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PLANTWIDE CONTROL STRUCTURE DESIGN OF THE METHOXY-METHYL-HEPTANE PROCESS

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A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering
Department of Chemical Engineering
Faculty of Engineering
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กันทรากร กตเวทิตาธรรม : การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ของกระบวนการเมทอกซี-เมทิล-เฮปเทน. (PLANTWIDE CONTROL STRUCTURE DESIGN OF THE METHOXY-METHYL-HEPTANE PROCESS) อ. ที่ปรึกษาวิทยานิพนธ์หลัก: ผศ.ดร.มนตรี วงศ์ศรี, 136 หน้า.

วิทยานิพนธ์นี้เสนอการออกแบบโครงสร้างการควบคุมทั้งโรงงานสำหรับกระบวนการเมทอกซี-เมทิล-เฮปเทน โดยใช้วิธีการออกแบบของวงศ์ศรี วิธีการออกแบบนี้ประกอบด้วยแปดขั้นตอน โดยเน้นการออกแบบในระดับทั้งโรงงานซึ่งทำให้โรงงานมีสภาวะการทำงานนิ่ง และการจัดการกับสิ่งรบกวนชนิดความร้อนและมวลสารเพื่อการควบคุมคุณภาพ โดย 2-เมทอกซี-2-เมทิลเฮปเทนเกิดจากปฏิกิริยาระหว่างเมทานอล กับ 2-เมทิล-1-เฮปทีน โดยกระบวนการนี้ประกอบด้วยเครื่องปฏิกรณ์แบบถังกวนต่อเนื่องหนึ่งเครื่อง หอกลั่นสามหอ และสายรีไซเคิลหนึ่งสาย สายรวมของสายป้อนกับสายรีไซเคิลของ 2-เมทิล-1-เฮปทีน ถูกควบคุมและเป็นอัตราส่วนกับสายเมทานอล สิ่งรบกวนชนิดมวลสารของ 2-เมทิล-1-เฮปทีน ถูกผลักให้ไหลออกทางด้านบนของหอกลั่นที่สองตามสายรีไซเคิล เพื่อรักษาความบริสุทธิ์ของ 2-เมทอกซี-2-เมทิลเฮปเทน ที่ออกจากหอกลั่นที่สาม สารทุกตัวถูกควบคุมตามตำแหน่งของตัวบ่งบอกปริมาณของสารนั้นๆ โครงสร้างการควบคุมทั้งโรงงานที่ออกแบบได้มีสมรรถนะเทียบได้กับการออกแบบของ Luyben

ภาควิชา วิศวกรรมเคมี ลายมือชื่อนิสิต
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KANTARAKORN KATAWETITATHUM: PLANTWIDE CONTROL STRUCTURE DESIGN OF THE METHOXY-METHYL-HEPTANE PROCESS. ADVISOR: ASST. PROF. MONTREE WONGSRI, D.Sc., 136 pp.

The design of plantwide control structure for the methoxy-methyl-heptane process using Wongsri's design procedure is studied. The eight steps of the design procedure focus on plantwide level design which is establishing a fixture plant and thermal and material disturbance managements for quality control. The process involves the reaction of methanol with 2-methyl-1-heptene to form 2-methoxy-2-methylheptane. The flowsheet features a continuous stirred tank reactor, three distillation columns, and one recycle stream. The combined feed of fresh and recycled 2-methyl-1-heptene is regulated and is ratioed to the fresh methanol. 2-methyl-1-heptene disturbance is pushed away via the distillate of the second column and recycled to maintain 2-methoxy-2-methylheptane purity in the third column. All components are handled at their identified quantifiers. The designed plantwide control structure performance is compared with the Luyben's design.

Department : Chemical Engineering Student's Signature
Field of Study : Chemical Engineering Advisor's Signature
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CHAPTER I

INTRODUCTION

1.1 Importance and Reasons for Research

Most of chemical processes consist of many units connected into a process. To ensure that those units in the processes are operated at the desired conditions, the process control systems are required to keep the chosen controlled variables at its desired set points by adjusting the manipulated variables. This is a primary objective of the process control. In addition, the control system must make the process operate safely and efficiently, while satisfy the environmental constraints.

In the past, all of the control loops were established individually for each unit in the plant. Then the units were combined together into an entire plant; therefore, any conflicts among the control loops somehow had to be reconciled (Luyben, Tyreus, & Luyben, 1997). Furthermore, the presence of material and energy recycles in the process leads to more interactions, and hence, the need for a perspective beyond the individual units. Thus, the better methodologies which can deal with the highly integrated processes in a more efficient way are necessary. This brings about the concept of plantwide control which demands plantwide perspective while designing plantwide control systems (Konda, Rangaiah, & Krishnaswamy, 2005).

During the period from the early 1990s, many plantwide control methodologies have been developed and applied to typical chemical processes. These methodologies can be classified based on the approach used to develop the plantwide control structure as heuristic-based, mathematics-based, optimization-based, and mixed approaches (Larsson & Skogestad, 2000; Konda, Rangaiah, & Krishnaswamy, 2003). One of the most popular heuristic based methods to date is that of Luyben et al. (1997). They proposed a comprehensive nine-step procedure that makes use of experience and basic process understanding for their effective usage. Then, Skogestad (2004) presented a systematic procedure which is a mathematical and optimization-based method. Though this method is rigorous, it is not easy to formulate and require extensive computations especially for complex chemical processes. As a result, the heuristic-based methods are still attractive as they are easier to understand and implement (Vasudevan, Rangaiah, Konda, & Tay, 2009). To improve heuristic-based methods, Konda et al. (2005) proposed an integrated framework of heuristics and simulation. Though this procedure has been successfully applied to several processes, their approach is still difficult to follow and not suitable for inexperienced users. Hence, to overcome this disadvantage, in 2009, Wongsri presented the eight-step procedure which is uncomplicated and straightforward.

So far, the Wongsri's design procedure has been successfully applied to several processes and also improved continuously. However, there is still a need to test its applicability to other complex industrial processes. With this motivation, the need arises to choose a suitable process that is complex and integrated to make it a suitable test-bed for the application of this procedure. As mentioned earlier, one process that has received little attention in the past is the 2-methoxy-2-methylheptane (MMH) plant.

Luyben (2010a) presented a plantwide control structure for the MMH plant that is capable of effectively handling large disturbances in production rate and operating parameters. However, in order to test the applicability of the Wongsri's design procedure (2012) and to develop the base case control structure for comparison, plantwide control structures design of the MMH process using Wongsri's design procedure (2012) is considered in this research.

1.2 Research Objective

To design the plantwide control structures for the 2-methoxy-2-methylheptane process using Wongsri's design procedure (2012).

1.3 Scopes of Research

1. The information about the flowsheet, the economics, the reaction kinetics and the design production rate of the 2-methoxy-2-methylheptane process is given by Luyben (2010a).
2. Wongsri's design procedure (2012) is applied to the 2-methoxy-2-methylheptane process in order to obtain the new control structures.
3. HYSYS process simulation software is used to achieve steady-state and dynamic simulation models for the 2-methoxy-2-methylheptane process.
4. The new design control structures are compared with the work proposed by Luyben (2010a).

1.4 Contributions of Research

1. Steady state and dynamic models of the 2-methoxy-2-methylheptane process by HYSYS process simulation software.
2. The new plantwide control structures for the 2-methoxy-2-methylheptane process by Wongsri's design procedure (2012).
3. Evaluation of the new plantwide control structures.

1.5 Research Procedures

1. Study the plantwide process control theory, the 2-methoxy-2-methylheptane process, the relevant information, including HYSYS tutorial and manual.
2. Simulate the steady state and dynamic of the 2-methoxy-2-methylheptane process according to the work proposed by Luyben (2010a).
3. Study the Wongsri's design procedure (2012).
4. Design the new control structures.
5. Simulate the dynamic of the designed control structures.
6. Evaluate the dynamic performance of all control structures.
7. Analyze the simulation results.
8. Conclude the thesis.

1.6 Research Framework

This thesis is divided into six chapters as follows:

Chapter I: Provide an introduction, objective, scopes, contributions and research outline.

Chapter II: Present some relevant literature about the previous works on plantwide control and the 2-methoxy-2-methylheptane.

Chapter III: Background information of Luyben's plantwide control theory and plantwide control structure design procedure of Wongsri (2012).

Chapter IV: Description of the 2-methoxy-2-methylheptane process via HYSYS process simulation software.

Chapter V: Description of step-by-step application of Wongsri's design procedure (2012), dynamic simulation results and comparison of the designed control structures with that proposed by Luyben (2010a).

Chapter VI: Conclusion of this research and recommendations.

CHAPTER II

LITERATURE REVIEW

Many works and researches in the fields of process control and process design have contributed essential ideas and concepts for developing the plantwide process design procedure. This chapter presents some relevant literature about the previous works on plantwide control and MMH process.

2.1 Previous Works on Plantwide Control

Luyben (1994) presented a mathematical analysis of the snowball effect in three kinetic systems: a simple binary first-order reaction $A \rightarrow B$, consecutive first-order reactions $A \rightarrow B \rightarrow C$, and a second-order reaction $A+B \rightarrow C$, and showed analytically that why his control structure can prevent snowballing and why the conventional structure leads to severe snowballing. Numerical results confirm that the snowball problems can be prevented using a plantwide control structure that places a flow controller somewhere in a liquid recycle loop. That is to say, in processes with one recycle, the flow rate of reactor effluent can be set, and in processes with two or more recycle streams, the flow rate of each recycle can be fixed.

Luyben (1996) illustrated the calculation of the design degrees of freedom and the control degrees of freedom, including the number of design optimization variables, for a number of complex processes with 11 case studies, and also illustrated that the number of design and control degrees of freedom are equal. Conceptually, the determination of the design degrees of freedom is more difficult than the control degrees of freedom, especially in the complex industrial processes. Therefore, the design degrees of freedom can be determined from the control degrees of freedom owing to their equivalence. In addition, he showed the effects of various types of flowsheets and physical properties, and found that the complexity of the phase equilibrium and the physical properties does not affect the degrees of freedom at all.

Luyben et al. (1997) presented the nine basic steps of a general heuristic design procedure which generates an effective plantwide control structure for processes involving reaction and separation sections. They outlined each step in general terms and summarized their justification for the sequence of steps. The method was illustrated in applications to three industrial process examples: the vinyl acetate monomer process, the Eastman process, and the HDA process. The procedure produces a workable plantwide control strategy for a given process design. Nonetheless, their approach is heuristic and experiential which need experience and basic process understanding for their effective usage, so in case of inexperienced users often face difficulties while adopting this method.

Larsson and Skogestad (2000) reviewed on the plantwide control with emphasis on the five tasks: selection of controlled variables, manipulated variables, measurements, control configuration and controller type, and ended up proposing the six steps of a plantwide design procedure which follows the mathematical and optimization-based approach. The procedure is divided into two main parts: top-down analysis and bottom-up design. The first two steps are top-down analysis that is used to obtain primary controlled (self-optimizing) variables, whereas the last four steps are bottom-up design that is used to determine secondary controlled variables and pairing the structure of control system.

Skogestad (2004) presented the eight steps of a systematic approach based on self-optimizing control for plantwide control of chemical plants, which is an expanded version of the plantwide control design procedure of Larsson and Skogestad (2000). The implementation of this procedure still consists of two main parts. The first four steps are top-down analysis that starts by formulating operational objectives and identifying the dynamic and steady-state (economic) degrees of freedom while the last four steps which are bottom-up design are still the same. This method is rigorous, but it is not easy to formulate and require extensive computations especially for complex chemical processes.

Konda et al. (2005) proposed an integrated framework of heuristics and simulation by addressing the limitations related to the nine-step heuristic procedure of Luyben et al. (1997). This improved heuristic method consists of eight levels. Each level improved heuristic methods, nonlinear steady-state and dynamic simulation models of the plant are used to take the decision or support the decision suggested by heuristics. They have successfully applied the procedure to the HDA process. Results show that a viable control system can be generated which synergizes the powers of both heuristics and simulation. The main advantage of this integrated framework of simulation and heuristics is that the use of nonlinear simulation tools such as HYSYS makes it easier to apply the more difficult heuristics. However, their approach is still difficult to follow and not suitable for inexperienced users.

Araujo and Skogestad (2008) discussed the application of the plantwide design procedure of Skogestad (2004) to the ammonia synthesis process. They started with a top-down analysis and followed by the bottom-up design. The final control structures resulted in good dynamic performance. Though this method is rigorous and has already been successfully applied to the ammonia synthesis process, it is the mathematical and optimization-based method that is not easy to formulate and require extensive computations especially for complex chemical processes. In addition, the solution might be affected by the model assumptions and details.

Detjareansri (2009) presented the plantwide control structures for alkylation process using Wongsri's design procedure (2009). The designed control structures are evaluated the dynamic performance and compared with control structure of Luyben by two types of disturbances: material and thermal disturbances. She designed eight plantwide control structures. All the designed control structures have a good performance because it can handle disturbances entering the process and maintain product quality as compared by integral absolute error (IAE) and total energy use low.

Sophonudomsub (2012) presented the plantwide control structures of ammonia production process using Wongsri's design procedure (2012). Two new control structures obtained (CS1 and CS2) are evaluated and compared with the control structure of Araujo and Skogestad (2008). The disturbances used in the evaluation are gas feed flowrate, feed temperature, and methane composition in feed changes. The new control structure, CS2, resulted in good dynamic performance for the feed flowrate and feed temperature changes. For methane composition in feed change, all control structures give comparable good performances.

Thongkam (2012) presented the plantwide control structures of acetone process via dehydrogenation of 2-propanol using Wongsri's design procedure (2012). Four new control structures obtained (CS1 through CS4) are evaluated the dynamic performance and compared with control structure of Luyben by two types of disturbances: material (flowrate and composition) and thermal disturbances. The results show that the designed control structures, the CS1 and CS3 are able to handle the material and thermal disturbances nearby the control structure of Luyben and the CS3 is the best designed control structure. The Wongsri's procedure is a useful, uncomplicated and heuristic-based method that can be followed easily and is suitable for beginners

2.2 Previous Works on the MMH Process

Griffin et al. (2009) studied the effect of competing reversible reactions on the optimum operating policies for plants with recycle and presented etherification chemistry of the MMH process as a case study, in order to illustrate the shift in operating policy that is driven by high and low values of the equilibrium constant. The chemistry involves two competing reactions, one producing the desired product and the second producing undesired products. Their paper provided the reaction kinetics and the desired production rate, including sketchy information about the process flow diagram and the economics. Nevertheless, control issues were not explored by these authors.

Luyben (2010a) studied on the MMH process by using the information given in Griffin et al. (2009) as the basis for his study. Due to the fact that the cost of the 2-methyl-1-heptene (MH) raw material and the values of the products are quite uncertain, the approach is adopted to design the process for a specified yield of MMH. For a given yield, there are optimum values of reactor size and recycle flow rate that minimize total annual cost. Lastly, he explored the economics and the dynamics of this process. As well as a reasonable conceptual design presented, a plantwide control structure is also developed that is capable of effectively handling large disturbances in production rate and operating parameters. However, many alternative configurations of columns or other plantwide control structures exist that are not studied in this paper.

Luyben (2010b) proposed a simple heuristic approach to determine economic optimum designs of chemical process with reaction and separation sections. The minimum recycle flow rate is determined by using very large reactors. After that, the actual recycle flow rate is set at 1.1 to 1.2 times the minimum, depending on the cost of catalyst, the relative volatilities, and the complexity of the separation section. He tested the economic optimum design of the MMH process presented in Luyben (2010a) on this heuristic. Result shows that the correct optimum-to-minimum recycle ratio in the MMH process is 1.08, which satisfies the proposed heuristic method.

CHAPTER III
THEORIES

3.1 Introduction

One of the biggest challenges to the successful development of a chemical process is finding an effective plantwide control structure. All of the units in a process must “dance together” in a stable harmonious manner. Small ripples in the reaction section should not be transmitted into the separation section, and vice versa. Anyway, the goals for an effective plantwide process control system include (1) safe and smooth process operation; (2) tight control of product quality in the face of disturbances; (3) avoidance of unsafe process conditions; (4) a control system run in automatic, not manual, requiring minimal operator attention; (5) rapid rate and product quality transitions; and (6) zero unexpected environmental releases.

The development of a plantwide control structure is not a trivial task. Typical processes can have many variables that must be controlled and many valves that must be driven by some control signal. Single-input–single-output proportional-integral controllers are widely used in industry. A process may have 30 to 50 loops to configure (select controlled/manipulated variable pairings and controller tuning constants). With 30 loops there are 30-factorial possible combinations of the variables. So an exhaustive enumeration of all possible pairings is untenable. Common sense, experience, and process control wisdom can reduce the possible pairings to a manageable number with dynamic performance that can be evaluated using dynamic simulation (Luyben, 2011).

In an industrial environment, a plant's control strategy should be simple enough, at least conceptually, so that everyone from the operator to the plant manager can understand how it works. The more complex the process, the more desirable it is to have a simple control strategy. This view differs radically from much of the current academic thinking about process control, which suggests that a complex process demands complex control. The first law of plantwide control is that it is easy to find a control structure that will not work! There are several alternative plantwide control structures that do work. The best structure depends on the control objectives of the plant, which in turn depend on the business objectives of the company. For example, if the product from the plant is to be provided to a downstream customer at whatever flowrate the customer desires at any point in time, an “on-demand” plantwide control structure must be developed. The inventory loops (liquid levels and pressures) would be set up to work their way backwards from the product leaving the process to the fresh feed streams coming into the process. Reaching a solution to the complex plantwide control problem is a creative challenge. It demands insight into and understanding of the chemistry, physics, and economics of real processes. However, it is possible to employ a systematic strategy (or engineering method) to get a feasible solution.

This chapter describes some basic concepts and features of the plantwide control problem and then outlines both the nine basic steps of a general heuristic design procedure (Luyben et al, 1997) and the new eight-step plantwide control structure design procedure of Wongsri.

3.2 Plantwide Control Fundamentals

The common topology consists of reaction sections and separation sections. Streams of fresh reactants enter the plant by being fed into the reaction section (or sometimes into the separation section) through a heat exchanger network. The reactor effluent usually contains a mixture of reactants and products. It is fed into a separation section where the products are separated by some means from the reactants. Due to their economic value, reactants are recycled back to upstream units toward the reactor. As well as recycle streams returned back to upstream units, thermal integration is also frequently done, Energy integration can link units together in locations anywhere in the flowsheet where the temperature levels permit heat transfer to occur. The reaction and separation sections are thus often intimately connected. If conditions are altered in the reaction section, the resulting changes in flowrates, compositions, and temperatures affect the separation section and vice versa.

3.2.1 Integrated processes

Three basic features of integrated chemical processes are necessary to be considered for control system of the entire plant: (1) the effect of material recycle, (2) the effect of energy integration, and (3) the need to account for chemical component inventories. If we did not have to worry about these issues, then we 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.

3.2.1.1 Material recycle

Material is recycled for six basic and important reasons.

1. *Increase conversion:*

For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints. Hence 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 like $A \longrightarrow B \longrightarrow C$, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much undesirable product C. As a result, the concentration of B is kept moderately low in the reactor and a large recycle of A is required.

4. *Provide thermal sink*:

In adiabatic reactors and in reactors where cooling is difficult and exothermic heat effects are large, it is often essential to feed excess material to the reactor so that the reactor temperature increase will not be too large. High temperature can cause several unpleasant events: it can bring about thermal runaways, it can deactivate catalysts, it can create 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 as to keep the concentration of the other reactant low. If this limiting reactant is not kept in low concentration, it could react to produce undesirable products. Thus the excess reactant must be separated from the product components in the reactor effluent stream and recycled back to the reactor.

6. Control properties:

In many polymerization reactors, conversion of monomer is limited 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.

3.2.1.2 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 cost. For energy-intensive processes, the savings can be quite significant.

3.2.1.3 Chemical component inventories

A plant's chemical species can be characterized into three types: reactants, products, and inerts. A material balance for each of these components must be satisfied. However, 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 via reaction or leave as an impurity or purge. On account of their value, we must ensure that every mole of reactant fed to the process is consumed by the reactions. This is an important concept and is generic to many chemical processes.

From the viewpoint of individual units, chemical component balancing is not a problem because exit streams from the unit automatically adjust their flows and compositions. However, when we connect units together with recycle streams, the entire system behaves almost like a pure integrator in terms of the reactants. If additional reactant is fed into the system without changing reactor conditions to consume the reactant, this component will build up gradually within the plant because it has no place to leave the system. Plants are not necessarily self-regulating in terms of reactants. We might expect that the reaction rate will increase as reactant composition increases. However, in systems with several reactants, increasing one reactant composition will decrease the other reactant composition with an uncertain net effect on reaction rate. Eventually the process will shut down when manipulated variable constraints are encountered in the separation section.

3.2.2 Units in series

If process units are arranged in a purely series configuration with no recycle of material or energy, the plantwide control problem is greatly simplified. That is, it can be effectively broken up into the control of each individual unit operation. 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 whereas 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 (flowrate changes to achieve different throughputs) and its upstream neighbor

3.2.3 Effects of recycle

Most real processes include recycle streams. In this case the plantwide control problem becomes much more complex and its solution is not intuitively obvious. The presence of recycle streams profoundly alters the plant's dynamic and steady-state behavior. There are 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. This has two manifestations, one steady state and one dynamic. Both effects have implications for the inventory control of components.

3.2.3.1 Time constants in recycle systems

One of the basic issues with recycle stream is that they can produce a drastic slowdown in the dynamic response of the entire integrated plant. That is, any change in a recycle process can take a long time to line out back to steady state. Distillation columns and reactors normally have transient responses that last for tens of minutes to several hours. Inserting a recycle stream can lengthen the transient response of the coupled process to days.

