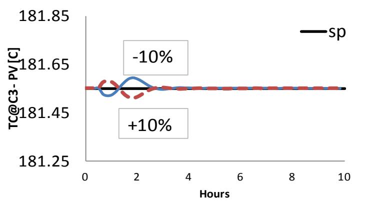
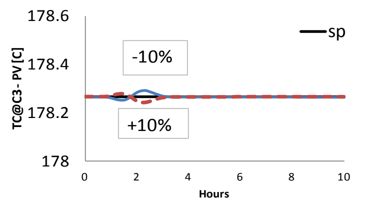
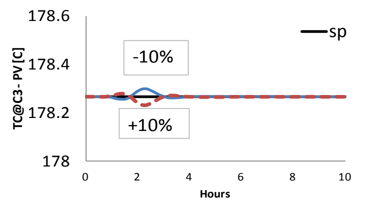
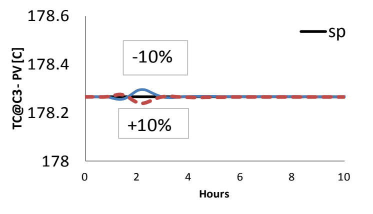
	BC	CS1	CS2	CS3
a.TC@CSTR				
b.TC@C1				
c.TC@C2				
d.TC@C3				

Table 5.10 (Continue) Dynamic responses with feed composition change

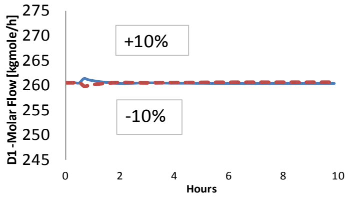
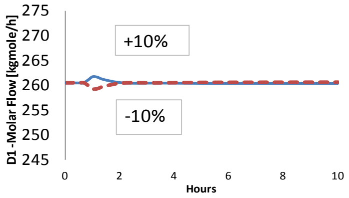
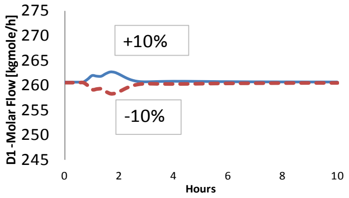
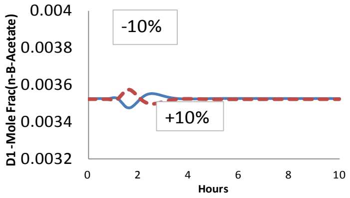
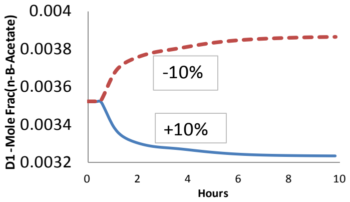
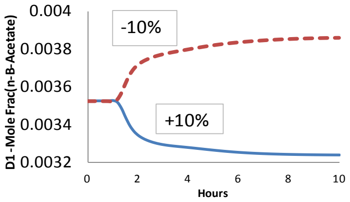
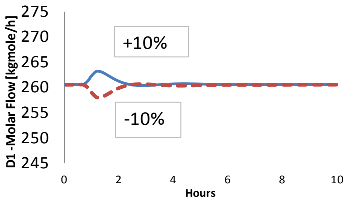
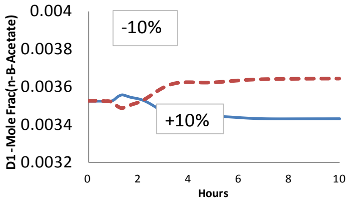
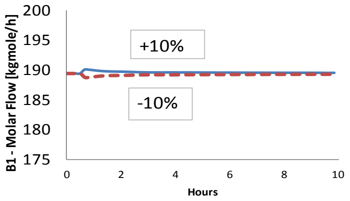
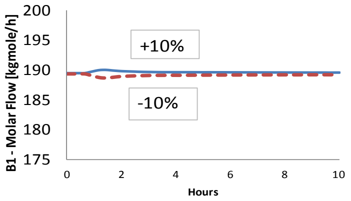
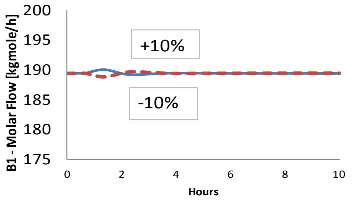
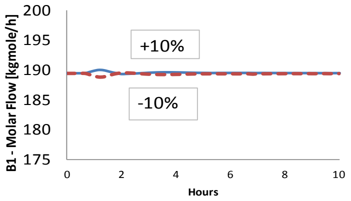
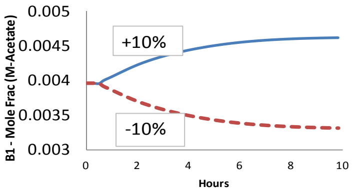
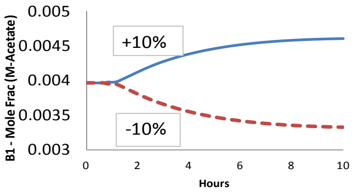
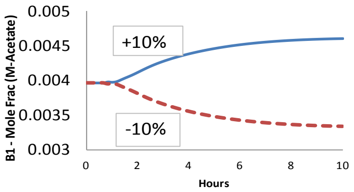
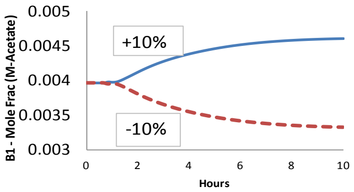
	BC	CS1	CS2	CS3
e.D1 Molar flow				
f.D1 Butyl acetate mole fraction				
g.B1 Molar flow				
h.B1Methyl acetate mole fraction				