3.2.3.2 Snowball effects

The flowrates of recycle streams are often very sensitive to small disturbances. This is called the “snowball” effect. A small change in some variable, for instance fresh feed flowrate, can produce a very large change in the resulting flowrate of the recycle stream. Amplification factors of 3 are quite common, that is, a 10% change in feed flowrate results in a 30% change in recycle flowrate. It is important to note that this is not a dynamic effect; it is a steady-state phenomenon. But it does have dynamic implications for disturbance propagation and for inventory control. It has nothing to do with closed-loop stability. Nevertheless, this does not imply that it is independent of the plant's control structure. In contrast, the extent of the snowball effect is very strongly dependent upon the control structure used.

Snowballing occurs because the conditions in the reactor have to change to accommodate the disturbance. Increasing fresh feed 10% requires that reaction rates in the reactor must increase by 10%. If the volume and the temperature in the reactor are fixed, the only way a 10% increase in reaction rate can be attained is by significant changes in the compositions of reactants in the reactor. Higher reactant concentrations are needed, which means that the recycle of reactant must increase.

The large swings in recycle flowrates are undesirable in a plant because they can overload the capacity of the separation section or move the separation section into a flow region below its minimum turndown. Thus it is important to choose a plantwide control structure which avoids this effect. A simple practical way to prevent drastic changes in the loading of the separation section is to use a plantwide control structure that places a flow controller somewhere in a liquid recycle loop.

3.2.4 Management of fresh feed streams

A key feature of plantwide control structures is where and how the fresh feed streams are introduced into the process. Assuming that the separation section is doing its job of keeping the losses of reactants to negligible amounts, the reactant components that are fed into the process in the fresh feed streams must be completely consumed by the reactions occurring in the reaction section. If we attempt to feed into the process more than can be reacted, the system will fill up with excess reactant and shut down. So managing the fresh feeds is a critical issue that the control structure must effectively handle.

If the fresh feed is a gas, it may be fed into a circulating gas loop, perhaps on pressure control. The system pressure gives a good indication of whether or not the gaseous reactant is being consumed at the rate we are feeding it. Rising pressure says too much is being fed. Dropping pressure say too little is being fed. So the pressure controller will effectively handle the issue of feeding exactly enough gaseous reactant.

If the fresh feed is a liquid, it may be fed directly into the reaction section or it may be fed into the separation section at a location where the component tends to accumulate. Distillation column bases or reflux drums are common locations. The liquid level gives an indication of whether or not the liquid reactant is being consumed at the rate we are feeding it. Increasing liquid level says too much is being fed. Dropping liquid level says we need to feed in more.

The fresh feed management problem becomes more complex when there are several reactant components involved in the chemistry. Then an almost perfect stoichiometric balance among the reactants must be maintained.

3.2.5 Design and control degrees of freedom

One of the central problems in developing a steady-state process flowsheet is finding the number of variables that must be specified to completely define the process. This number is called the design degrees of freedom. They are easily calculated by simply subtracting the number of equations from the number of variables. However, for typically complex industrial processes, there are many hundreds of variables and equations, and it is not a trivial job to make sure that the correct variables and equations have been defined. Once the plant has been specified, the design of a control structure requires that the control degrees of freedom be known. This is the number of variables that can be controlled. It is very easy to calculate this number, even for quite complex processes, because it is equal to the number of manipulated variables (the number of control valves in the process). Certainly, it is vital that good engineering practices are followed in installing all control valves. For example, there should never be two control valves in series in a liquid-filled line.

The determination of the design degrees of freedom is more difficult than the control degrees of freedom, especially in the complex industrial processes. Luyben (1996) has illustrated that the number of design degrees of freedom is equal to the number of control degrees of freedom. Hence, the design degrees of freedom can be determined from the control degrees of freedom.

In satisfying the control degrees of freedom we use one to set production rate. All liquid levels (except in recycle systems) and all gas pressures must be controlled, so these controlled variables consume an equivalent number of degrees of freedom. Additional degrees of freedom are used to control product qualities and to satisfy safety, environmental, and regulatory constraints. Any remaining degrees of freedom can be used to achieve optimum operation (e.g., minimize energy consumption, maximize yield, etc.) or to improve dynamic performance (e.g., maintain purities in recycle streams, hold pressures or temperatures at intermediate locations in the flowsheet, etc.).

3.3 Plantwide Control Design Procedure

In this section the nine basic steps of a general heuristic plantwide control design procedure (Luyben et al, 1997) are outlined in general terms. The procedure was developed after many years of work and research in the fields of process control and process design. Listed below are some of the fundamental concepts and techniques which form the basis of the procedure.

3.3.1 Basic concepts of plantwide control

3.3.1.1 Buckley basics

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

1. Material balance control
2. Production quality control

He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loops is established, using the flowrates of the liquid and gas process streams. The idea is to establish the inventory control system by setting up this "hydraulic" control structure as the first step. Note that most level controllers should be proportional-only (P) to achieve flow smoothing. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated. He tries to make these as small as possible so that good, tight control is achieved, but stability constraints impose limitations on the achievable performance.

3.3.1.2 Douglas doctrines

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

1. Minimize losses of reactants and products.
2. Maximize flowrates through gas recycle systems.

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

3.3.1.3 Downs drill

Jim Downs (1992) has insightfully pointed out the importance of looking at the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. We must ensure that all components (reactants, products, and inerts) have a way to leave or be consumed within the process. Most of the problems occur in the consideration of reactants, especially when several chemical species are involved. Since we usually want to minimize raw material costs and maintain high-purity products, most of the reactants fed into the process must be chewed up in the reactions. And the stoichiometry must be satisfied down to the last molecule. Chemical plants often act as pure integrators in terms of reactants. Any imbalance in the number of moles of reactants involved in the reactions will lead to the process gradually filling up with the reactant component which is in excess.

3.3.1.4 Luyben laws

As a result of a number of case studies of many types of systems, three laws have been developed:

1. A stream somewhere in all recycle loops should be flow controlled so as to prevent the snowball effect.

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

3. If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995).

3.3.1.5 Richardson rule

Bob Richardson suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense since it provides more muscle to achieve the desired control objective. An analogy is that it is much easier to maneuver a large barge with a tugboat than with a life raft. The point is that the bigger the handle you have to affect a process, the better you can control it. This is why there are often fundamental conflicts between steady-state design and dynamic controllability.

3.3.1.6 Shinskey schemes

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

3.3.1.7 Tyreus tuning

The use of P-only controllers (usually the controller gain equal to 1.67) is strongly recommended for liquid levels whereas the use of PI controllers is suggested for other control loops. The relay-feedback test is a simple and fast way to obtain the ultimate gain (K_u) and ultimate period (P_u). Then either the Ziegler-Nichols settings or the Tyreus-Luyben (1992) settings can be used:

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

The use of PID controllers should be limited to those loops where two criteria are both satisfied: (1) the controlled variable should have a very large signal-to-noise ratio and (2) tight dynamic control is really essential from a feedback control stability perspective. The classical example of the latter is temperature control in an irreversible exothermic chemical reactor.

3.3.2 Steps of plantwide process control design procedure

The plantwide control design procedure satisfies the overall conservation of energy and mass. In addition, this procedure accounts for non-conserved entities within a plant such as chemical components (produced and consumed) and entropy (produced). Such procedure will generate a workable plantwide control strategy, which is not necessarily the best solution. Since the design problem is open-ended, the procedure will not produce a unique solution. In this section each step of the design procedure is discussed in detail.

Step 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.

Step 2: Determine control degrees of freedom

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

Step 3: Establish energy management system

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

Step 4: Set production rate

Establish the variables that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate. Often design constraints require that production be set at a certain point. An upstream process may establish the reactant feed flow sent to the plant. A downstream process may require on-demand production, which fixes the product flow rate from the plant. If no constraint applies, then the valve that provides smooth and stable production-rate transitions and rejects disturbances is selected. Often a variable that has the least effect on the separation section is selected, but also has a rapid and direct effect on reaction rate in the reactor without hitting an operational constraint. This may be the feed flow to the separation section, the flow rate of a recycle stream, the flow rate of initiator or catalyst to the reactor, the reactor heat removal rate, the reactor temperature, and so forth.

Throughput changes can only be achieved by altering, either directly or indirectly, conditions in the reactor. To obtain higher production rates, overall reaction rates must be increased. 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).

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

Select the “best” valves to control each of the product-quality, safety, and environmental variables. We want tight control of these important quantities for economic and operational reasons. Therefore we should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants and the latter prevents problems with the range ability of the manipulated variable (control valve saturation). In addition, the magnitudes of various flow rates also come into consideration according to Richardson rule.

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

Determine the valve to control each inventory variable. These variables include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit. Inventory may also be controlled with fresh reactant makeup streams. Liquid fresh feed streams may be added to a location where level reflects the amount of that component in the process. Gas fresh feed streams may be added to a location where pressure reflects the amount of that material in the process.

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 flows in the recycle loop are controlled by levels. For gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields.

Step 7: Check component balances

Identify how chemical components enter, leave, and are generated or consumed in the process. In this step, control loops are installed to prevent the accumulation of individual chemical species in the process. Without control, chemical species often build up, especially in material recycle loops.

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations. That is, the remaining degrees of freedom are assigned to ensure that adequate local control is provided in each process unit. For example, a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust fuel flow rate to a furnace supplying energy to the reactor. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

Step 9: Optimize economics or improve dynamic controllability

Establish the best way to use the remaining control degrees of freedom. That is to say, after satisfying all of the basic regulatory requirements, we usually have additional degrees of freedom involving control valves that have not been used and set points in some controllers that can be adjusted. These can be used either to optimize steady-state economic process performance or to improve dynamic response.

3.4 Wongsri's Design Procedure (2012)

The new plantwide control design procedure is heuristic-based and systematic. It emphasizes on maintaining the plant operating conditions, i.e. establishing a fixture plant. The amount of components is accounted by regulating the material quantifiers which are locations within the plant indicating the amount of the components. The material quantifier is a more general term than the material inventory, it includes flowrate. Additionally, the entered disturbance must be forced to leave the process plant at the nearest exits to avoid disturbance propagation through the plant. The plantwide control structure design is indeed a structural decision about placing control loops though out the plant to above objectives. It is divided into two levels: plant level and unit level designs. The procedure is carried out in eight steps. The major steps deal with plant level design. Step 1 gathers the process plant information and the control objective of the process plant. Step 2 analyzes the available degrees of freedom, heat and material pathways, and reaction and separation sections; locates the material quantifiers. Step 3 establishes the fixture plant to ensure that all chemical components are accounted for. Step 4 ensures the heat and material disturbances are rejected to environment, compensated within, or directed to the designated pathways. Step 5 is about unit level design, i.e. design the rest of the control loops using only unit level information. Step 6 conserves the thermal energy via the heat exchanger network. This step creates the heat integrated process design alternatives (HIPs). Step 7 optimize economics and/or improve control performance. Step 8 Validate the designed control structures by rigorous dynamic simulation.

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

Step 2: Plant analysis

2.1 Control degree of freedom (CDOF)

List manipulated variables (control degree of freedom, CDOF). The manipulated variables can be obtained using the guideline given in Table 3.1 and the guideline for pairing the controlled variables with the manipulated variables is presented in Table 3.2

Table 3.1 Degree of freedom for simple units

Unit	DOF / unit
Independent stream	1
Heater, cooler, pump, and compressor	1
Process-to-process heat exchanger with a by-pass stream	1
Adiabatic plug flow reactor	0
Non-adiabatic plug flow reactor	1
Adiabatic flash separator	2
Simple distillation column	5

2.2 Heat pathways

Three different "heat pathways" introduced in Luyben (1999) are also useful in plant analysis from a plantwide perspective. The first pathway is from inside the process and flows out to the environment heat generated by exothermic reactions and by degradation of mechanical work. A second pathway carries heat from utilities into the process and to the environment. The third pathway is internal to the process. The heat flow is circular and its magnitude depends upon the heating and cooling needs and the amount of heat integration implemented. The level of heat circulated of the third pathway can be adjusted to optimize the energy used (step 7). The heat pathway is used to design control loops to reject the disturbances or to maintain the product qualities. The fourth pathway is introduced here. This pathway is accounted for the enthalpies entered and leaved the plant via process stream.

Table 3.2 Guideline pairing of manipulated and controlled variables

No.	Guidelines
1	A control and manipulated variables must have strong causal relationship (high gain).
2	The manipulated variables should not be far from the control variables (zero or minimal dead time).
3	The time constant of the quality loops should be short and the time constant of the inventory loops should be last.
4	The manipulated variables should not be saturated for the whole range of the disturbances.
5	The manipulation of the manipulated variables should not have or have less effects on others variables (low gains with the remainder of the variables).

2.3 Material pathways

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

2.4 Material quantifiers

The notion of material quantifier is also introduced here. In order to regulate a component balance in a process plant, a place representing the amount of material in the plant must be identified to provide its handle. The features of material recycle and chemical component inventories mentioned above which have profound implications for a plant's control strategy (Luyben et al, 1997) can be handled quite readily by making use of quantifiers. By locating a quantifier, we can regulate the quantity of a component quantified by using its handle.

2.5 Reaction section

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

2.6 Separation section

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

Step 3: Establish fixture plant

The principal idea of establishing a fixture plant is to have an entire plant fluid-filled and a material-balanced. This idea is similar to creating hydraulic control structure proposed by Buckley. By establishing a fixture plant we mean creating a material-balanced process plant by control the components at their quantifiers or handles:

3.1 Keep the materials entered combined with reentered fixed

$$q_i(t) + q_r(t) = \text{constant} \tag{3.1}$$

This leaves the recycle streams free to adjust; one degree of freedom is added to the process. However, if the composition of the recycle stream differs from the fresh feed significantly, each stream should be flow-controlled separately:

$$q_i(t) = \text{constant} \tag{3.2}$$

$$q_r(t) = \text{constant} \tag{3.3}$$

In this settlement, the flow of the recycle cannot be used to regulate the inventory of its upstream unit, e.g., the level of the reflux drum or the column pressure.

3.2 Regulate the production rate

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

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

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

$$q_o(t) = -\frac{dq}{dt} \tag{3.4}$$

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

$$q_p(t) = -\frac{dq}{dt} \tag{3.5}$$

$$q_p(t) = \text{constant} \tag{3.6}$$

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

Step 4: Disturbance management

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

4.1 Heat disturbance management

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

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

4.1.2) Manage the thermal disturbance that related to quality in order to maintain the product specification constraints

4.2 Material disturbances

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

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

How to direct material disturbance? At a splitter (e.g. a distillation column), we must decide which paths to push extra loads or disturbances to. It is depend on how we want to manage the extra loads to keep the plant running smoothly and the quality of the products. For example, we don't want to push the extra loads to the product stream. It is always designable to reject the disturbance out of the process plant as soon as possible. Thirdly, we prefer to keep the recycle flow constant in the case that its composition differs significantly from the make-up feed. However if this is not allowed, we must trade-off between pushing the extra loads to the recycle stream and keeping it constant. Note that this material disturbance direction policy is applicable to light key and heavy key for a simple column. Providing side streams, we can manage the disturbance direction policy to non-key components.

Ratio Control on Feeds. Add ratio control to accommodate the variation of one of the fresh feed in the case that the two feeds must be proportional.

Single-end Control, Which End? Since the distillation columns, usually the one-point control is common. To control top or bottom temperatures, depend on the material disturbance rejection policy. The control policy of a distillation column is to reject or direct disturbances to the designated pathways. For example, a recycle distillate flow must be maintained. Product purity must be maintained.

Fixing Reflux flow, Reflux Ratio or Reflux to feed. To aid in making this choice, a series of dynamic simulation runs can be made in which the effects of changes in composition, temperature, total flow and component flow of distillation column feed.

Single-end or dual-end control. If there are two locations with large changes in the temperature profiles when the sensitivity test is performed (see Step 2.6), so it may be possible to use dual-temperature control if this structure is required.

Step 5: Design the rest of the control loops

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

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

Step 6: Energy management via heat exchanger networks

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

Step 7: Optimize economics and/or improve control performance. For example, the controls scheme/structure of the reactor (e.g. temperature/composition sensor location), the control scheme of the distillation column (e.g. reflux to feed ratio control), the optimal operating temperatures of the reactors, the recycle flow rates, the sequence of separation, etc. If the opportunity of optimization exists, we might backtrack to the previous step as dictated.

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

CHAPTER IV
METHOXY-METHYL-HEPTANE PROCESS

4.1 Introduction

The chemical 2-methoxy-2-methylheptane (MMH) is an ether with molecular formula $C_9H_{20}O$. It has been proposed as a great alternative gasoline additive to replace methyl tert-butyl ether (MTBE) in order to avoid groundwater contamination due to its higher molecular weight and the lower solubility in water. The production of MMH involves liquid phase reversible reaction of methanol (MeOH) with unsaturated compound 2-methoxy-2-methylheptene (MH). The molecular structures of these components are shown in Figure 4.1.

$$\begin{array}{ccccc} \mathrm{CH_3OH} & + & \mathrm{C_8H_{16}} & \leftrightarrow & \mathrm{C_9H_{20}O} \\ \mathrm{(MeOH)} & & \mathrm{(MH)} & & \mathrm{(MMH)} \end{array} \tag{4.1}$$

There is also an undesirable irreversible reaction of methanol and MH to form dimethyl ether (DME) and 2-methyl-2-heptanol (MHOH). Thus the system has two undesirable products.

$$\begin{array}{ccccccc} \mathrm{2CH_3OH} & + & \mathrm{C_8H_{16}} & \rightarrow & \mathrm{C_2H_6O} & + & \mathrm{C_8H_{18}O} \\ \mathrm{(MeOH)} & & \mathrm{(MH)} & & \mathrm{(DME)} & & \mathrm{(MHOH)} \end{array} \tag{4.2}$$

The overall reaction rates have units of kmol s^{-1} kg^{-1}. Concentrations are in terms of mole fractions.

$$\mathrm{R_1 = k_{1F}x_{MeOH}x_{MH} - k_{1R}x_{MMH}} \tag{4.3}$$

$$\mathrm{R_2 = k_2(x_{MeOH})^2} \tag{4.4}$$

Table 4.1 gives the kinetic parameters for these reactions on the basis of the information given in Griffin et al. (2009).

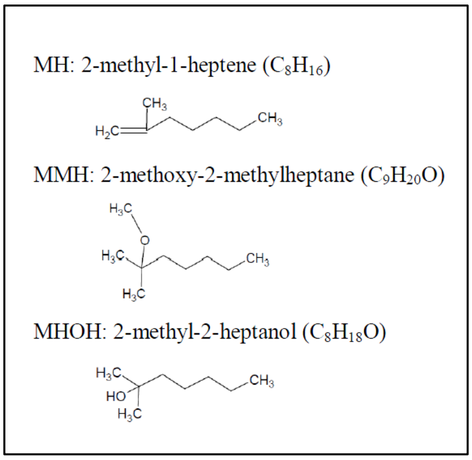


Figure 4.1 Molecular structures

The activation energies of these two competing reactions favor high reactor temperature, which is limited by catalyst activity to 400 K. Notice that the activation energy of the forward MMH reaction is larger than that of the reverse reaction, which means that high reactor temperatures should favor conversion.

Table 4.1 Kinetic parameters

		R_1		R_2
		forward	reverse	
k_0	kmol s^{-1} $kg_{cat.}^{-1}$	6.7×10^{7}	2.1×10^{-6}	1.3×10^{9}
E_A	kJ/kmol	90000	900	105900
concentrations	mole fraction	$x_{MH}x_{MEOH}$	x_{MMH}	$(x_{MeOH})^2$

4.2 Process Description

Figure 4.2 shows the flowsheet of the process. It features a 12 m^3 continuous stirred tank reactor (CSTR), three distillation columns, and one recycle stream. The equipment sizes and conditions are the economic optimum developed by Luyben (2010a).

4.2.1 Reactor

The reactor operates at 400 K and 15 atm. A fresh methanol stream (MeOH) is fed at 50 kmol/h. Fresh 2-methyl-1-heptene (MH) is fed to the reactor at 49.51 kmol/h and combined with a recycle stream from a downstream distillation column to give a total of 129.5 kmol/h of MH fed to the reactor.

4.2.2 Column C1

The reactor effluent is fed on stage 7 of a 10-stage distillation column (C1). HYSYS notation is used with the stages numbered from the top down. The top tray is 1 and the bottom tray is 10. The column operates at 10 atm. The distillate product is a small stream of 0.2805 kmol/h of 97 mol % DME. A reflux ratio of 0.43 is required to achieve the specified separation. The reboiler duty is 1.244 MW, but the condenser duty is only 0.0237 MW because of the very small distillate flow rate and low reflux ratio. The column diameter is 0.78 m. The reboiler temperature is high (501.9K), which requires the use of high-pressure stream (42 bar, 527 K).

4.2.3 Column C2

The bottoms is fed to a second distillation column (C2) that separates the product MMH from the recycle MH. The distillate is 79.99 kmol/h with a composition of 0.1 mol % MMH, 4.78 mol % MeOH, and 95.12 mol % MH. The bottoms is a mixture of the product MMH and the impurity MHOH. The bottoms specification is 0.05 mol % MH. The column has 40 stages and is fed on stage 22. It operates under vacuum conditions (0.4 atm). Operation at 0.4 atm gives the smallest total annual cost (See Luyben (2010a)). A reflux ratio of 1.79 is required to achieve the specified separation. The column consumes 0.8231 MW in the reboiler and is 2.24 m in diameter. The reboiler temperature is 416.2 K, so medium-pressure stream can be used in the reboiler (11 bar, 457 K).

4.2.4 Column C3

The third column (C3) has 20 stages and is fed on stage 8. The distillate is the MMH product (49.47 kmol/h) with a purity of 99.9 mol % MMH. The bottoms is 0.2685 kmol/h of byproduct MHOH with a purity of 99.9 mol %. The column operates under vacuum conditions (0.1 atm). Operation at this pressure gives the smallest total annual cost (See Luyben (2010a)). The reflux ratio is 0.33, and the reboiler duty is 0.3857 MW. The column diameter is 1.98 m. The reboiler temperature is 418.7 K, so medium-pressure stream is used in the reboiler.

4.3 Process Modeling and Steady State Simulation

Our modeling and simulation are performed in HYSYS process simulation software. The "UNIQUAC" physical properties model is used in all units of the process. Since MMH and 2-methyl-2-heptanol (MHOH) are not in HYSYS databank, pseudo components were generated from the molecular structures of these two molecules. Although the reaction is liquid phase and there is no phase change in the CSTR, HYSYS requires that a CSTR have both liquid and vapor exit streams, so we must install a vent line and a control valve in the simulation. A small flow of inert gas (nitrogen) is used in the reactor vessel so that the pressure can be maintained while achieving the desired reactor temperature. The N_2 fed to the reactor is 5 kmol/h. Some nitrogen is removed through the vent line whereas there is still an amount of N_2 in the liquid fed to the first column. Hence a partial condenser is used to remove the rest of nitrogen. The HYSYS flowsheet of the process, stream conditions and equipment data are shown in appendix A. In the following chapters, we will use the flowsheet given in Figure 4.2 due to the fact that there are no N_2 and two vent streams in the real plant.

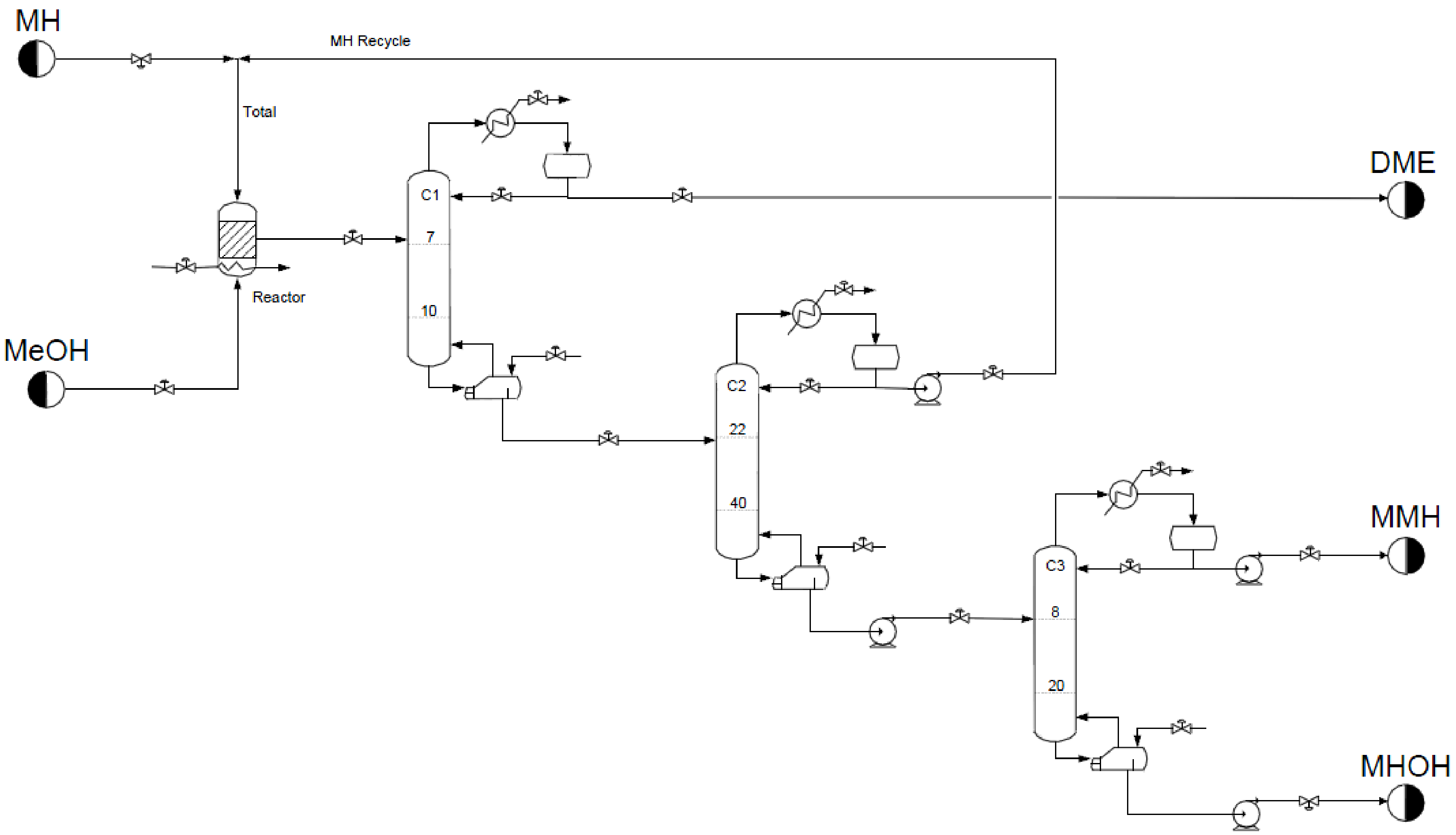


Figure 4.2 MMH flowsheet

CHAPTER V
NEW CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION

The eight-step procedure of Wongsri (2012) is applied to the 2-methoxy-2-methylheptane process in order to obtain the new control structures. The step-by-step application of this procedure is discussed in this chapter. The designed control structures are evaluated the dynamic performance compared with that proposed by Luyben (2010a).

5.1 New Control Structures Design

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

The process information has been discussed in the previous chapter, and as for equipment data and stream conditions, they are shown in appendix A.

Control objectives:

1. Provide smooth and stable plant operation and reject disturbances efficiently.
2. Product quality of MMH is better than 99.8 mol%.
3. MMH production capacity is about 62,000 tons /year.

Step 2: Plant analysis

2.1 Control degree of freedom (CDOF)

The control degrees of freedom are the number of variables that can be controlled in the process, and it is important to know this number when developing a control system for the process. It is very easy to calculate this number, even for quite complex processes, because it is equal to the number of manipulated variables. The available manipulated variables (control degree of freedom, CDOF) for this process are listed in Table 5.1. The total control degree of freedom are 23.

Table 5.1 The control degree of freedom for the MMH process

Unit	Manipulated variable	Quantity	CDOF
Independent streams	Flow rate	2	2
Pumps	Power	4	4
Reactor	Reactor effluent Coolant flow rate to the jacket	1	2
Distillation columns	Condenser heat removal Bottoms flow rate Distillate flow rate Reboiler heat input Reflux flow rate	3	15
Total CDOF			23

2.2 Heat pathways

From a plantwide perspective we can discern four different heat pathways in the MMH process. See Figure 5.1 for an illustration. The first pathway has its origins at the CSTR and flows to the environment via a cooling jacket surrounding the reactor. The second heat pathway carries heat from reboiler heat input and pump power into the process and to the environment via condenser heat removal. This pathway goes through the process and is needed to satisfy the thermodynamic work requirements of separation. The third pathway is the heat circulated in the process, as shown in Figure 5.1. The fourth pathway is accounted for the enthalpies entered and leaved the plant via process stream. The first three pathways are related to the fourth pathway as shown in the red points on the positions of their intersections.

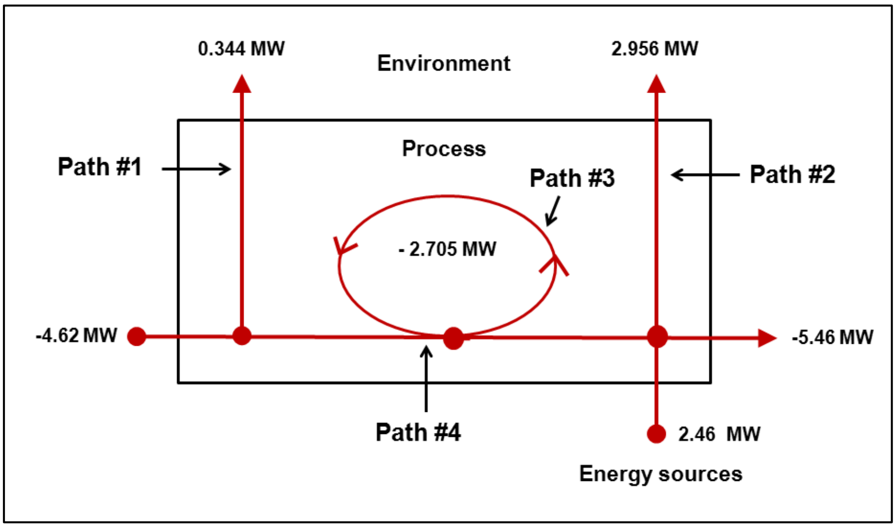


Figure 5.1 Heat pathways

2.3 Material pathways

Material pathway is the flow path of a component from an entry point or an originated point to an exit point or an end point. The material pathway is useful for component balance and in control design. There are five components involved in the MMH process, so there are five material pathways in the process as well. The limiting reactant methanol and the total MH (fresh feed plus recycle, which is the distillate from column C2) are fed to react in the reactor. The remaining MH is separated by column C2 and recycled back to the process. Certainly, DME, MMH and MHOH are generated at the reactor. DME is separated by column C1 whereas MMH and MHOH are separated from each other by column C3. Each material pathway is shown in Figure 5.2. The red, orange, green, dark blue, and violet lines are the methanol, MH, DME, MMH, and MHOH pathways, respectively.

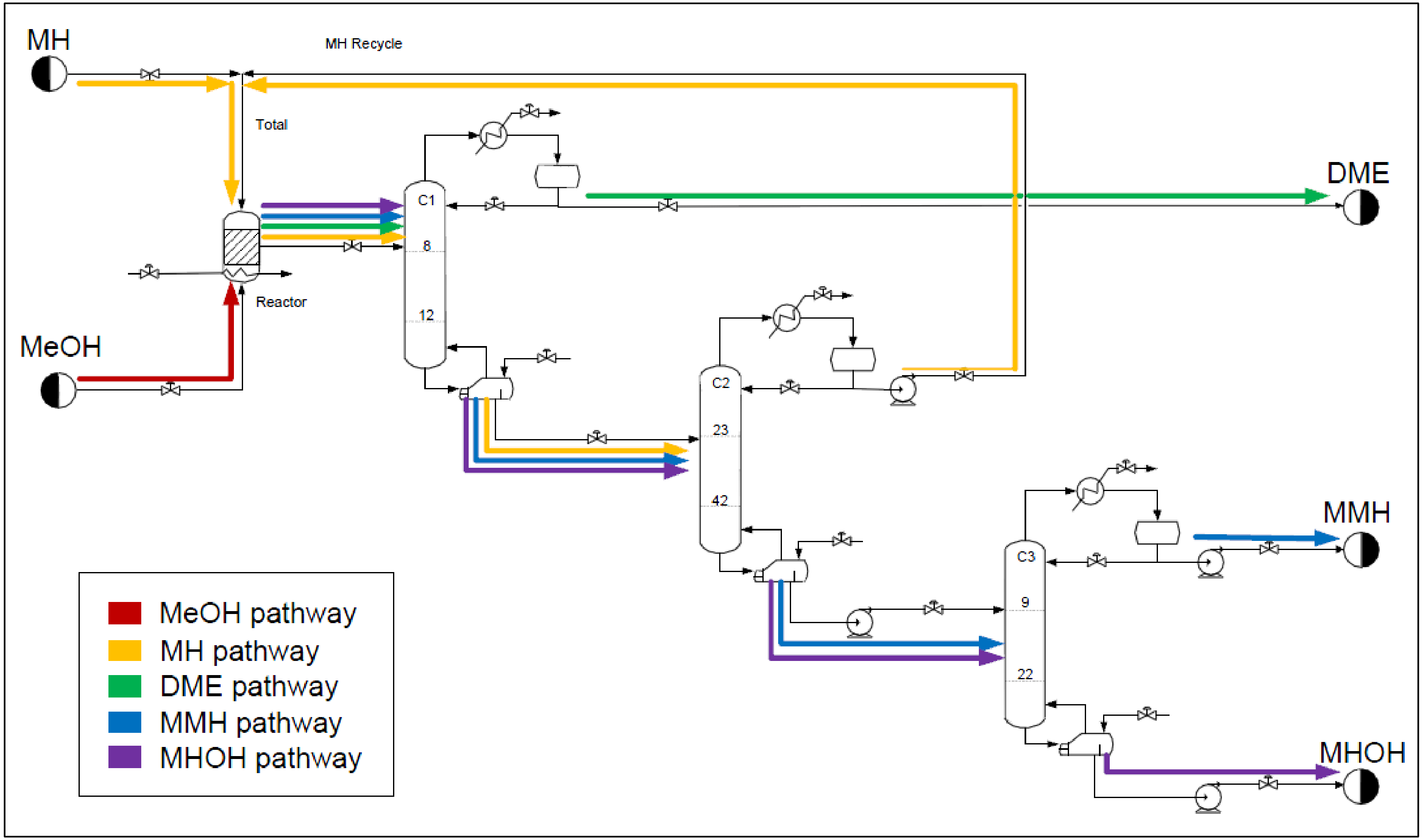


Figure 5.2 Material pathways

2.4 Material quantifiers

Material quantifier is the best place that represents the amount of material in the process. From the material pathways shown in Figure 5.2, the quantifiers of each component can be now located. By locating a quantifier, we can regulate the quantity of a component quantified by using its handle. Methanol is the limiting reactant, so methanol quantifier is its flowrate entering the reactor. The fresh feed of MH is combined with a recycle stream to give a total flow of MH fed to the reactor, so MH quantifier is the total flow of MH into the reactor. DME is separated by column C1 as the distillate product, so DME quantifier is the reflux-drum level in column C1. Similarly, MMH and MHOH are separated from each other by column C3 as the distillate and the bottoms, respectively. Hence, MMH quantifier is the reflux-drum level in column C3 and MHOH quantifier is the reboiler level in column C3. The quantifiers of each component are shown in Figure 5.3. The red, orange, green, dark blue, and violet circles are the methanol, MH, DME, MMH, and MHOH quantifiers, respectively.

2.5 Reaction section

The reaction section of a chemical plant is typically the heart of the process. Here is where the basic chemical transformations of raw materials into products are conducted. The reaction section for the process is shown in Figure 5.4. The reactor is a continuous stirred-tank reactor (CSTR) using a jacket for cooling. The reactions are simultaneous and exothermic. The reaction kinetics has been shown in the previous chapter. The jacket heat-transfer area is 11.07 m^2 with an overall heat-transfer coefficient of 0.8486 kW m^{-2} K^{-1} and a cooling duty of 0.344 MW. The flow rate of cooling water is 1232 kmol/h with an inlet temperature of 350 K. Throughput changes can be achieved only by altering, either directly or indirectly, conditions in the reactor. To obtain higher production rates, we must increase overall reaction rates. This can be accomplished by raising temperature (higher specific reaction rate), or increasing reactant concentrations. Our first choice for setting production rate should be to alter one of these variables in the reactor. The variable we select must be dominant for the reactor.

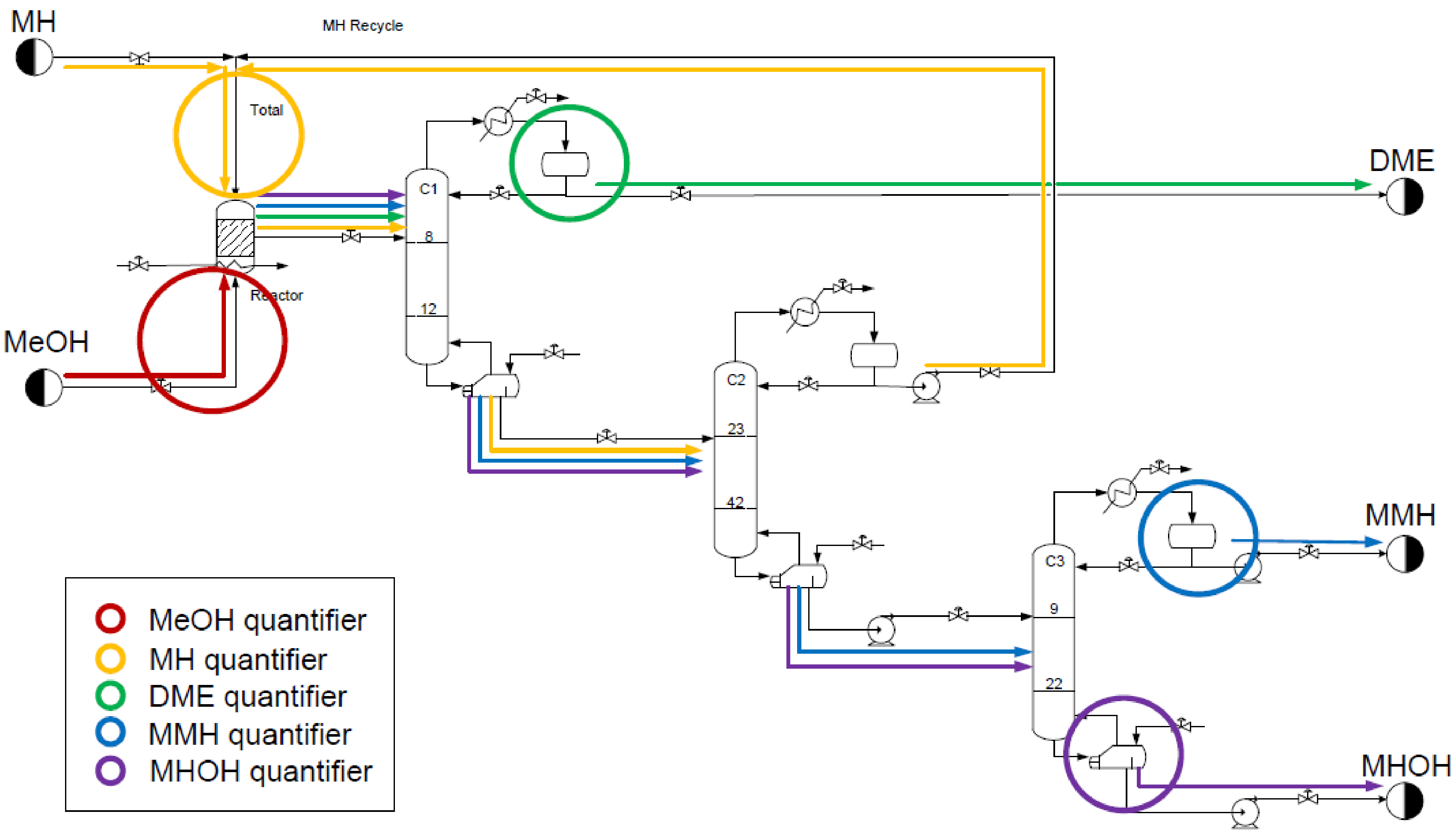


Figure 5.3 Material quantifiers

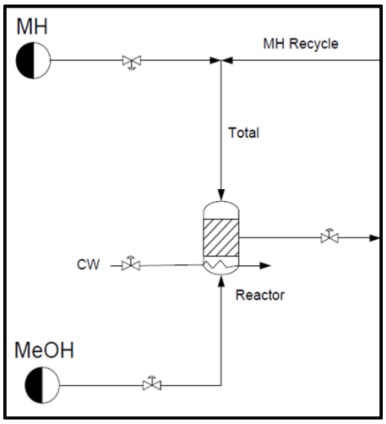


Figure 5.4 Reaction section

Dominant reactor variables always have significant effects on reactor performance. Temperature is often a dominant reactor variable. The concentration of methanol in the reactor must be kept low by using a large excess of MH in the reactor for yield reason, so it cannot be changed freely. Therefore, temperature is identified as the dominant reactor variable which may be used to set the desired production rate.

2.6 Separation section

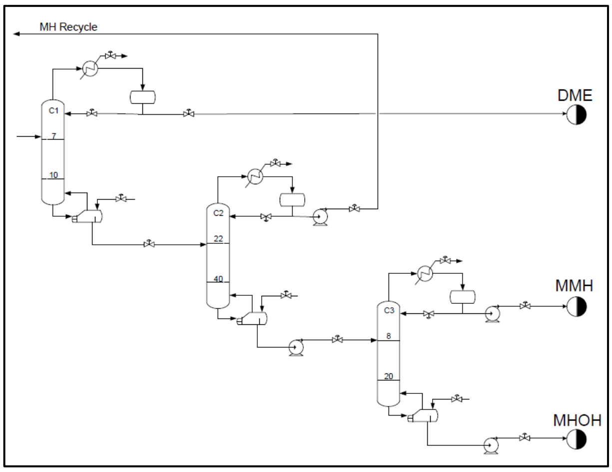


Figure 5.5 Separation section

The separation section of the process has the job of taking the reactor effluent and producing recycle, byproduct and product streams at their required purities. It features three distillation columns, as shown in Figure 5.5.

One of the most important issues in distillation control is the location of the tray on which temperature is to be controlled. There are many methods for making this selection, but a simple and effective approach that we use in this study is to find the tray which has the largest changes in temperature from the initial steady state through the sensitivity test. For each column, the sensitivity test is done on the changing of total flow, composition (the light-key component varied), temperature, and component flow (the light-key component varied) while keeping the reboiler heat duty and reflux flow or reflux ratio constant in order to find the tray where there is the largest change in temperature from the original steady state. The tray with largest changes in temperature may be a good location to use for temperature control.