Table 5.10 (Continue) Dynamic responses with feed composition change

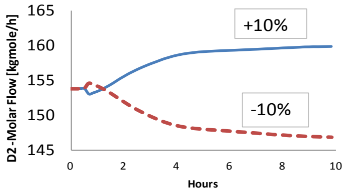
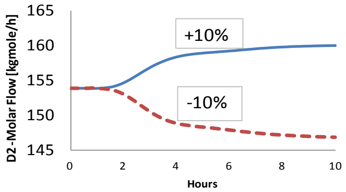
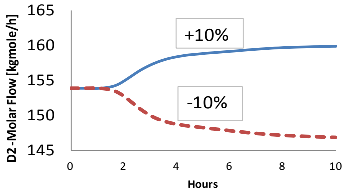
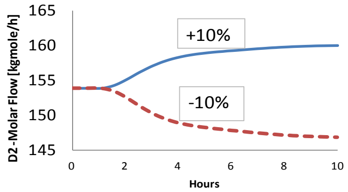
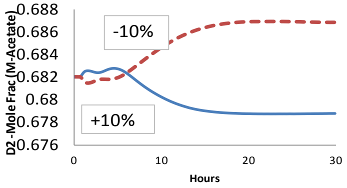
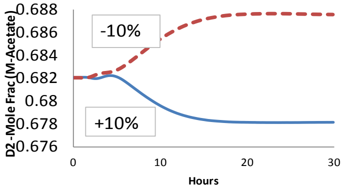
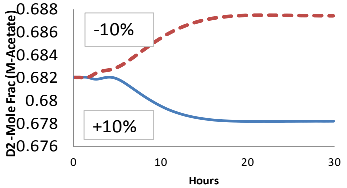
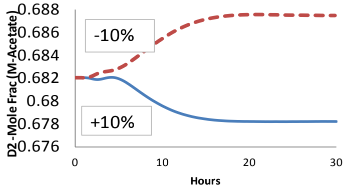
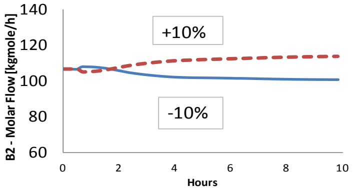
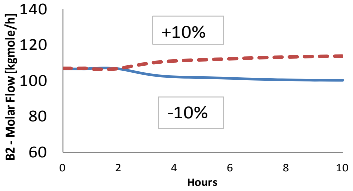
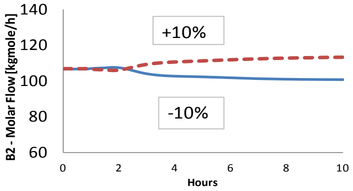
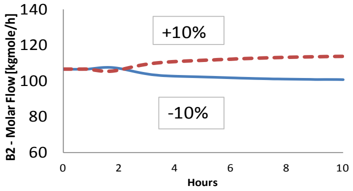
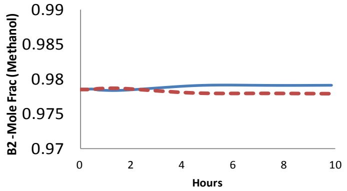
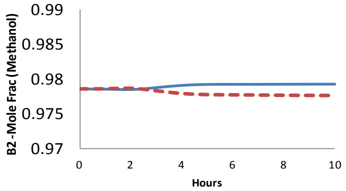
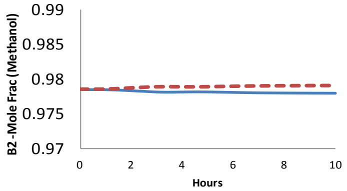
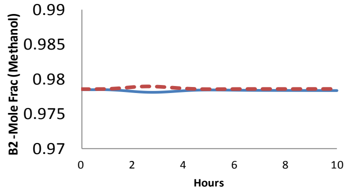
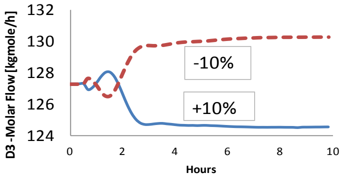
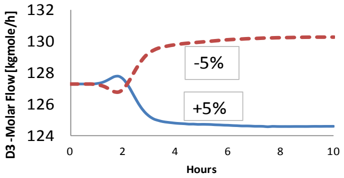
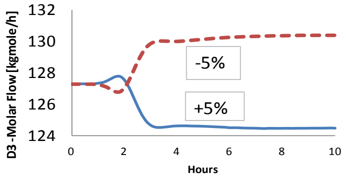
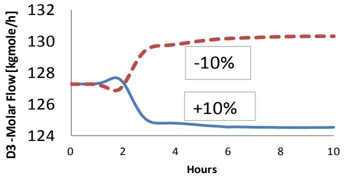
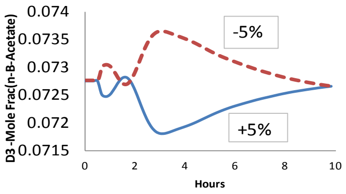
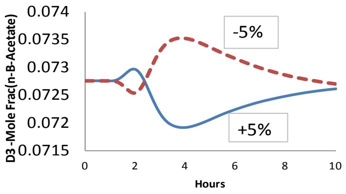
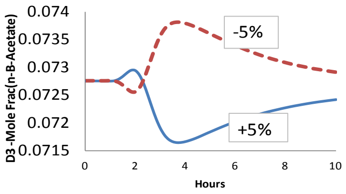
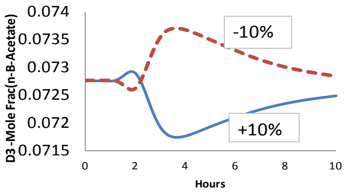
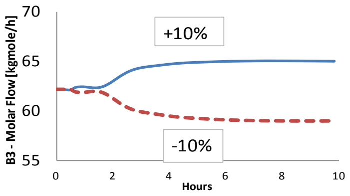
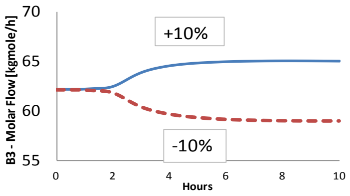
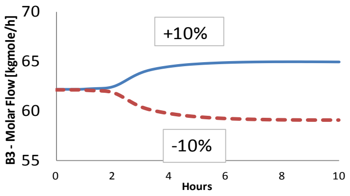
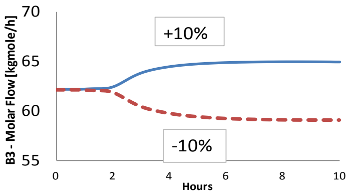
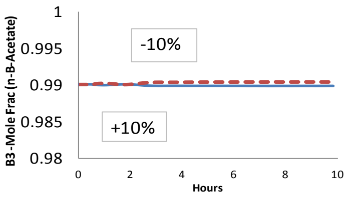
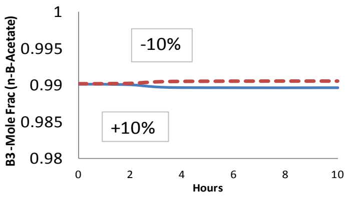
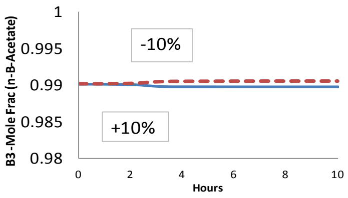
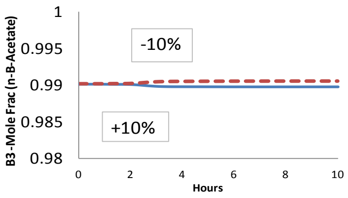
	BC	CS1	CS2	CS3
i.D2 Molar flow				
j.D2 Methyl acetate mole fraction				
k.B2 Molar flow				
l.B2Methanol mole fraction				