Column C1

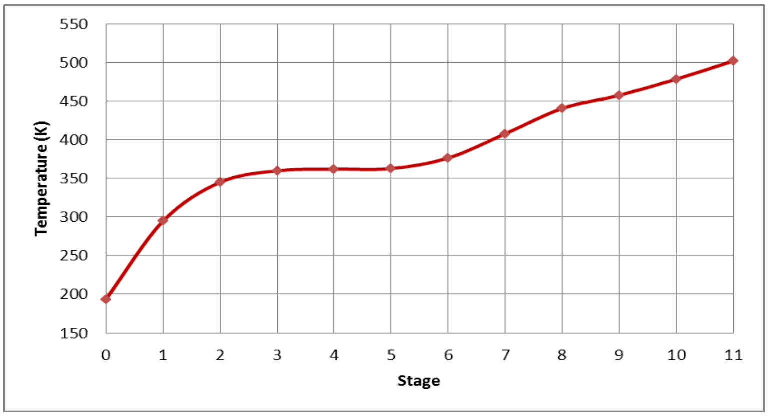


Figure 5.6 Temperature profile in column C1

Figure 5.6 shows the temperature profile in column C1. The resulting changes in the tray temperatures from the original steady state while keeping the reboiler heat duty (Q_R) and reflux flow (R) constant are shown in Figure 5.7 and examined to see which tray has the largest change in temperature. Looking at the temperature profiles given in Figures 5.7a, 5.7b, and 5.7c, we can see that there are significantly changes in the temperature profiles in the rectifying section of the column, so the tray in this section is focused. Tray 2 is selected to control because it is the most disturbed point (the best place) that can efficiently detect the occurrence of disturbances. And as for figure 5.7d,

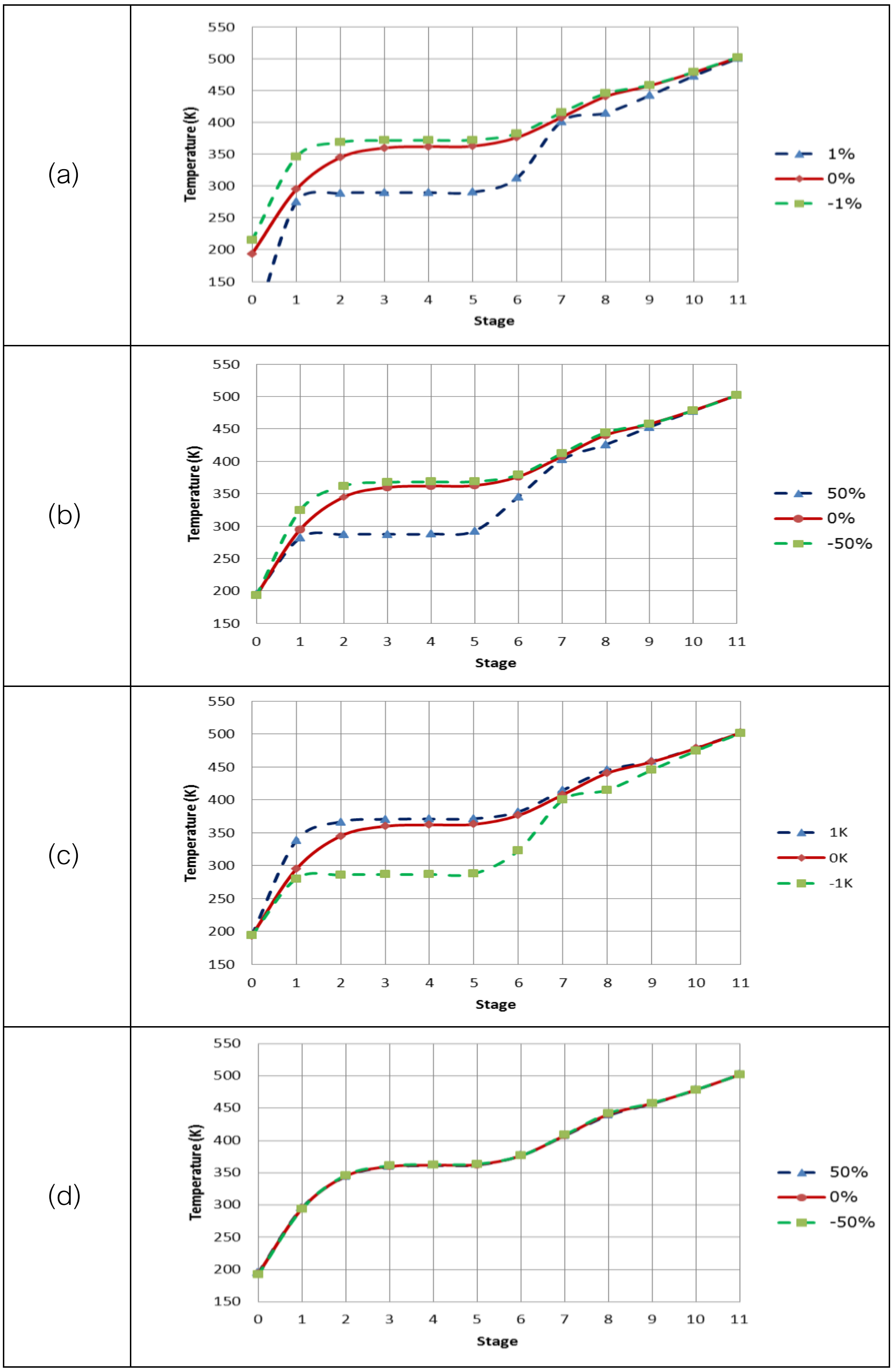


Figure 5.7 Temperature profile in column C1 with Q_R and R fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

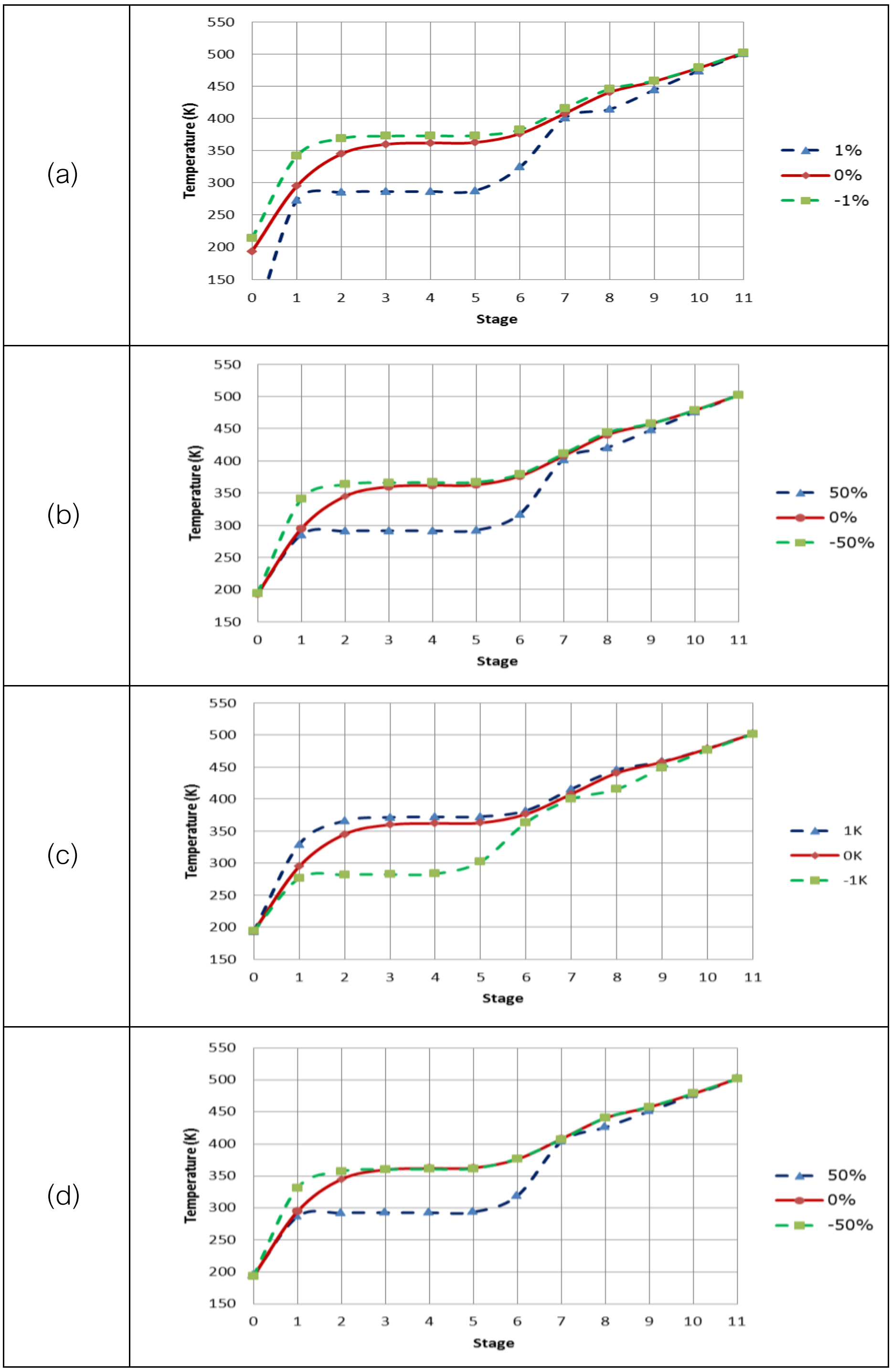


Figure 5.8 Temperature profile in column C1 with Q_R and RR fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

the temperature profile looks as though it doesn't change since the component flow of the light-key component DME in feed is very small in comparison with the total feed flow and Q_R with R are also constant, so its changes don't result in the temperature profile change much.

The procedure is repeated for keeping the reboiler heat duty (Q_R) and reflux ratio (RR) constant. The disturbances are the same as those used in Figure 5.7. The resulting changes in the tray temperatures are shown in Figure 5.8. Similarly, looking at the temperature profiles given in Figures 5.8a, 5.8b, 5.8c and 5.8d, we can see that there are significantly changes in the temperature profiles in the rectifying section of the column. It is the same as before, tray 2 is selected to control.

Column C2

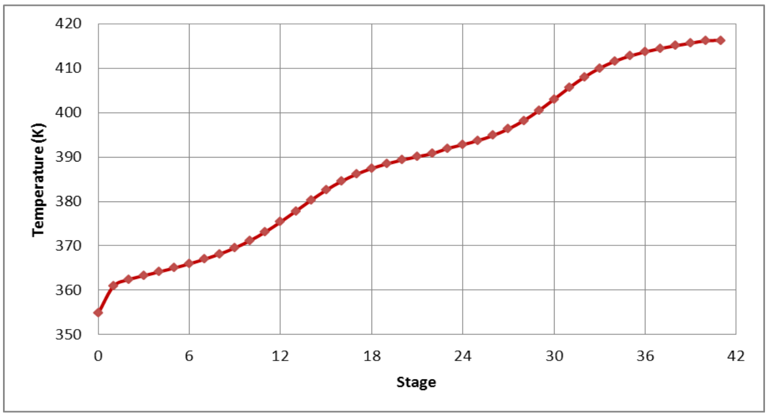


Figure 5.9 Temperature profile in column C2

Figure 5.9 shows the temperature profile in column C2. The resulting changes in the tray temperatures while keeping Q_R with R and Q_R with RR constant are shown in Figures 5.10 and 5.11, respectively. Looking at the temperature profiles given in Figures 5.10 and 5.11, we can see that there are significantly changes in the temperature profiles in both the rectifying and stripping sections of the column, so the trays in two sections are focused. The trays which have the largest change in temperature are trays 13 and 30. That means there are two most disturbed points in the temperature profile, so one or both of these trays can be selected to control.

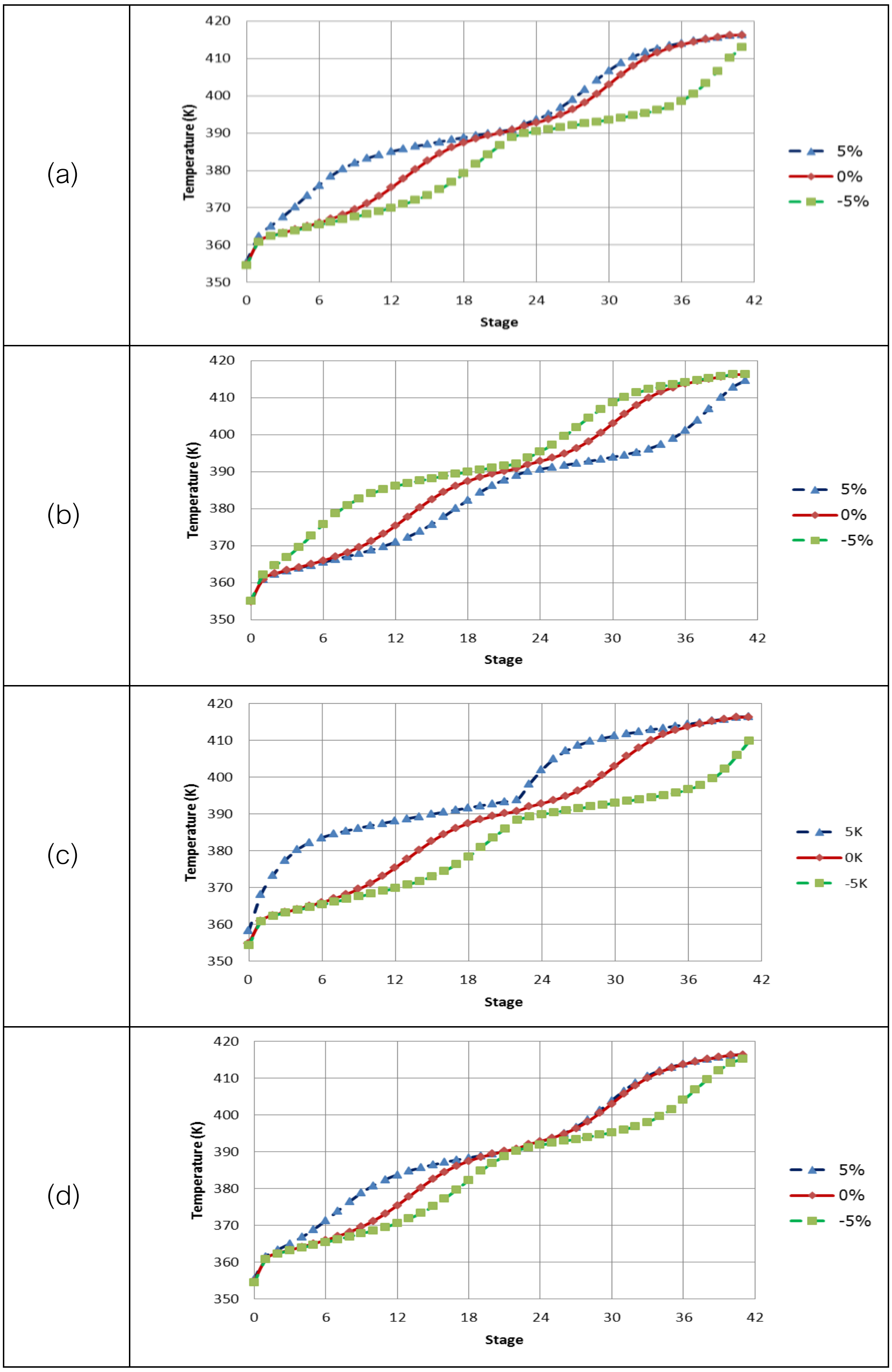


Figure 5.10 Temperature profile in column C2 with Q_R and R fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

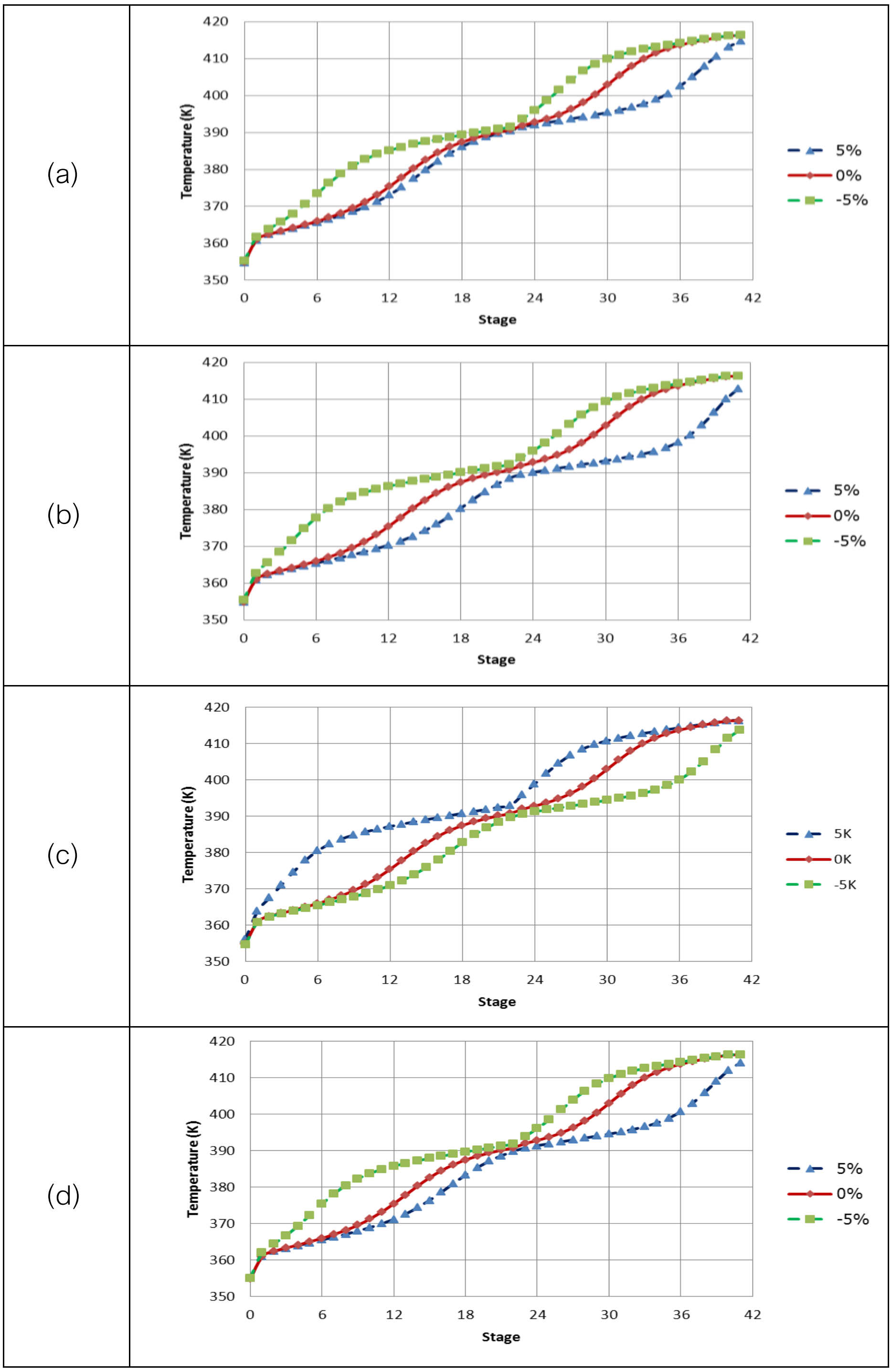


Figure 5.11 Temperature profile in column C2 with Q_R and RR fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

Column C3

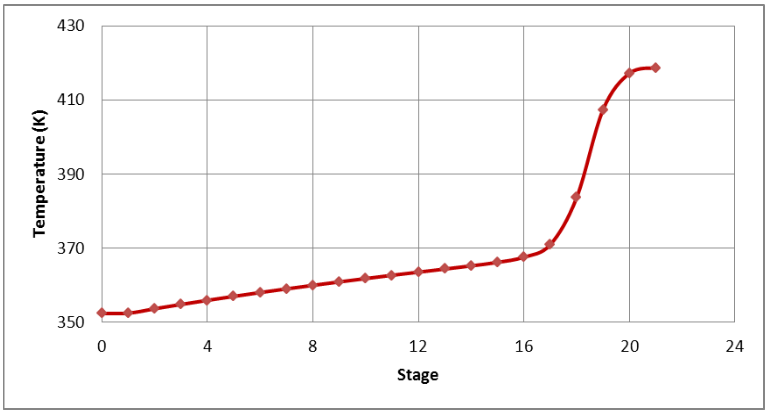


Figure 5.12 Temperature profile in column C3

Figure 5.12 shows the temperature profile in column C3. The resulting changes in the tray temperatures while keeping Q_R with R and Q_R with RR constant are shown in Figures 5.13 and 5.14, respectively. Looking at the temperature profiles given in Figures 5.13 and 5.14, we can see that there are significantly changes in the temperature profiles in the stripping section of the column, so the tray in this section is focused. Tray 18 is clearly the most sensitive sensor location, so tray 18 is selected to control.

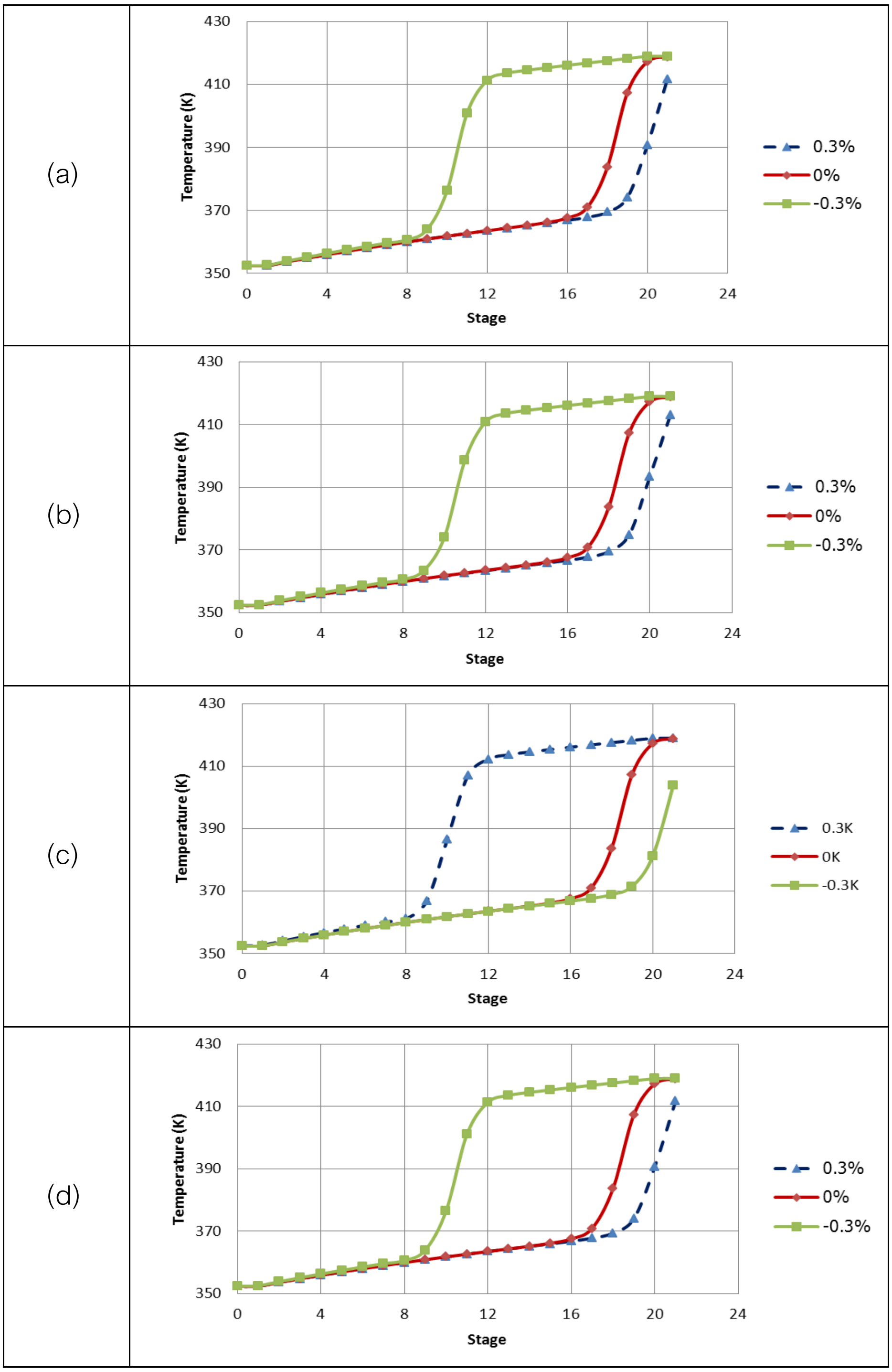


Figure 5.13 Temperature profile in column C3 with Q_R and R fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

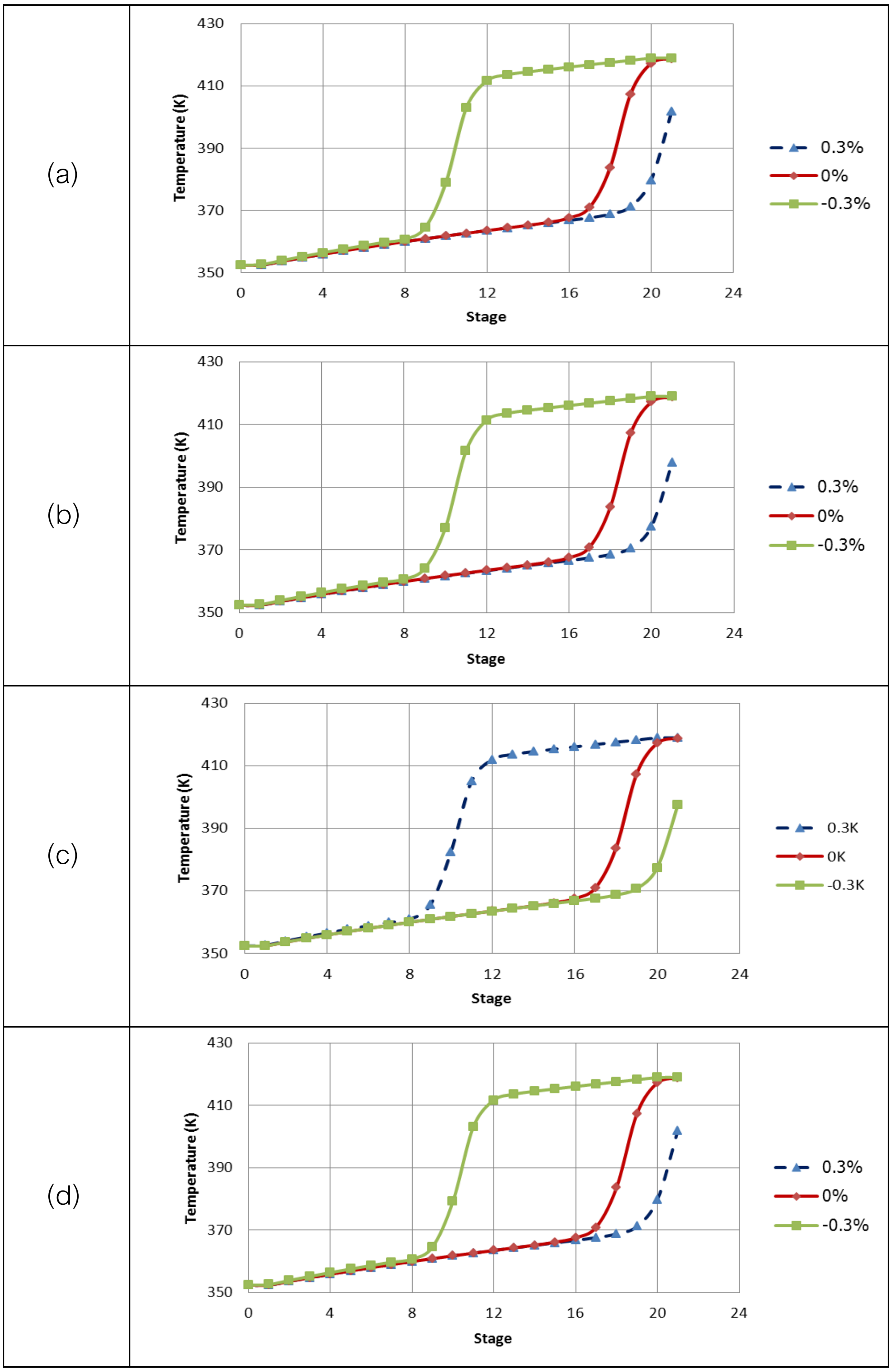


Figure 5.14 Temperature profile in column C3 with Q_R and RR fixed when (a) total flow, (b) composition (c) temperature, and (d) component flow changes

In addition to sensitivity test, another useful method that we use is to find the tray where there is the largest change in temperature for a change in the manipulated variable. We fix the reflux ratio and make a small change in the reboiler heat input. The resulting changes in the tray temperatures from the original steady state are calculated. The procedure is repeated for fixing the reboiler heat input and make a small change in the reflux ratio. The tray with the largest temperature changes is the most “sensitive” and is selected to be controlled.

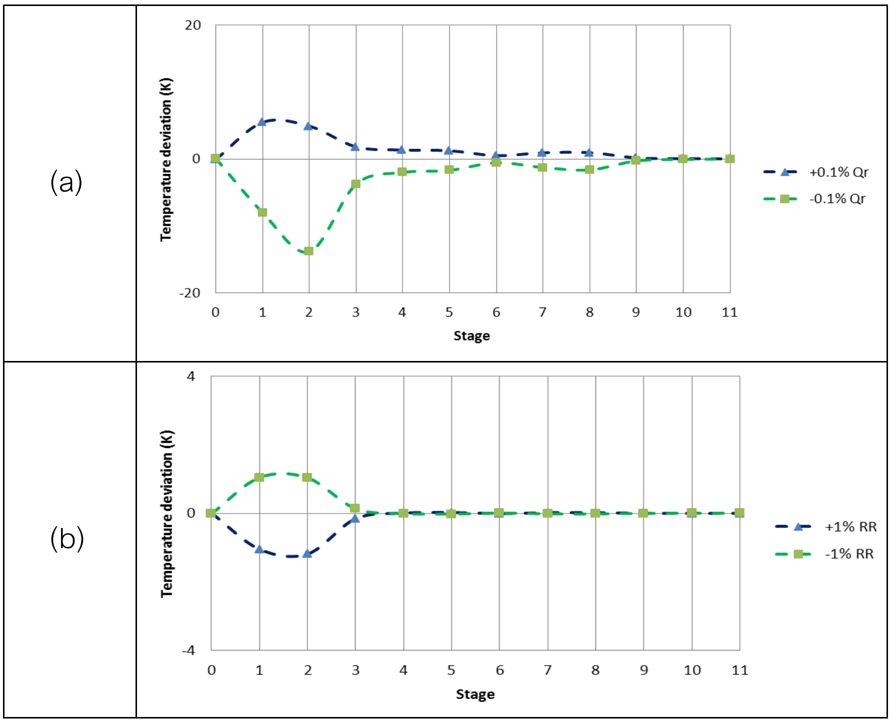


Figure 5.15 Column C1 sensitivity when (a) Q_R changed with RR fixed, and (b) RR changed with Q_R fixed

Figure 5.15a and 5.15b give the resulting changes in the tray temperatures in column C1 (temperature deviation term) for a small change in the reboiler heat input (Q_R) with the reflux ratio (RR) fixed and a small change in RR with Q_R fixed, respectively. These curves show that tray 2 is sensitive to changes in the reboiler heat input and reflux ratio. Therefore tray 2 is selected to control. This method recommends the same control tray location as sensitivity test.

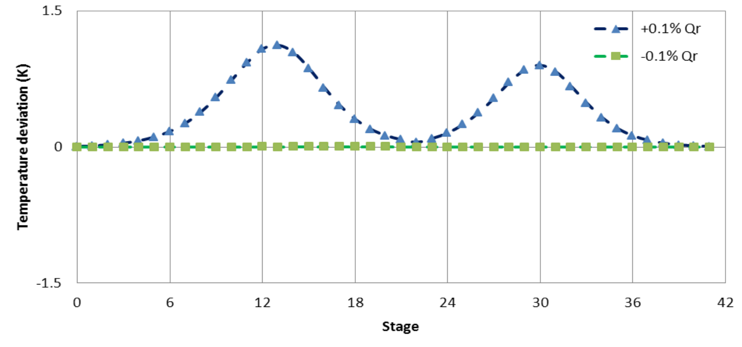
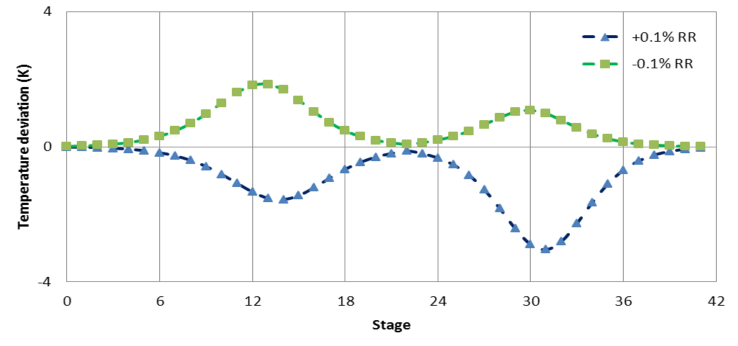
(a)	
(b)	

Figure 5.16 Column C2 sensitivity when (a) Q_R changed with RR fixed, and (b) RR changed with Q_R fixed

Figure 5.16a and 5.16b give the resulting changes in the tray temperatures in column C2 (temperature deviation term) for a small change in Q_R with RR fixed and a small change in RR with Q_R fixed, respectively. These curves show that tray 13 and 30 are sensitive to changes in the reboiler heat input and reflux ratio. So one or both of these trays can be selected to control. This method recommends the same control tray location as sensitivity test.

Figure 5.17a and 5.17b show the resulting changes in the tray temperatures in column C3 (temperature deviation term) for a small change in QR with RR fixed and a small change in RR with QR fixed, respectively. These curves show that tray 18 is sensitive to changes in the reboiler heat input and reflux ratio. Therefore tray 18 is selected to control. This method recommends the same control tray location as sensitivity test.

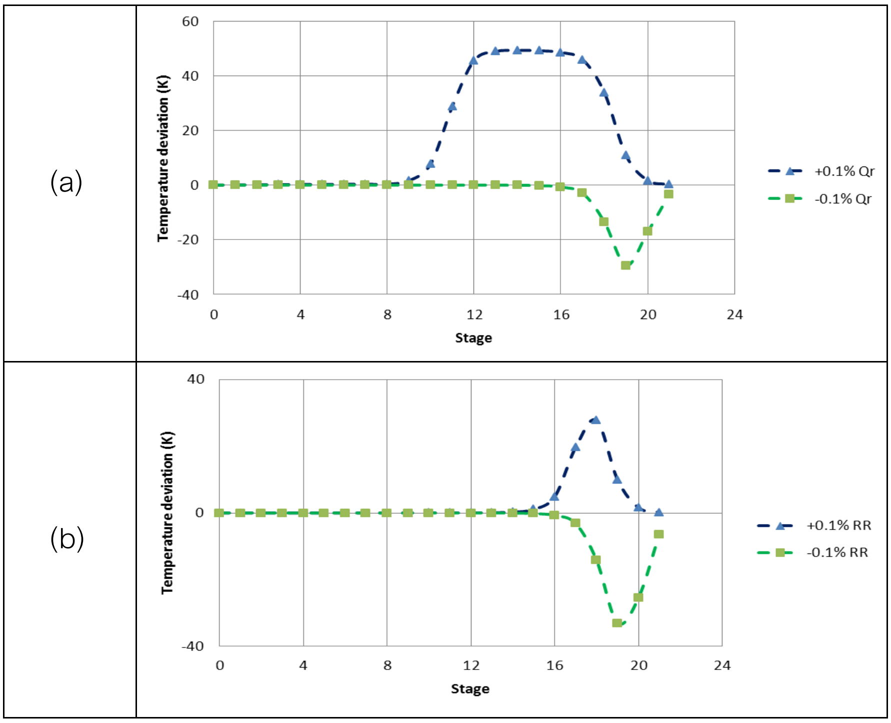


Figure 5.17 Column C3 sensitivity when (a) Q_R changed with RR fixed, and (b) RR changed with Q_R fixed

Step 3: Establish fixture plant

The material entered and in-process stream must be maintained to ensure that the plant is smoothly operated.

3.1 Keep the materials entered and reentered fixed

There are two streams of raw materials entering the process which need to be fixed: methanol feed and total flow of MH (MH feed plus MH recycle). That is to say, the fresh feed of methanol is flow-controlled into the reactor and the total flow of MH into the reactor is flow-controlled by manipulating the fresh feed of MH. Both flow controllers installed are shown in Figure 5.18

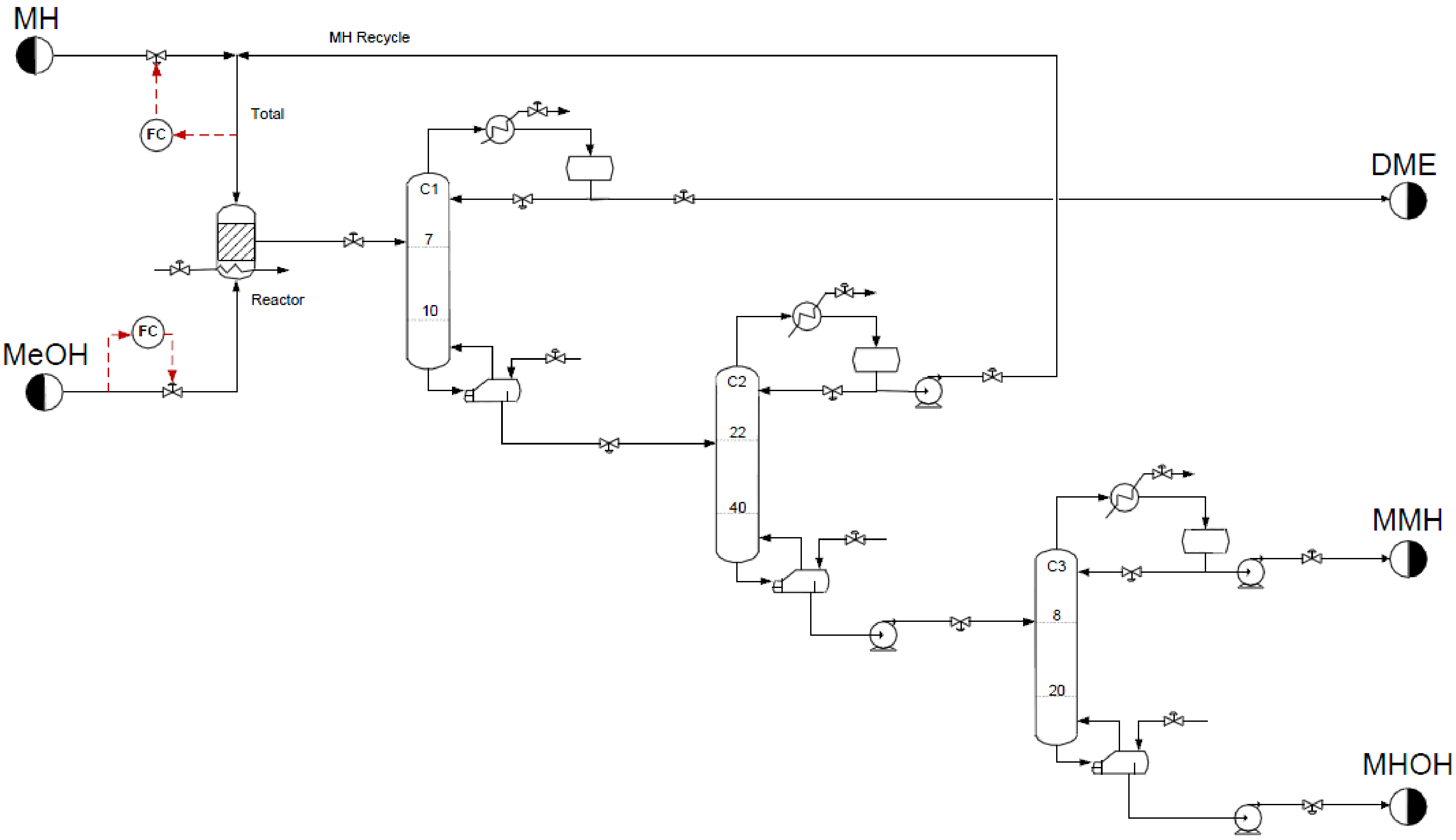


Figure 5.18 Flowsheet with controllers for step 3.1

3.2 Regulate the production rate

3.2.1) Consume the limiting reactant

The limiting reactant should be totally or extremely consumed at the reactor for the economic reason, but there are some situations where the limiting reactant is not totally consumed and remains its small amount in the reactor effluent. Hence the concentration of the limiting reactant should be controlled in order not to exceed the design point (for example, catalyst deactivation). In the process, the composition of the limiting reactant methanol in the reactor effluent is low (2.83 mol %). Two options of the cascade control structures that can be used to control this are proposed as follows:

- Option 1: The methanol composition in the reactor effluent is controlled by changing the setpoint of the reactor temperature controller, as shown in Figure 5.19.
- Option 2: The methanol composition in the reactor effluent is controlled by changing the setpoint of the total flow of MH controller, as shown in Figure 5.20.

3.2.2) Regulate the production rate

The product rate (the flowrate of product MMH) can be regulated through step 3.2.1. If this is done and the production rate does not reach the objective or the production demand, two options of the control structures that may be able to be used to regulate the production rate are suggested as follows:

- Option 1: The production rate is regulated by manipulating the setpoint of the methanol feed flow controller (the cascade control structure), as shown in Figures 5.21.
- Option 2: The production rate is regulated by manipulating the feed into column C3. Now some of the inventory loops (the reboiler levels of columns C1 and C2, and the reactor liquid level) are controlled by manipulating the feed into each unit, as shown in Figures 5.22. Changes in throughput will propagate back through the process. Nevertheless, these are just the recommendations for this step. They are not used in this study.