Table 5.10 (Continue) Dynamic responses with feed composition change

	BC	CS1	CS2	CS3
m.D3 Molar flow				
n.D3 Butyl acetate mole fraction				
o.B3 Molar flow				
p.B3 Butyl acetate mole fraction				

3. Feed temperature change

Temperature of feed is changed by increasing feed temperature from 65.85°C to 75.86 °C and decreasing tmeperature from 65.85 °C to 55.85 °C.

Table 5.11 shows responses of variable disturbed by feed temperature changing. Reactor temperaturecontroller can control temperature in all of control structures. In base case control structure, the temperature deviation of reactor is larger than design control structures because in case of design control structures use PID controller.

Deviations of column C1, C2 and C3 tray temperature and time used for return to the set point in design control structures are smaller than base case because controlling tray temperature in design control structures use PID controller effecting smaller deviation.

Temperature change has no effect on bottom flows. Distillate flows are affected in the first period because of temperature deviation of each column.

Table 5.11 Dynamic responses with feed temperature change

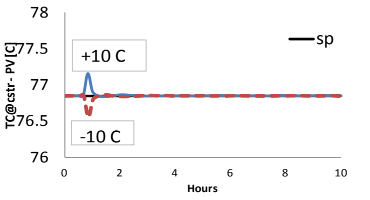
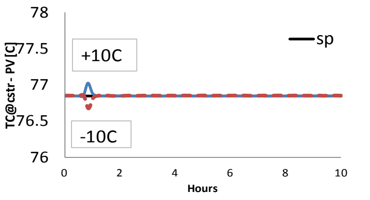
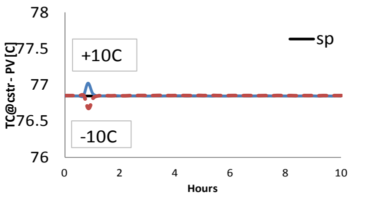
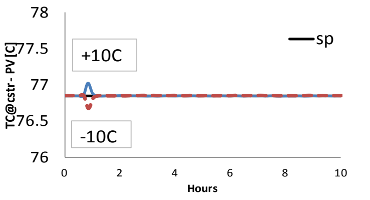
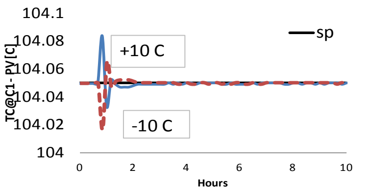
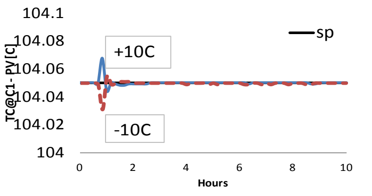
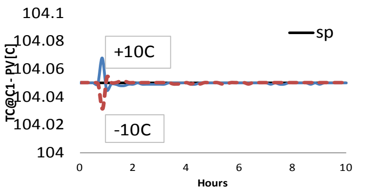
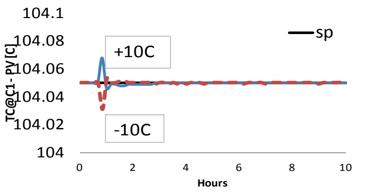
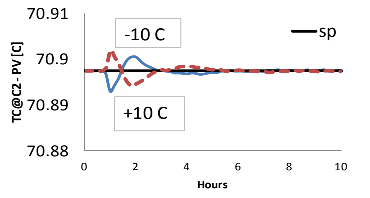
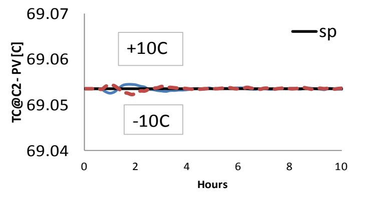
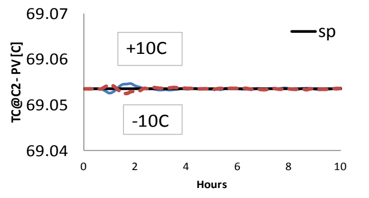
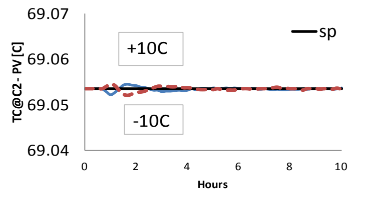
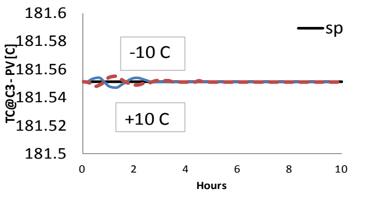
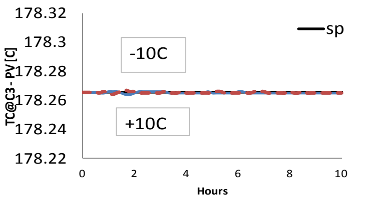
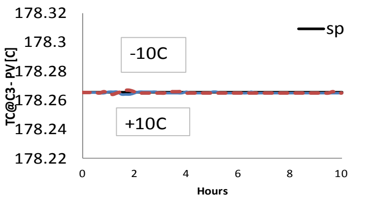
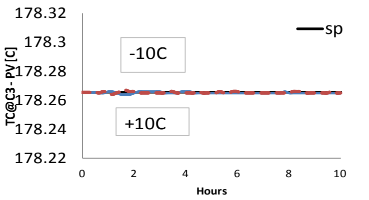
	BC	CS1	CS2	CS3
a.TC@CSTR				
b.TC@C1				
c.TC@C2				
d.TC@C3				

Table 5.11 (Continue) Dynamic responses with feed temperature change

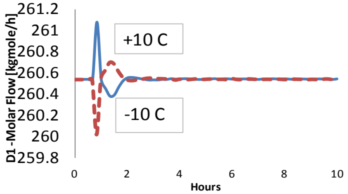
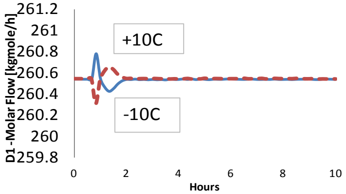
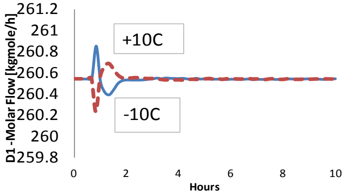
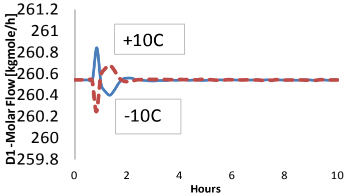
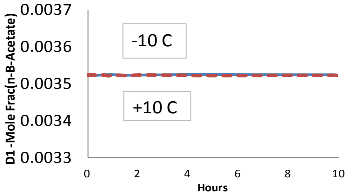
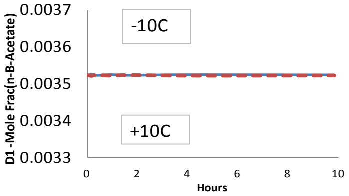
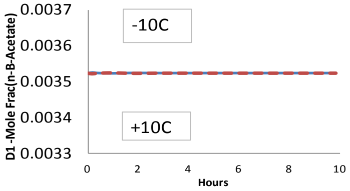
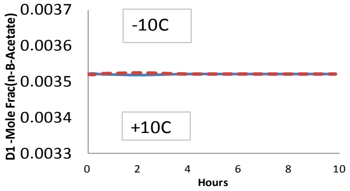
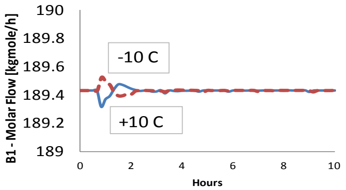
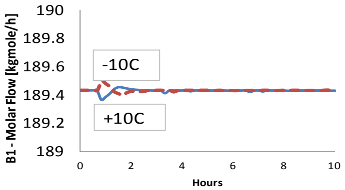
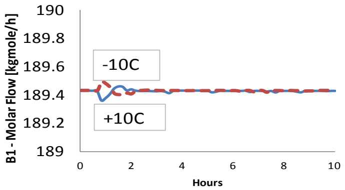
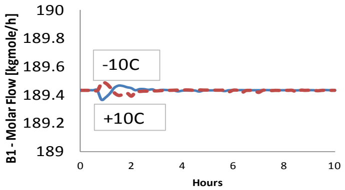
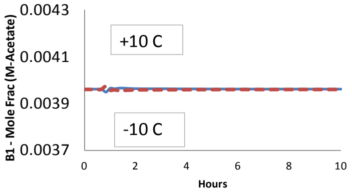
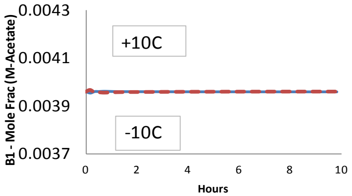
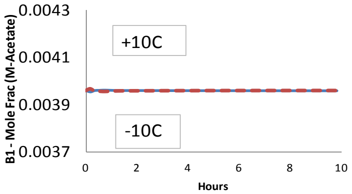
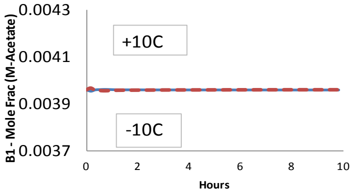
	BC	CS1	CS2	CS3
e.D1 Molar flow				
f.D1 Butyl acetate mole fraction				
g.B1 Molar flow				
h.B1Methyl acetate mole fraction				