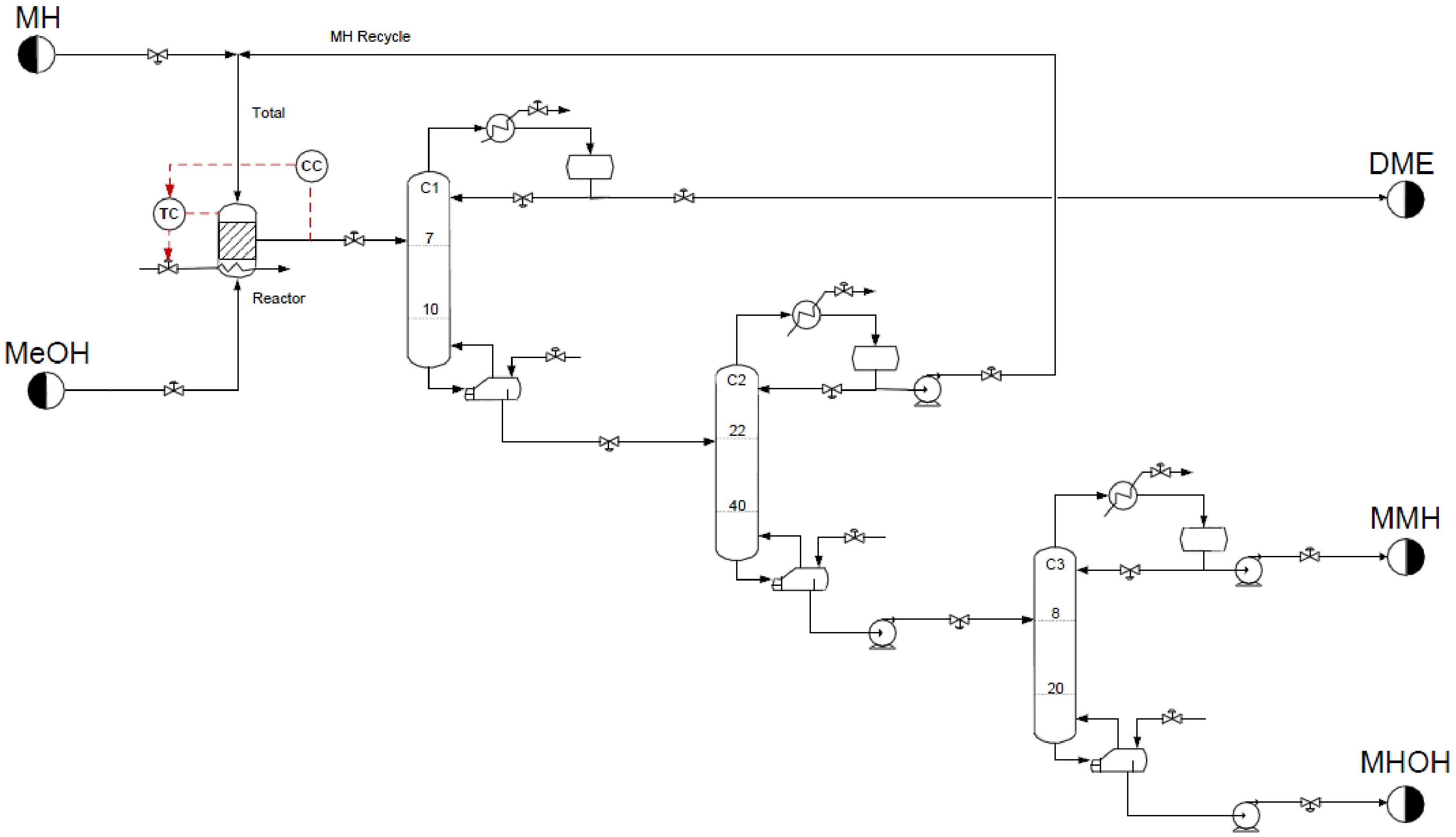


Figure 5.19 Flowsheet with controllers for step 3.2.1 (option 1)

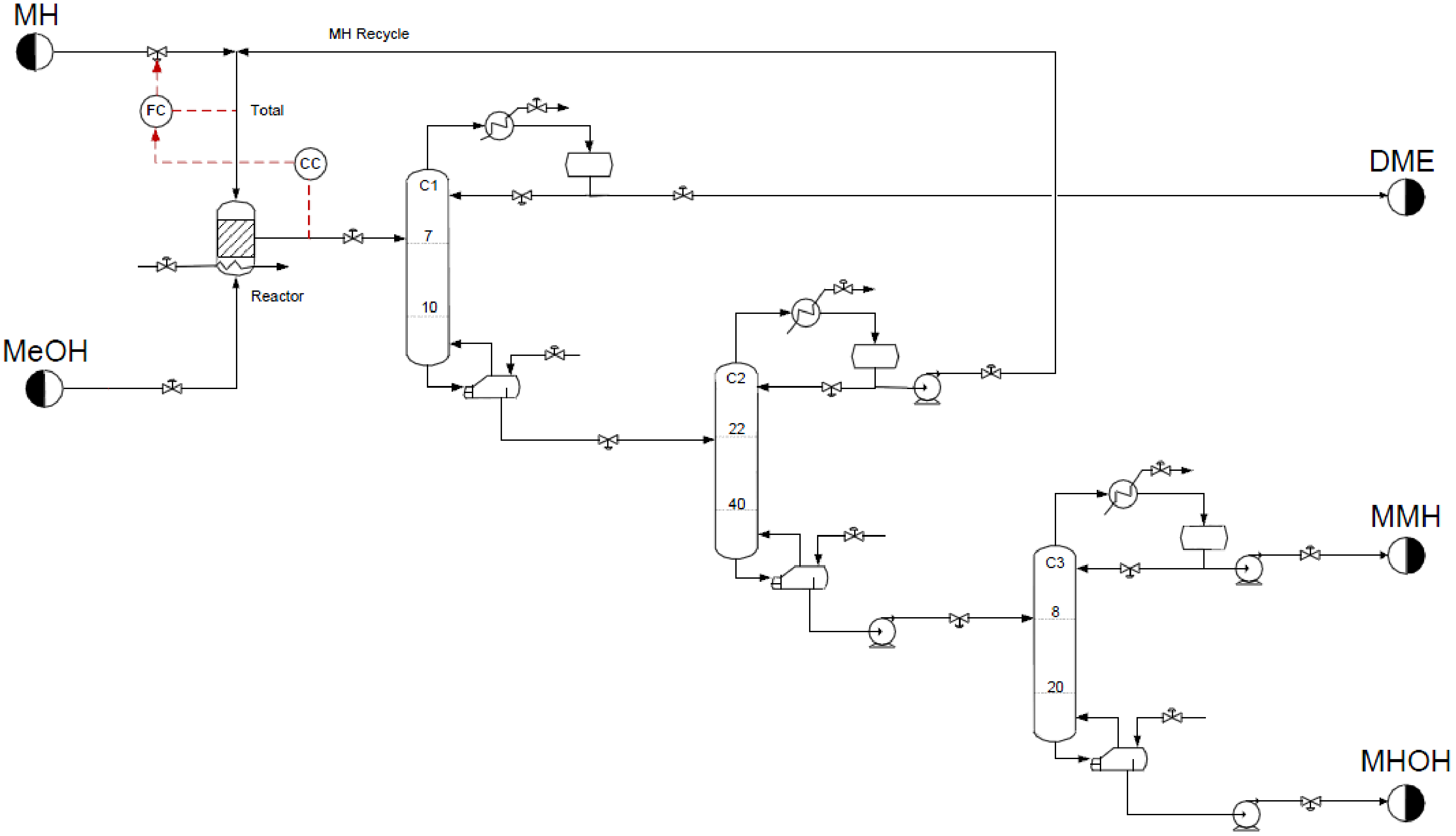


Figure 5.20 Flowsheet with controllers for step 3.2.1 (option 2)

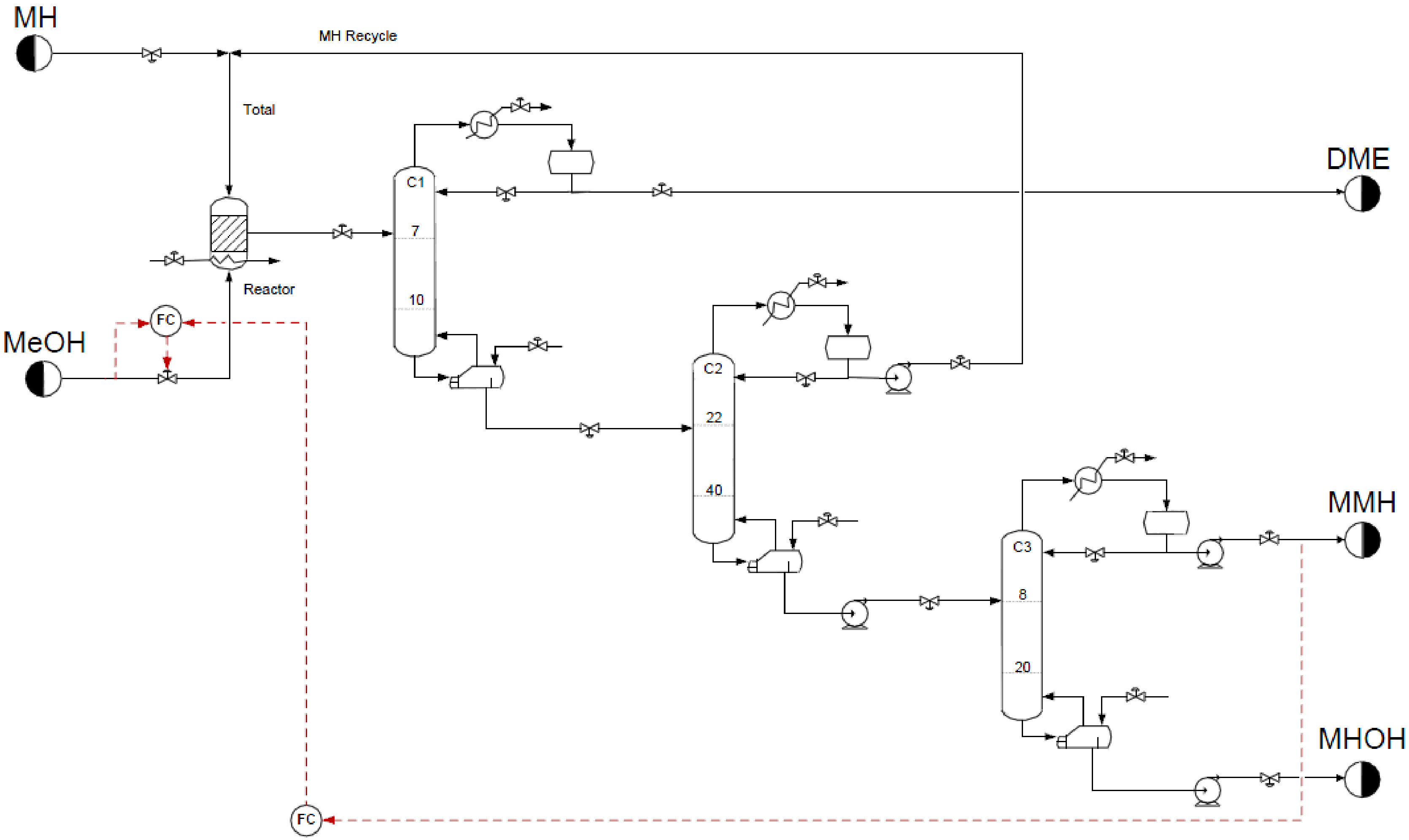


Figure 5.21 Flowsheet with controllers for step 3.2.2 (option 1)

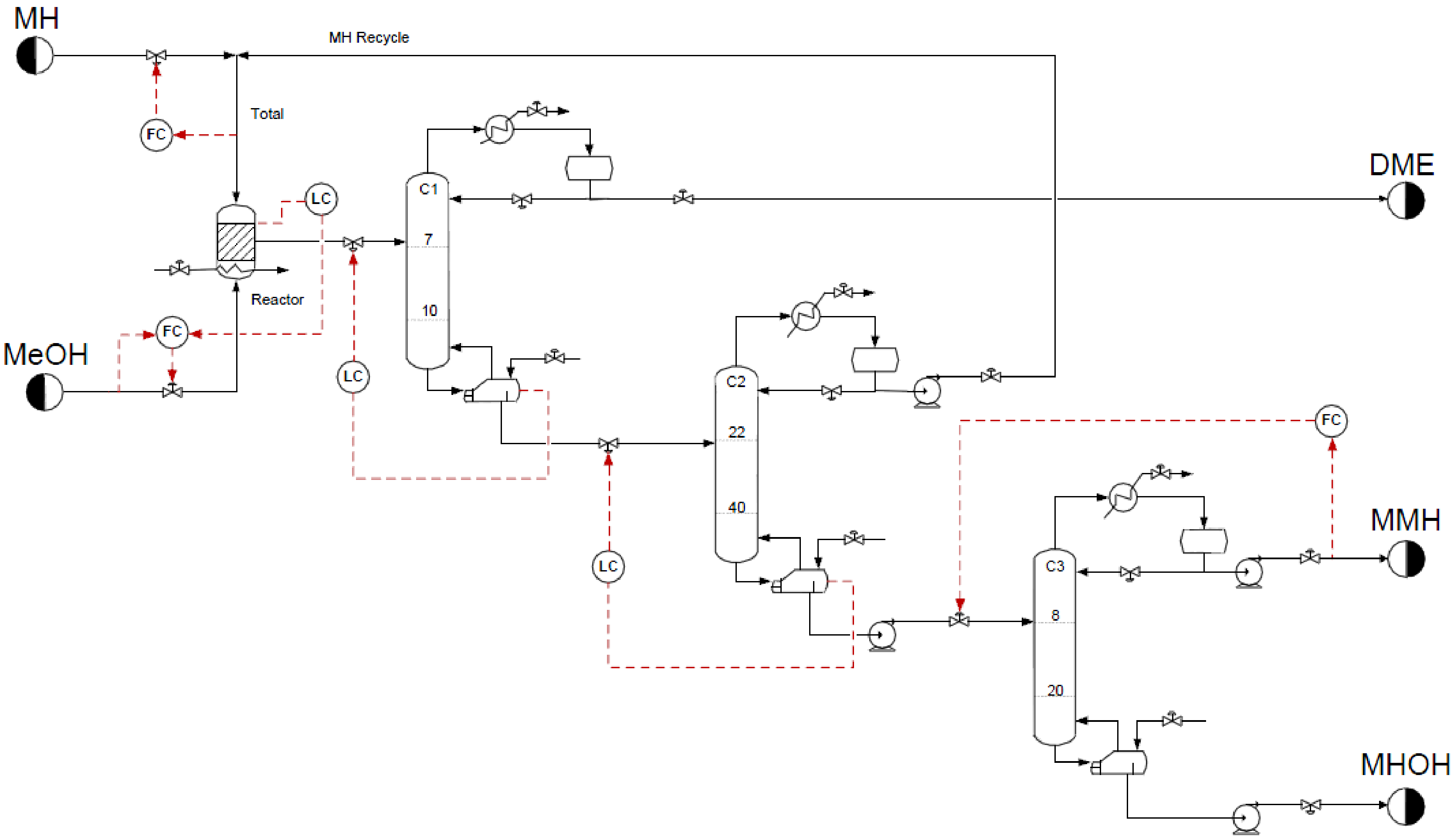


Figure 5.22 Flowsheet with controllers for step 3.2.2 (option 2)

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

In the process, there are one product and two byproduct streams: MMH product, DME and MHOH byproducts. The three exit material streams are adjusted the flow according to their accumulation. This provides three level controllers, as shown in Figure 5.23. The reflux-drum levels of columns C1 and C3 are controlled by manipulating the flow rates of DME byproduct and MMH product, respectively. In the same way, the reboiler level of column C3 is controlled by manipulating the flow rates of MHOH byproduct.

3.4 Control the amount of the rest of the component at their quantifiers, i.e. the indicators of the representative accumulation, for the rest of the components and design the control loops to regulate their inventories in the plant.

There are no other components left for quantification control because the quantifiers of all components have been regulated in the previous steps.

Step 4: Disturbances management

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

4.1 Heat disturbance management

4.1.1) Direct the heat disturbances that are not directly related to quality to the environment via the next and nearest exit points, usually heaters or coolers, to keep the thermal conditions of process stream fixed

Since there are no heaters or coolers in the process, the heat disturbances that are not directly related to quality cannot be directed to the environment. Nevertheless, in the next step (step 4.1.2), these heat disturbances entering the reactor and distillation columns will be managed in the form of heat disturbances that related to quality.

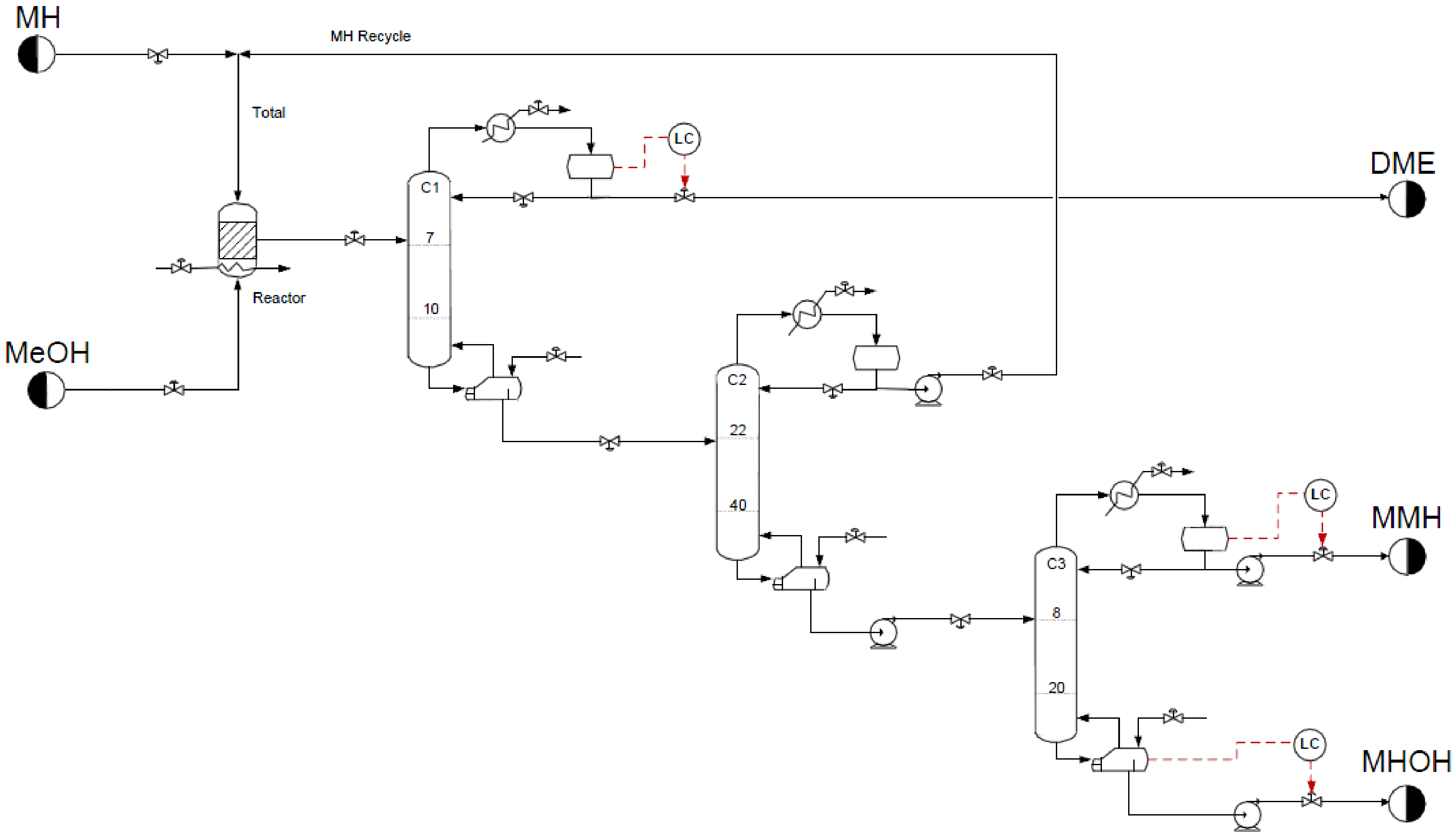


Figure 5.23 Flowsheet with controllers for step 3.3

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

To keep the product quality constant in the presence of heat disturbances, the reactor temperature controller and the column tray temperature controllers are needed to install in the plant. From the sensitivity test performed in step 2.6, the tray 2 in column C1 and tray 18 in column C3 are selected for single-end temperature control, and as for in column C2, trays 13 and 30 are two locations with large changes in the temperature profiles, so it is possible to use either single-end or dual-end temperature control. This issue will be resolved in the step 4.2.

Heat disturbance entering the reactor is managed by manipulating the flow rate of the cooling medium to the jacket so as to control the reactor temperature. Similarly, heat disturbances entering the columns C1, C2 and C3 are managed by manipulating the reboiler heat inputs in order to control stage temperatures in all three columns. Figure 5.24 shows four temperature controllers installed in the flowsheet.

4.2 Material disturbances management

In this step, we firstly discuss the development of effective distillation control structures. There are three inventory variables that must be controlled: pressure, liquid level in the reflux drum, and liquid level in the base. There are five control valves available: condenser cooling water, reboiler steam, reflux, distillate, and bottoms. Three of these must be used to control the three inventory variables. That leaves two control valves available to control two variables. Ideally, the two variables to control would be the compositions of the distillate (heavy-key impurity) and the bottoms (light-key impurity). These are the variables that were used to design the column in the first place. A “dual-composition” control structure is the ideal scheme but is seldom implemented in industry because online composition measurements are usually expensive, require high maintenance, and can introduce significant delays in the control loop, particularly if gas chromatographs are used. Therefore many distillation columns are controlled using temperature measurements, which are inexpensive, reliable, and relatively fast.

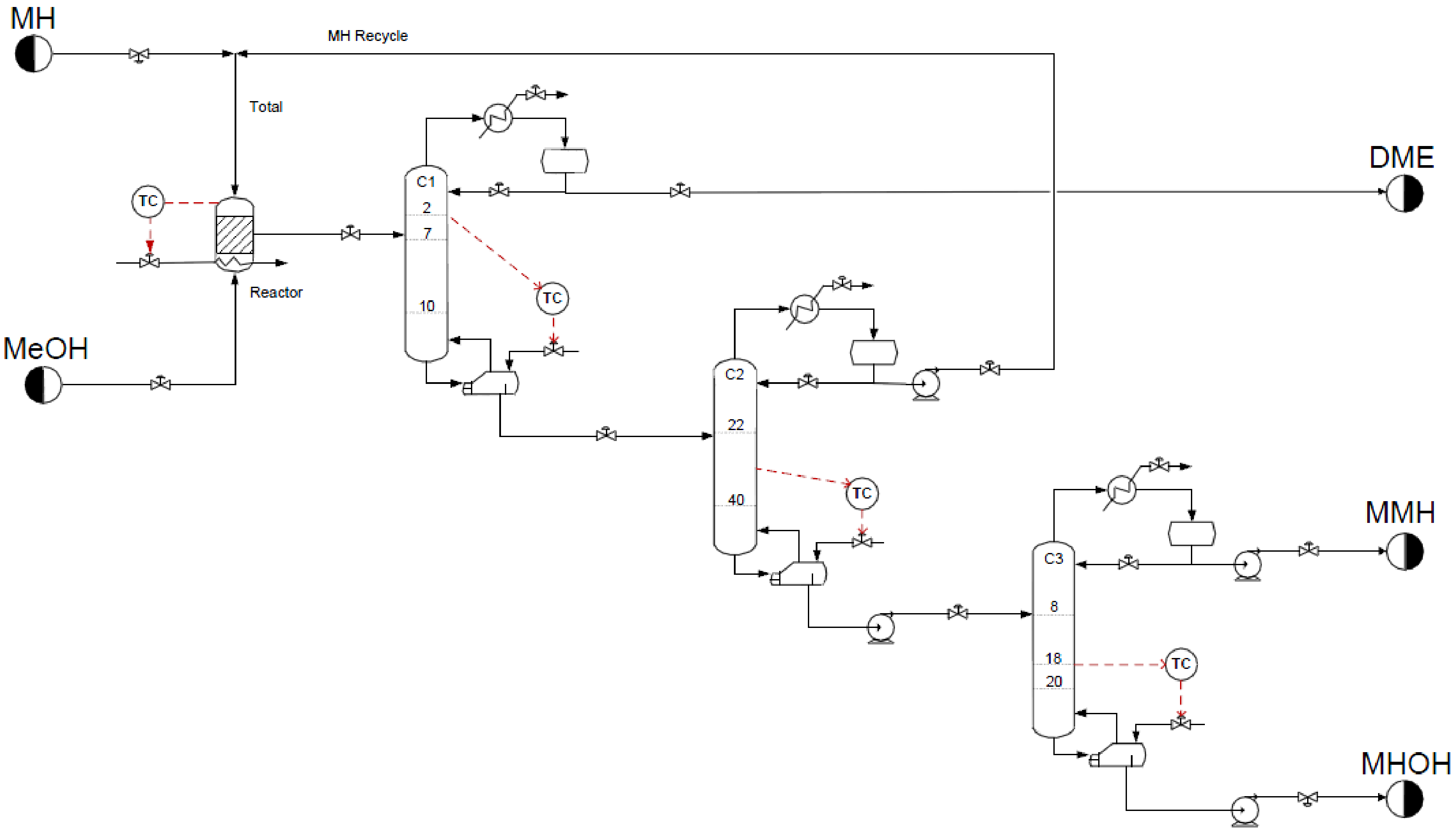


Figure 5.24 Flowsheet with controllers for step 4.1

Many industrial distillation columns use some type of single-end temperature control because of its simplicity and low maintenance cost. However, this simple structure may not provide effective control for some columns. Even if a single-end control structure is possible, we have to decide how to select the other control degree of freedom. The most common choices are holding a constant reflux flow (R) or holding a constant reflux ratio (RR) or holding a constant reflux-to-feed ratio (R/F). To aid in making this choice for each column, a series of dynamic simulation runs is made in which the effects of changes in component flow, composition, total flow and temperature of column feed. In case of column C2 which has two locations with large changes in the temperature profiles, if the results of these disturbance tests indicate that single-end control is inadequate, we may have to use a dual-end control structure.

Column C1

Figure 5.25 shows the alternative column C1 control structures: the R, RR, and R/F structures. The results of component flow (DME component varied), composition (DME component varied), total flow and temperature of column feed changes for these structures are compared in Figures 5.26, 5.27, 5.28, and 5.29, respectively. The red lines are the R results. The black lines are the RR results and the green lines are the R/F results. The solid lines are the results from increased disturbances, while the dashed lines are the results from decreased disturbances.

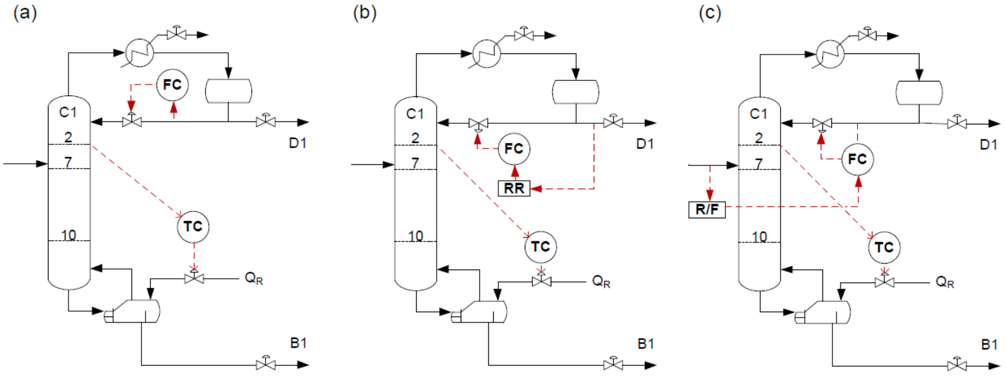


Figure 5.25 Alternative C1 control structures (a) R structure, (b) RR structure, and (c) R/F structure

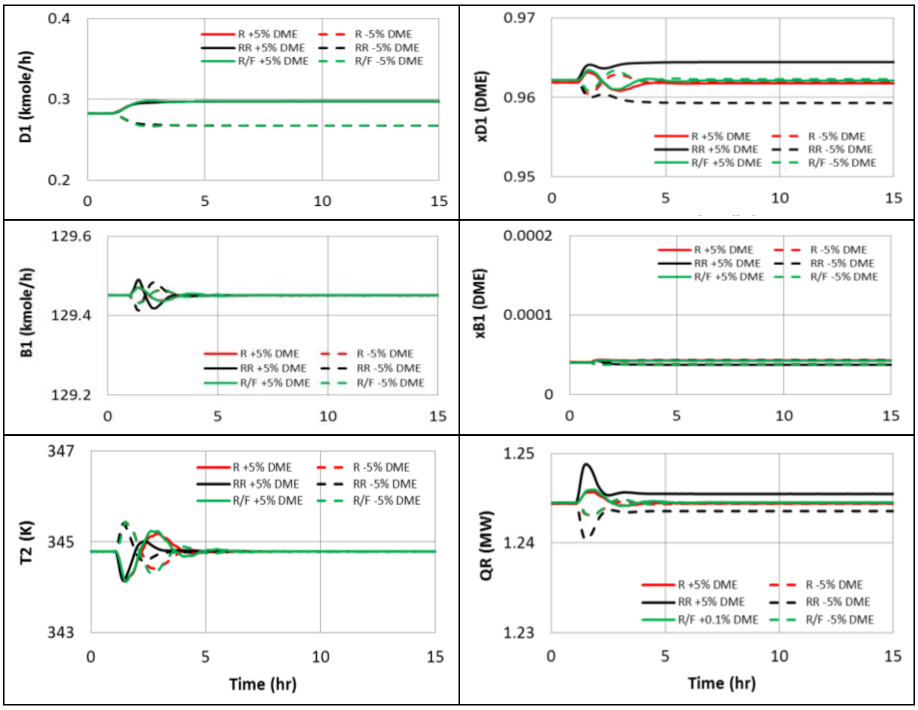


Figure 5.26 Comparison of alternative C1 control structures when component flow changes

Figure 5.26 and 5.27 give responses for disturbances in the DME component flow and DME composition of the column C1 feed, respectively. Now, we must decide which paths to push the extra loads or disturbances to. DME byproduct is separated in column C1 as the distillate product, so we will push the extra load of DME to the distillate stream. That is, the control structure that we select must reject the disturbance to this pathway and also maintain the impurity of DME in the bottoms. The first graphs on the right of both Figures show that when DME component flow or composition increased, the RR structure can push the extra load of DME to the distillate stream, while the DME impurity in the bottoms is maintained quite close to its desired level. Consequently, the RR results are better than the R and R/F results.

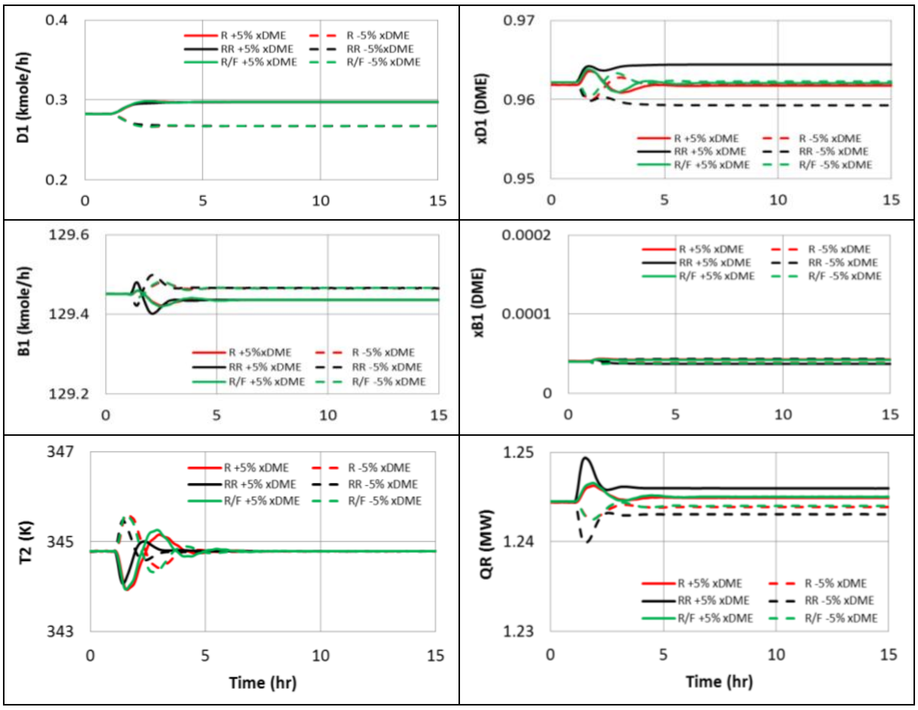


Figure 5.27 Comparison of alternative C1 control structures when composition changes

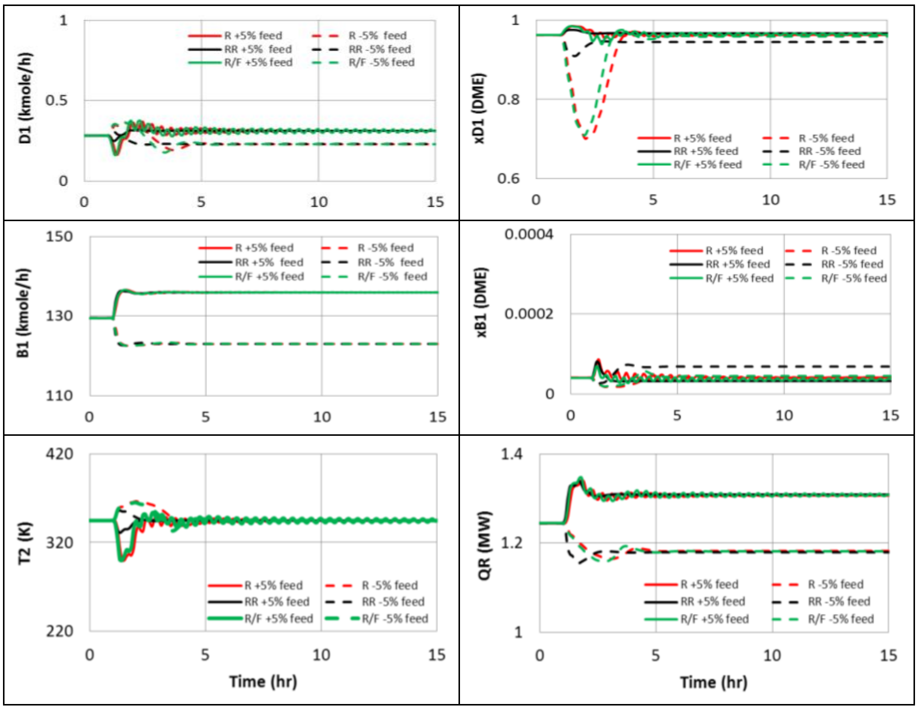


Figure 5.28 Comparison of alternative C1 control structures when total flow changes

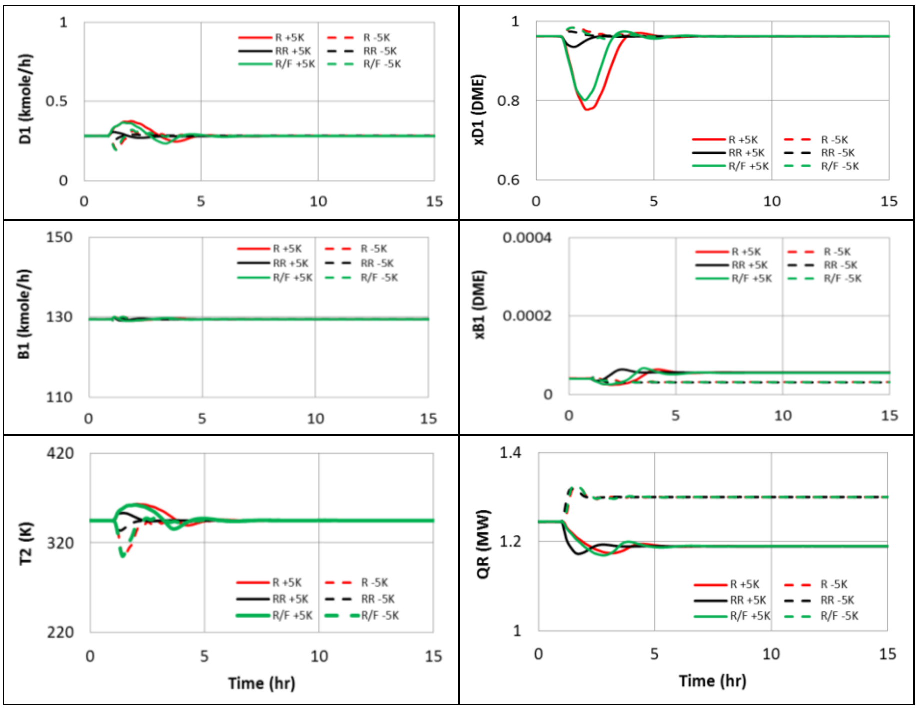


Figure 5.29 Comparison of alternative C1 control structures when temperature changes

Figure 5.28 and 5.29 show how variables in column C1 change for disturbances in the total flow and temperature of the column C1 feed, respectively. The control structure that we select must be able to maintain the DME purity in the distillate and the DME impurities in the bottoms to their specifications. Looking at the R and R/F results of both Figures, we can see that there are large transients in the temperature about 1-3 hours, which cause large temporary changes in the DME purity in the distillate. The DME impurities in the bottoms for three structures are not much different (very little changes). Clearly, the RR results are better than the R and R/F results. Therefore, the RR structure is selected in column C1 for disturbance management.

Column C2

As mentioned in step 2.6, trays 13 and 30 are the most disturbed points in the column C2 temperature profiles, so one or both of these trays can be selected to control. This provides four alternative control structures for single-end temperature control and one alternative control structure for dual-end temperature control as follows:

1. T13-R structure: The temperature on tray 13 is controlled by manipulating the reboiler heat input and reflux is flow-controlled.

2. T13-RR structure: The temperature on tray 13 is controlled by manipulating the reboiler heat input and the reflux ratio is maintained by manipulating reflux flow rate on the basis of the distillate flow rate.

3. T30-R structure: The temperature on tray 30 is controlled by manipulating the reboiler heat input and reflux is flow-controlled.

4. T30-RR structure: The temperature on tray 30 is controlled by manipulating the reboiler heat input and the reflux ratio is maintained by manipulating reflux flow rate on the basis of the distillate flow rate.

5. Dual-end structure: The tray 13 temperature is controlled by manipulating the reflux flow rate. The tray 30 temperature is controlled by manipulating the reboiler heat input.

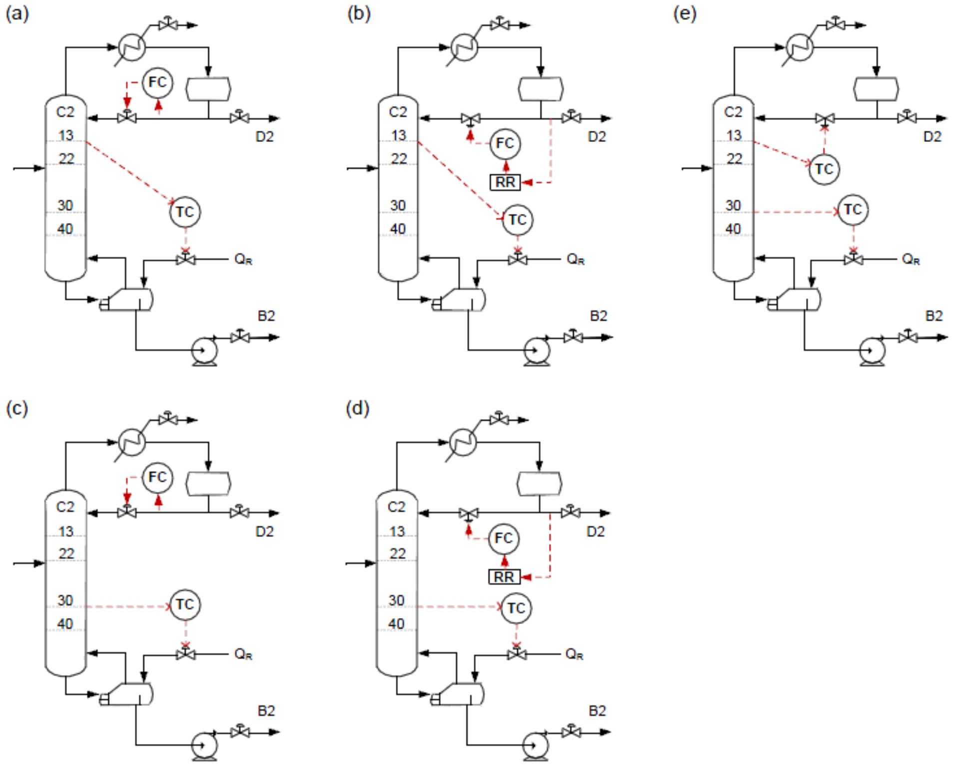


Figure 5.30 Alternative C2 control structures (a) T13-R structure, (b) T13-RR structure, (c) T30-R structure, (d) T30-RR structure, and (e) Dual-end structure

Figure 5.30 shows the alternative column C2 control structures. The results of component flow (MH component varied), composition (MH component varied), total flow and temperature of column feed changes for these structures are compared in Figures 5.31, 5.32, 5.33, and 5.34, respectively. The red, black, green, blue, and orange lines are the T13-R, T13-RR, dual, T30-R, and T30-RR results, respectively. The solid lines are the results from increased disturbances, while the dashed lines are the results from decreased disturbances.

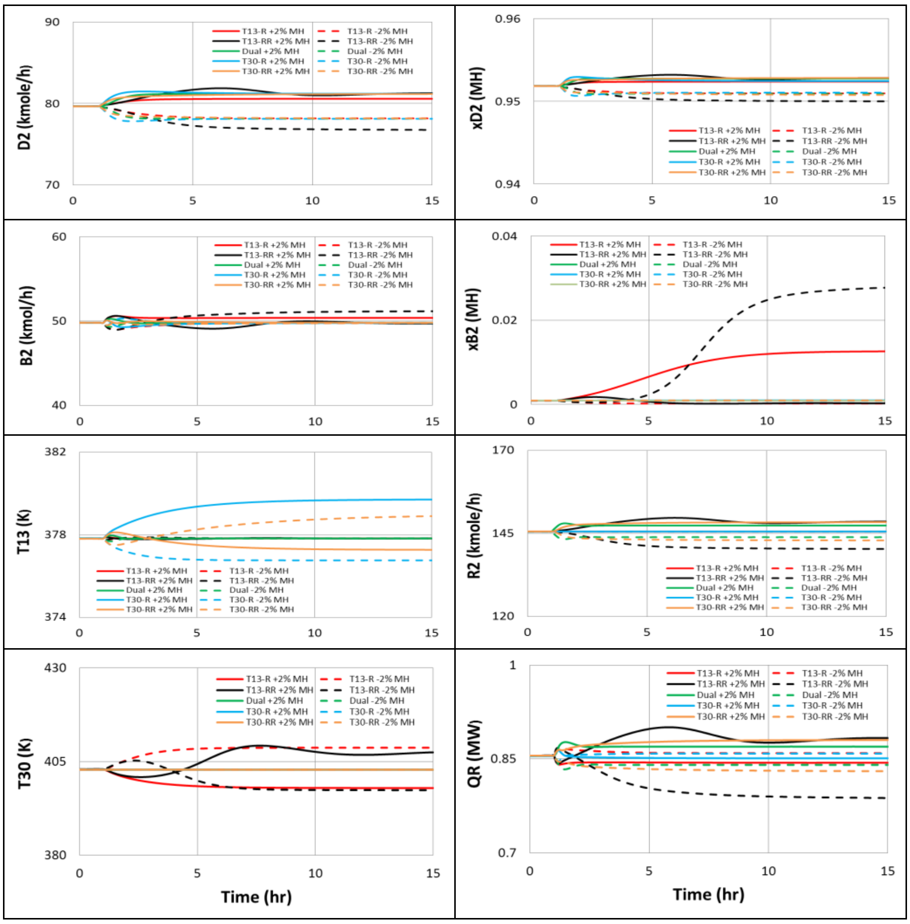


Figure 5.31 Comparison of alternative C2 control structures when component flow changes

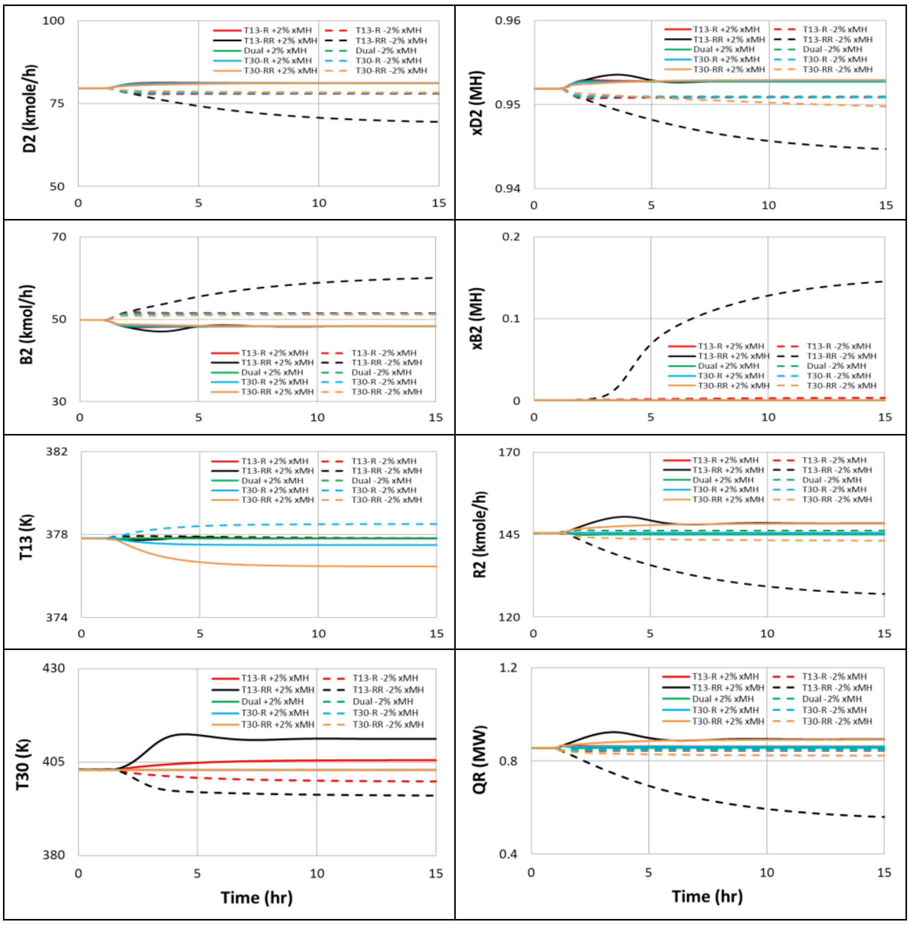


Figure 5.32 Comparison of alternative C2 control structures when composition changes

Figure 5.31 and 5.32 give responses for disturbances in the MH component flow and MH composition of the column C2 feed, respectively. Now, we must decide which paths to push the extra loads or disturbances to. As mentioned in the previous chapter, column C2 is used to separate the product MMH (bottoms) from the recycle MH (distillate). Pushing the extra load of MH to the bottoms will result in MMH product contamination in column C3, so the control structure that we select must reject the extra load to the recycle stream and also maintain the impurity of MH in the bottoms. The first graphs on the right of both Figures show that when MH component flow or composition increased, every structure can push the extra load of MH to the distillate stream, but the T13-R and T13-RR results cannot maintain the impurity of MH in the bottoms.