Table 5.11 (Continue) Dynamic responses with feed temperature change

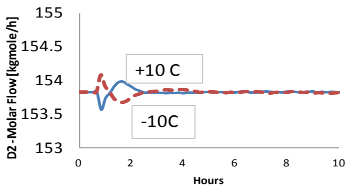
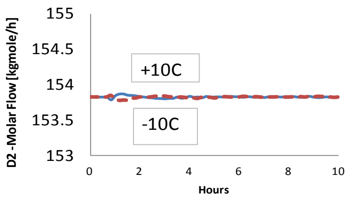
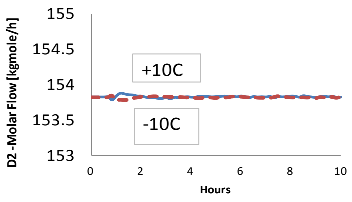
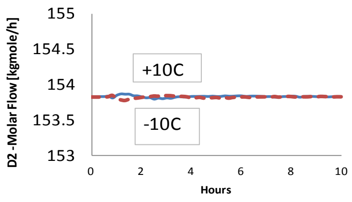
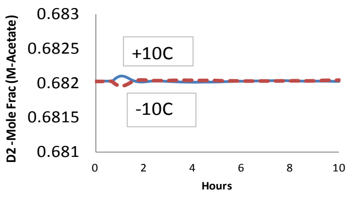
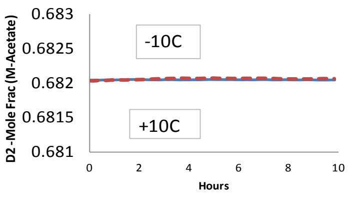
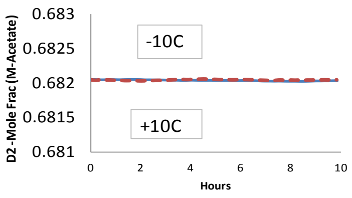
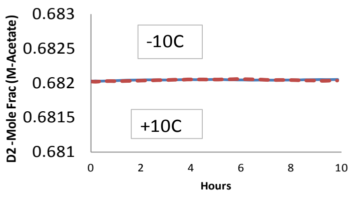
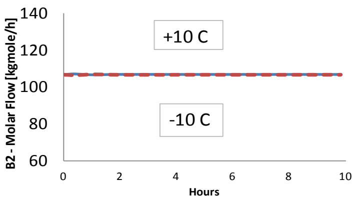
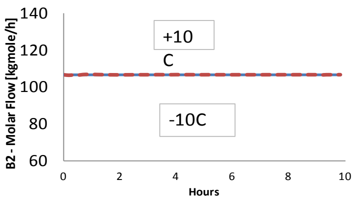
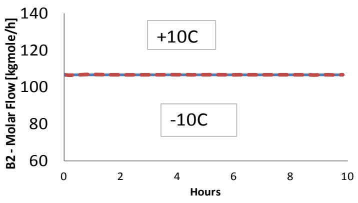
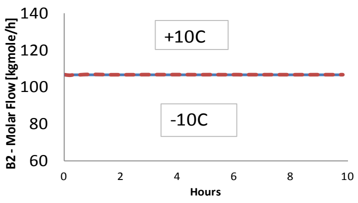
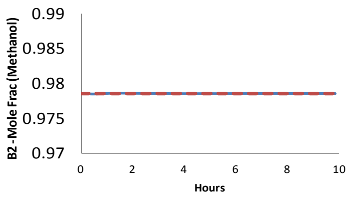
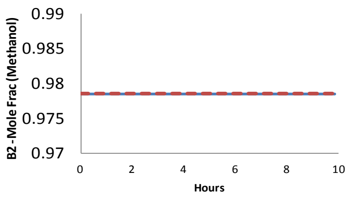
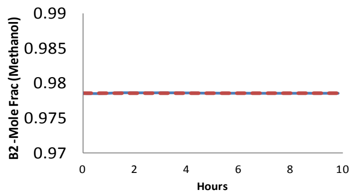
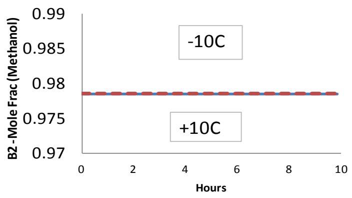
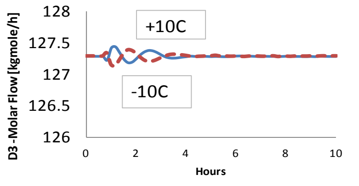
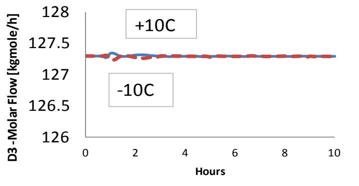
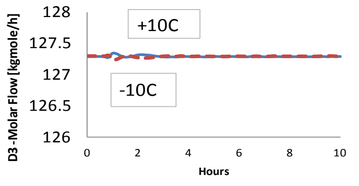
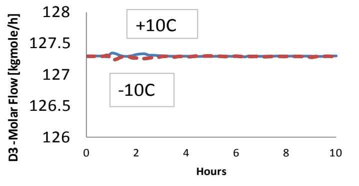
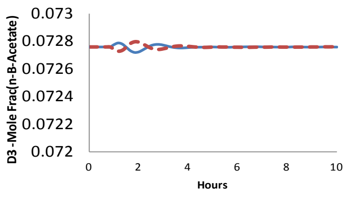
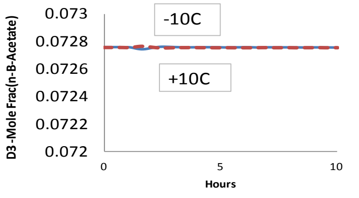
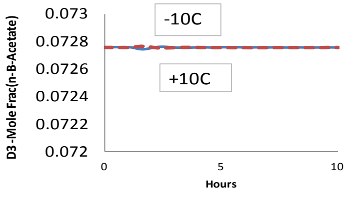
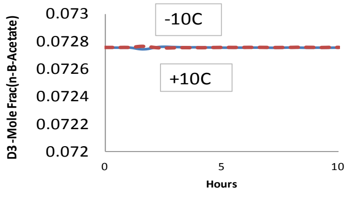
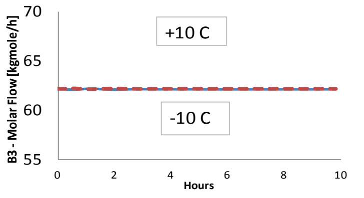
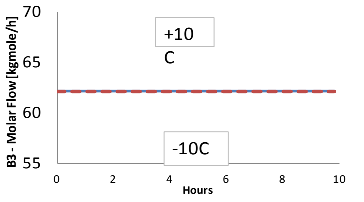
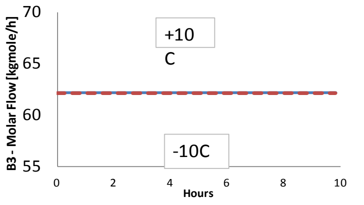
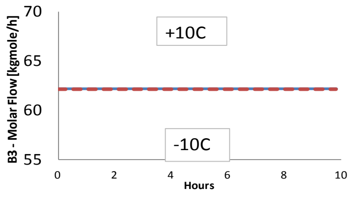
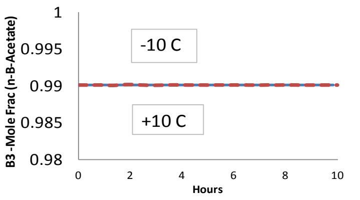
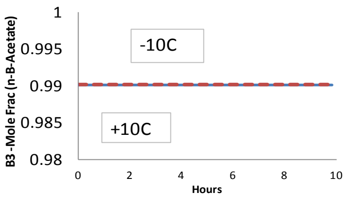
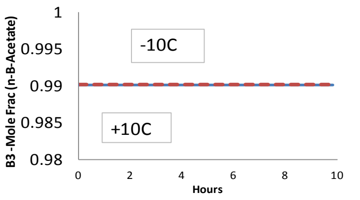
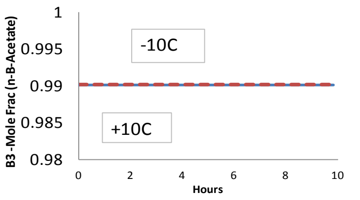
	BC	CS1	CS2	CS3
i.D2 Molar flow				
j.D2 Methyl acetate mole fraction				
k.B2 Molar flow				
l.B2Methanol mole fraction				

Table 5.11 (Continue) Dynamic responses with feed temperature change

	BC	CS1	CS2	CS3
m.D3 Molar flow				
n.D3 Butyl acetate mole fraction				
o.B3 Molar flow				
p.B3 Butyl acetate mole fraction				

5.2 Evaluation of the Dynamic Performance.

The dynamic performance index is focused on time related characteristics of the controller's response to setpoint changes or deterministic disturbances. There exist several candidate performance measures such as settling time and integral absolute error (IAE). Integral absolute error is well known and widely used. For the formulation of a dynamic performance as written below:

$$\text{IAE} = \int | e\,(t)\, | dt \qquad (5.1)$$

Note that $e(t) = y_{sp}(t) — y(t)$ is the deviation (error) of the response from the desired setpoint.

In this research, IAE method is used to evaluate the dynamic performance of the base case control structure and designed control structures. In the process, have many types of variables (temperature, pressure, and molar flow rate) so to compare it we must divide by span (the largest expected change in disturbance) of each variable. The IAE results consider in handle disturbances and maintain product qualityare used to evaluate the dynamic performance of the base case control structure and designed control structures. Control loops which are considered are safety loop.

Table 5.12 IAE of safety control loop with total feed change.

Controller	**Integral Absolute Error (IAE)**			
	BC	CS1	CS2	CS3
TC@CSTR	0.0192	0.0061	0.0060	0.0059
TC@C1	0.0036	0.0023	0.0025	0.0024
TC@C2	0.0159	0.0051	0.0050	0.0050
TC@C3	0.0030	0.0010	0.0011	0.0011
PC@C1	0.0017	0.0017	0.0017	0.0017
PC@C2	0.0008	0.0005	0.0005	0.0005
PC@C3	0.0001	0.0000	0.0000	0.0000
SUM	0.0442	0.0166	0.0166	0.0165

Table 5.13 IAE of safety control loop with feed composition change.

Controller	**Integral Absolute Error (IAE)**			
	BC	CS1	CS2	CS3
TC@CSTR	0.0060	0.0042	0.0045	0.0040
TC@C1	0.0006	0.0004	0.0007	0.0006
TC@C2	0.0030	0.0023	0.0023	0.0022
TC@C3	0.0007	0.0003	0.0004	0.0004
PC@C1	0.0017	0.0017	0.0017	0.0017
PC@C2	0.0003	0.0002	0.0002	0.0002
PC@C3	0.0000	0.0000	0.0000	0.0000
SUM	0.0122	0.0092	0.0097	0.0090

Table 5.14 IAE of safety control loop with feed temperature change.

Controller	**Integral Absolute Error (IAE)**			
	BC	CS1	CS2	CS3
TC@CSTR	0.0030	0.0019	0.0019	0.0019
TC@C1	0.0002	0.0001	0.0001	0.0001
TC@C2	0.0002	0.0002	0.0002	0.0002
TC@C3	0.0002	0.0000	0.0000	0.0000
PC@C1	0.0017	0.0017	0.0016	0.0017
PC@C2	0.0001	0.0001	0.0001	0.0001
PC@C3	0.0000	0.0000	0.0000	0.0000
SUM	0.0054	0.0040	0.0040	0.0040

From the IAE result the minimum IAE value is the value of case CS3.The smallest IAE of case CS3 shows the good controlling of the product purities and the good operation.

5.3 Utilities cost

Utilities costs are calculated from the duties used in cooling and heating and the works used in pumps and compressors. The cost of cooling water used in the process is $0.354/GJ. Price of $7.78/GJ for low pressure stream (column C1and C2) and $ 9.83/GJ for high pressure stream (column C3). The electric cost is $16.8/GJ.

Table 5.15 Utilities cost with methyl acetate total flow change

	BC	**CS1**	**CS2**	**CS3**
Low pressure stream ($/hr)	22.960	22.950	22.950	22.950
High pressure stream($/hr)	13.470	13.490	13.490	13.490
Work ($/hr)	0.021	0.021	0.021	0.021
Cooling water ($/hr)	35.100	35.150	35.150	35.150
Utilities cost ($/hr)	71.556	71.611	71.610	71.610

Table 5.16 Utilities cost with feed composition change

	BC	**CS1**	**CS2**	**CS3**
Low pressure stream ($/hr)	22.956	22.955	22.955	22.955
High pressure stream($/hr)	13.495	13.496	13.496	13.496
Work ($/hr)	0.0214	0.0214	0.0214	0.0214
Cooling water ($/hr)	34.880	34.879	34.884	34.882
Utilities cost ($/hr)	71.353	71.352	71.358	71.356

Table 5.17 Utilities cost with feed temperature change

	BC	**CS1**	**CS2**	**CS3**
Low pressure stream ($/hr)	22.961	22.961	22.961	22.961
High pressure stream($/hr)	13.493	13.493	13.493	13.493
Work ($/hr)	0.0214	0.0214	0.0214	0.0214
Cooling water ($/hr)	34.780	34.787	34.787	34.785
Utilities cost ($/hr)	71.256	71.264	71.263	71.261

From the utilities cost the minimum utilities cost is the value of case CS3.The smallest IAE of case CS3 shows the good controlling of the product purities and the good operation.

CHAPTER VI

CONCLUTIONS AND RECOMMENDATIONS

6.1 Conclusion

At dynamic simulation, this work has discussed control structure design for butyl acetate process, using new design procedure of Wongsri (2012). This procedure based on heuristics analysis. The precedence of control variables is established. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple, and straightforward.

The best control structure should handle disturbances entering the process and maintain product quality. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the material disturbances and the thermal disturbances.

For all disturbances, designed control structure III (CS3) is the best structure to handle disturbances.

New design procedure of Wongsri (2012) can find the appropriate set of controlled variables to achieve. The best control configurations depend on the direction of controlled variable with manipulated variable. Therefore this research establishes that the Wongsri's procedure, which combines heuristics, and dynamic simulation, a useful design procedure that leads to a good-performance plantwide control system.

6.2 Recommendation

Study and design the control structure of the other process in plantwide control via new design procedure of Wongsri's (2012).

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APPENDICES

APPENDIX A

EQUIPMENT DATA AND STREAM INFORMATION

Table A.1 Equipment data

Units operation	Properties	Size
Reactor	Height (m)	1.50
	Diameter (m)	2.25
Reflux drum column C1	Length (m)	2.1
	Diameter (m)	1.4
Reflux drum column C2	Length (m)	2.62
	Diameter (m)	1.74
Reflux drum column C3	Length (m)	2.88
	Diameter (m)	1.92
Reboiler column C1	Length (m)	3
	Diameter (m)	2
Reboiler column C2	Length (m)	2.34
	Diameter (m)	1.56
Reboiler column C3	Length (m)	3.6
	Diameter (m)	2.44

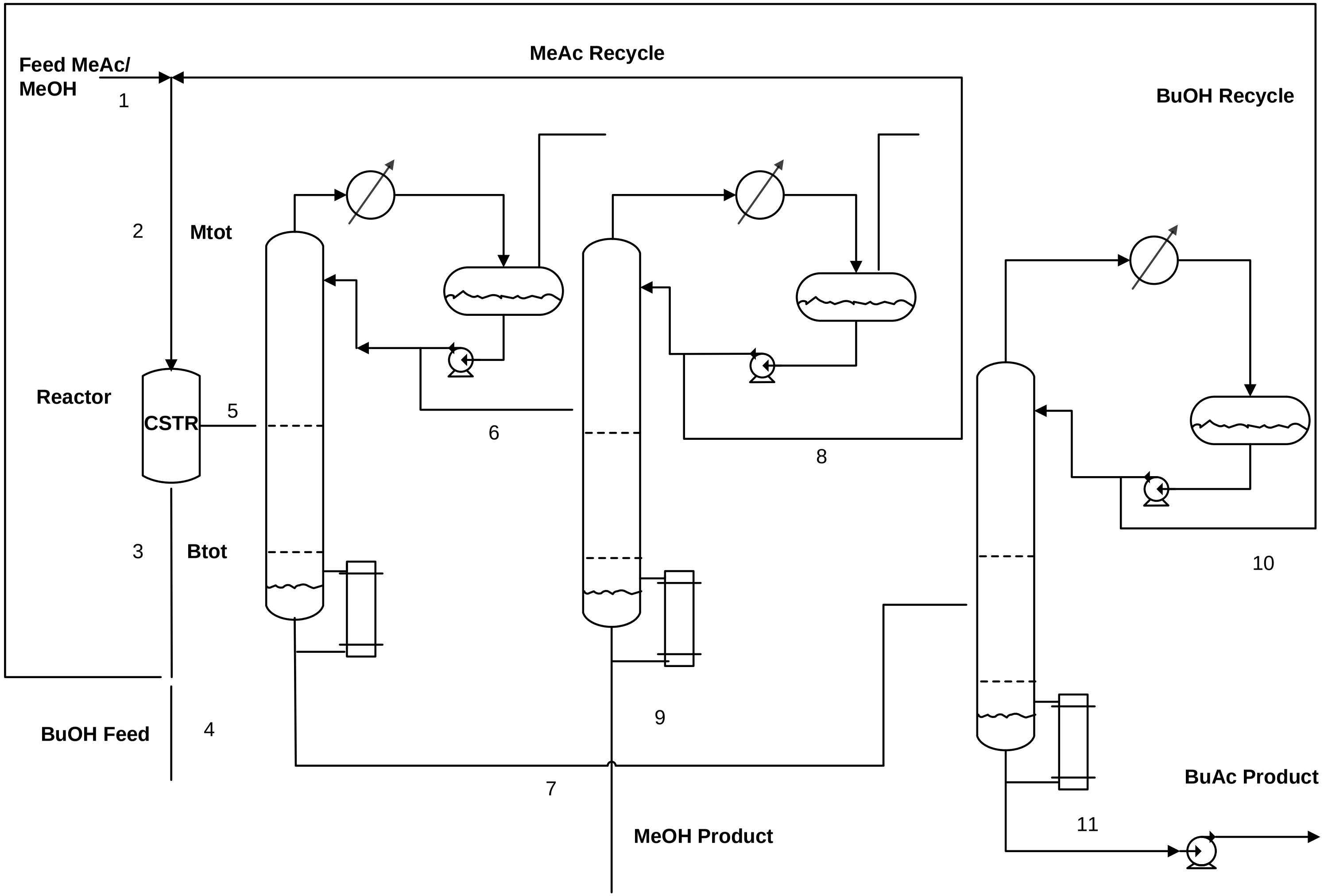

Figure A.1 Process flow sheet

Table A 2 Stream information

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
Flow(kgmole/hr)	107.47	261.30	190.75	63.46	452	260.5	189.4	153.8	106.7	127.3	62.14
Temperature (°C)	65.85	34.93	118.3	31.85	76.85	43.31	125.9	12.67	72.58	160.48	184.81
Pressure (atm)	6	5	5	6	5	1.2	1.4	1.1	1.2	4	4.3
Mole fraction											
Methyl acetate	0.6	0.65	0.004	0	0.237	0.407	0.004	0.683	0.010	0.006	0
Methanol	0.4	0.35	0.021	0	0.349	0.588	0.021	0.317	0.979	0.031	0
Butanol	0	0	0.927	1	0.254	0.001	0.601	0	0.003	0.890	0.010
Butyl acetate	0	0	0.049	0	0.160	0.004	0.374	0	0.009	0.073	0.990

APPENDIX B

TUNNING 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	τ_i
MeAc/MeOH feed	FCM	Total flow rate	Feed flow rate	PI	Reverse	261kgmole/hr	131-392	0.457	0.0346
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	0.73	95-286	0.3	0.026
CSTR reactor	TC	Temperature	Reactor duty	PI	Direct	76.85 ^oC	38-115	1.9	5.13
	LC	Liquid level	Effluence flow rate	P	Direct	1.12 m	0-2.25	2	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	1.2 atm	0.6-1.8	23.2	0.936
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	0.271	34-102	0.085	0.036
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.7 m	0-1.4	2	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1 m	0-3	2	-
	TC	Temperature tray 36	Reboiler duty	PI	Reverse	104 ^oC	52-156	3.5	13.4
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	1.1 atm	0.55-1.65	13.7	1.86
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.85 m	0-1.74	2	-
	LC	Reboiler level	Bottom flow rate	P	Direct	0.6 m	0-1.56	2	-
	TC	Temperature tray 25	Reboiler duty	PI	Reverse	70.9 ^oC	35-106	2.94	15.1
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	4 atm	2-6	24.4	0.267
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	1.8	160-478	0.087	0.036
	LC	Reflux drum level	Distillate flow rate	P	Direct	1.02 m	0-1.92	2	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.25 m	0-2.44	2	-
	TC	Temperature tray 41	Reboiler duty	PI	Reverse	181.6 ^oC	91-272	5.44	13.9

Table B.2 Type of controllers and tuning parameters of CS1

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	261kgmole/hr	131-392	0.457	0.0346	-
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	0.73	95-286	0.3	0.026	-
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	76.85 °C	38-115	2.76	5.13	0.37
	LC	Liquid level	Effluence flow rate	P	Direct	1.12 m	0-2.25	2	-	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	1.2 atm	0.6-1.8	23.2	0.936	-
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	0.271	34-102	0.085	0.036	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.7 m	0-1.4	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1 m	0-3	2	-	-
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	104 °C	52-156	5.1	13.4	0.967
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	1.1 atm	0.55-1.65	13.7	1.86	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.85 m	0-1.74	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	0.6 m	0-1.56	2	-	-
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	69.05 °C	34-103	3.6	13.5	0.974
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	4 atm	2-6	24.4	0.267	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	1.02 m	0-1.92	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.25 m	0-2.44	2	-	-
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	178.3 °C	89-267	6.6	15.3	1.104

Table B.3 Type of controllers and tuning parameters of CS2

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	261kgmole/hr	131-392	0.457	0.0346	-
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	0.73	95-286	0.3	0.026	-
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	76.85 °C	38-115	2.76	5.13	0.37
	LC	Liquid level	Effluence flow rate	P	Direct	1.12 m	0-2.25	2	-	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	1.2 atm	0.6-1.8	23.2	0.936	-
	CC	Butyl acetate composition	Reflux flow rate	PID	Direct	0.003504	0-0.007	18	0.7	0.05
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.7 m	0-1.4	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1 m	0-3	2	-	-
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	104 °C	52-156	5.1	13.4	0.967
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	1.1 atm	0.55-1.65	13.7	1.86	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.85 m	0-1.74	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	0.6 m	0-1.56	2	-	-
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	69.05° C	34-103	3.6	13.5	0.974
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	4 atm	2-6	24.4	0.267	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	1.02 m	0-1.92	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.25 m	0-2.44	2	-	-
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	178.3 °C	89-267	6.6	15.3	1.104

Table B.4 Type of controllers and tuning parameters of CS3

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
MeAc/MeOH feed	FCM	Total feed flow rate	Feed flow rate	PI	Reverse	261kgmole/hr	131-392	0.457	0.0346	-
Butanol feed	FCB	B_{tot}/M_{tot}Ratio	Feed flow rate	PI	Reverse	0.73	95-286	0.3	0.026	-
CSTR reactor	TC	Temperature	Reactor duty	PID	Direct	76.85 °C	38-115	2.76	5.13	0.37
	LC	Liquid level	Effluence flow rate	P	Direct	1.12 m	0-2.25	2	-	-
Column C1	PC	Condenser pressure	Condenser duty	PI	Direct	1.2 atm	0.6-1.8	23.2	0.936	-
	TC	Temperature tray 8	Reflux flow rate	PID	Direct	78.25 °C	40-120	11.1	23.5	1.7
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.7 m	0-1.4	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1 m	0-3	2	-	-
	TC	Temperature tray 36	Reboiler duty	PID	Reverse	104 °C	52-156	5.1	13.4	0.967
Column C2	PC	Condenser pressure	Condenser duty	PI	Direct	1.1 atm	0.55-1.65	13.7	1.86	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.85 m	0-1.74	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	0.6 m	0-1.56	2	-	-
	TC	Temperature tray 23	Reboiler duty	PID	Reverse	69.05 °C	34-103	3.6	13.5	0.974
Column C3	PC	Condenser pressure	Condenser duty	PI	Direct	4 atm	2-6	24.4	0.267	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	1.02 m	0-1.92	2	-	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.25 m	0-2.44	2	-	-
	TC	Temperature tray 38	Reboiler duty	PID	Reverse	178.3 °C	89-267	6.6	15.3	1.104

VITAE

Mr.OrachaRattananipon was born in Nakhon Si Thammarat, Thailand on February 12, 1987. She received the Bachelor Degree of Science, field of Chemical Engineering from Thammasat University in 2009. After that she entered the Graduate School of Chulalongkorn University to pursue the Master of Engineering in Chemical Engineering and completed in 2011.