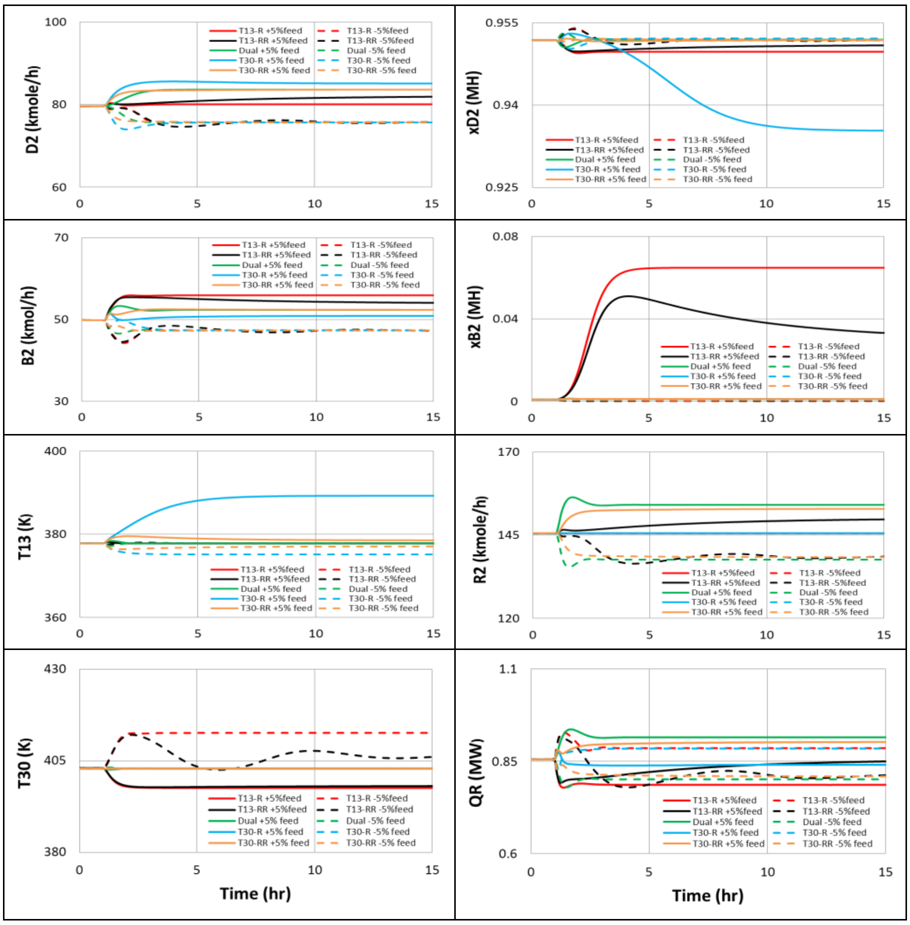


Figure 5.33 Comparison of alternative C2 control structures when total flow changes

Figure 5.33 and 5.34 show how variables in column C2 change for disturbances in the total flow and temperature of the column C2 feed, respectively. The control structure that we select must be able to maintain the MH purity in the distillate and the MH impurities in the bottoms to their specifications. Looking at the first and second graphs on the right of both Figures, we can see that the MH purity in distillate and MH impurity in bottoms in the dual results are maintained closest to the desired levels. Also, the tray 13 and 30 temperatures are well-controlled. That is, the dual results are the best in these alternative C2 control structures. Therefore, the dual-end structure is selected in column C2 for disturbance management.

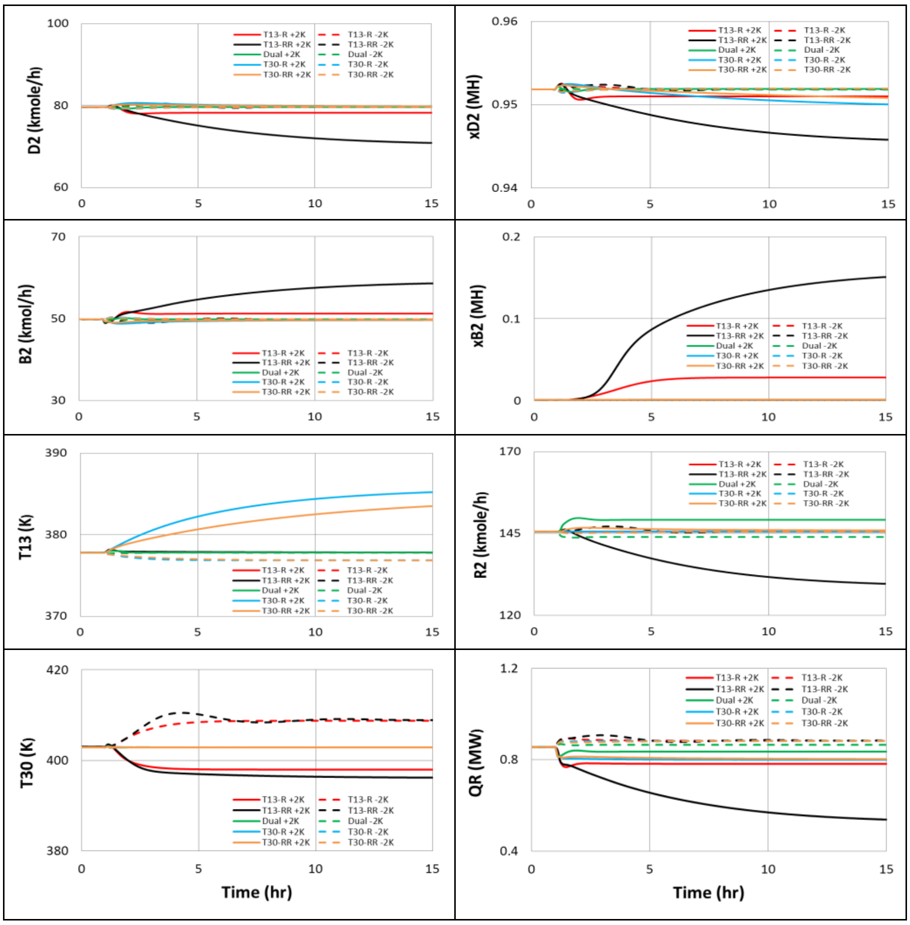


Figure 5.34 Comparison of alternative C2 control structures when temperature changes

Column C3

Column C3 is used to separate the MMH product from the MHOH byproduct. Since the MMH product is the distillate, controlling the tray temperature by manipulating reflux flow rate may provide the better product quality control. If this structure is possible, we have to decide how to select the other control degree of freedom. The common choices are holding a constant heat duty (Q_R) or holding a constant boilup ratio (Q_R/B). This provides five alternative control structures for single-end temperature control: the R, RR, R/F, Q_R, and Q_R/B structures, as shown in Figure 5.35. The results of component flow (MHOH component varied), composition (MMH component varied), total flow and temperature of column feed changes for these structures are compared in Figures 5.36, 5.37, 5.38 and 5.39, respectively. The red, black, green, blue, and orange lines are the R, RR, Q_R, Q_R/B and R/F results, respectively. The solid lines are the results from increased disturbances, while the dashed lines are the results from decreased disturbances.

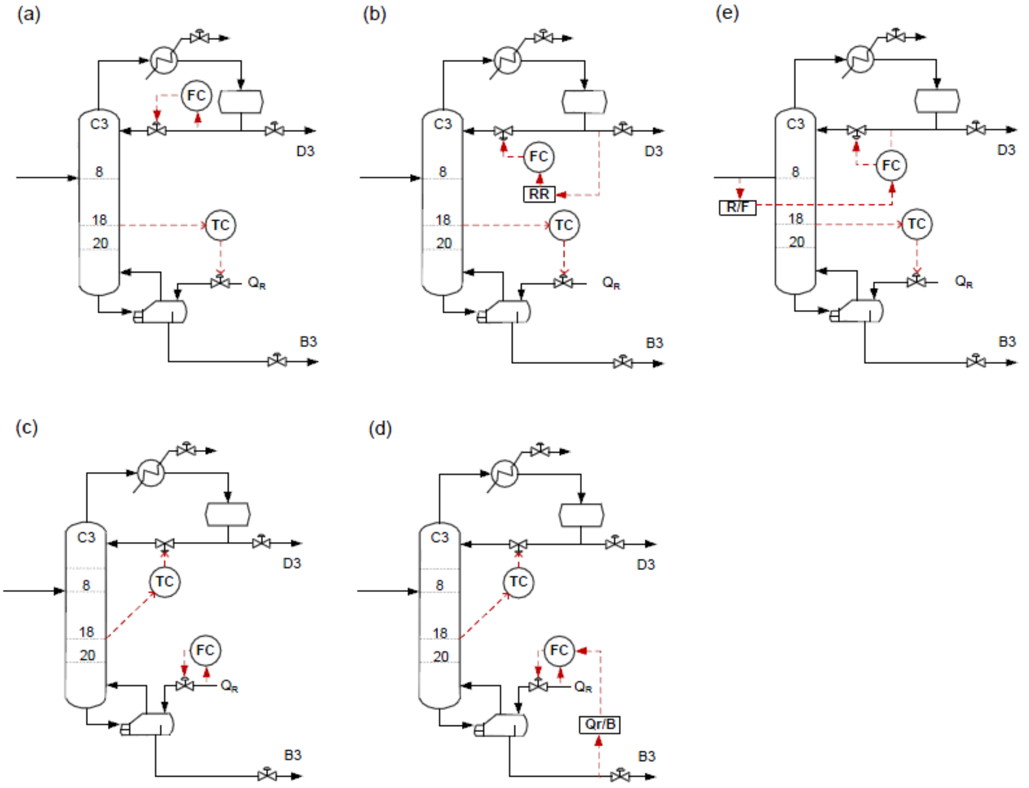


Figure 5.35 Alternative C3 control structures (a) R structure, (b) RR structure, (c) Q_R structure, (d) Q_R/B structure, and (e) R/F structure

Figure 5.36 and 5.37 give responses for disturbances in the MHOH component flow and MMH composition of the column C3 feed, respectively. The purity of MMH product is focused for this column. That is, the control structure that we select must be able to maintain the purity of MMH product to its specification. The first graphs on the right of both Figures show that the R, RR, Q_R and R/F results are quite the same, but in the Q_R/B results, the purity of MMH product cannot be maintained close to its specification.

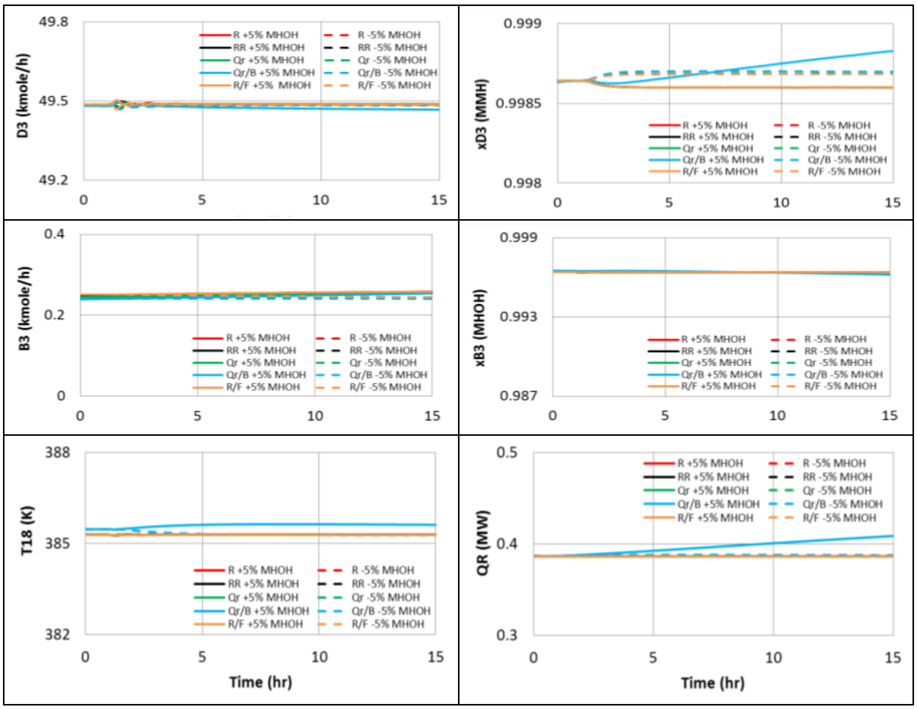


Figure 5.36 Comparison of alternative C3 control structures when component flow changes

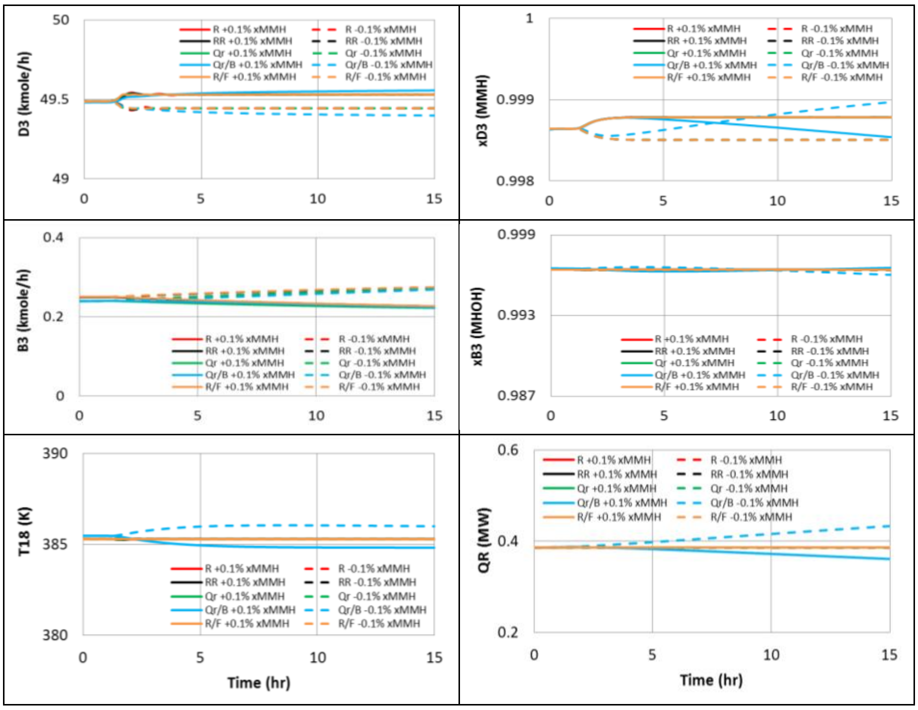


Figure 5.37 Comparison of alternative C3 control structures when composition changes

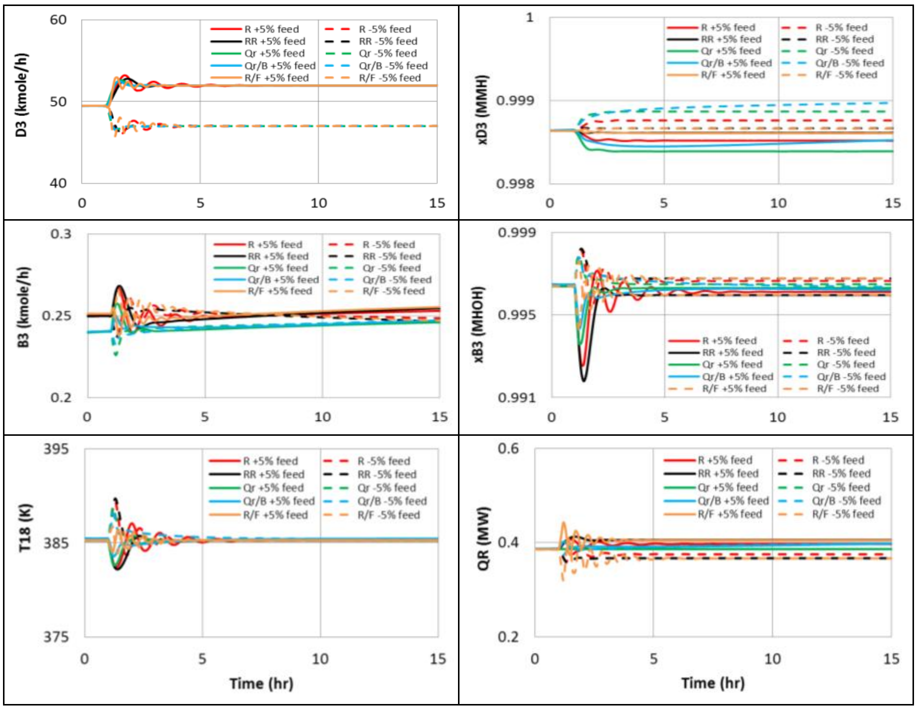


Figure 5.38 Comparison of alternative C3 control structures when total flow changes

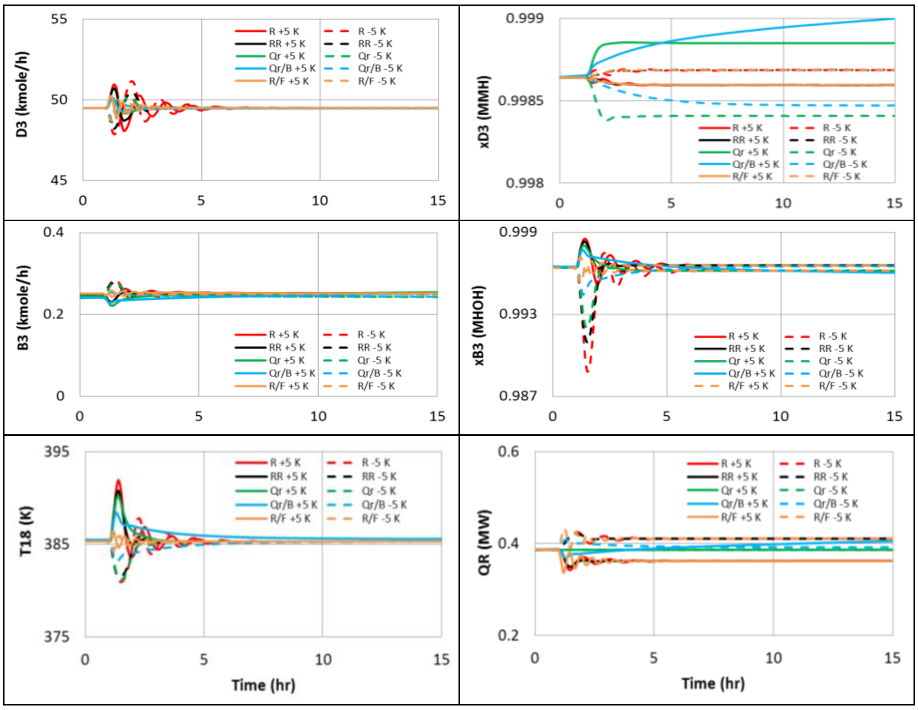


Figure 5.39 Comparison of alternative C3 control structures when temperature changes

.

Figure 5.38 gives responses for disturbances in the total flow of the C3 feed. Looking at the first graph on the right, we can see that the MMH purity in the RR and R/F results are maintained closest to their specifications, but the RR result gives responses smoother than R/F results.

Figure 5.39 shows how variables in column C3 change for disturbances in the temperature. The first graph on the right shows that the MMH purity in the R, RR and R/F results are the same and maintained very close to its specification, so the R, RR and R/F results are better than the Q_R and Q_R/B results. From the responses in Figures 5.36 through 5.39 analyzed, we can conclude that the RR results are the best. Consequently, the RR structure is selected in column C3 for disturbance management.

Figure 5.40 shows the selected control structures in columns C1, C2, and C3 for disturbance management. They are just the control structures in each column for this step. Then, the other loops added to manage the material disturbances will be discussed.

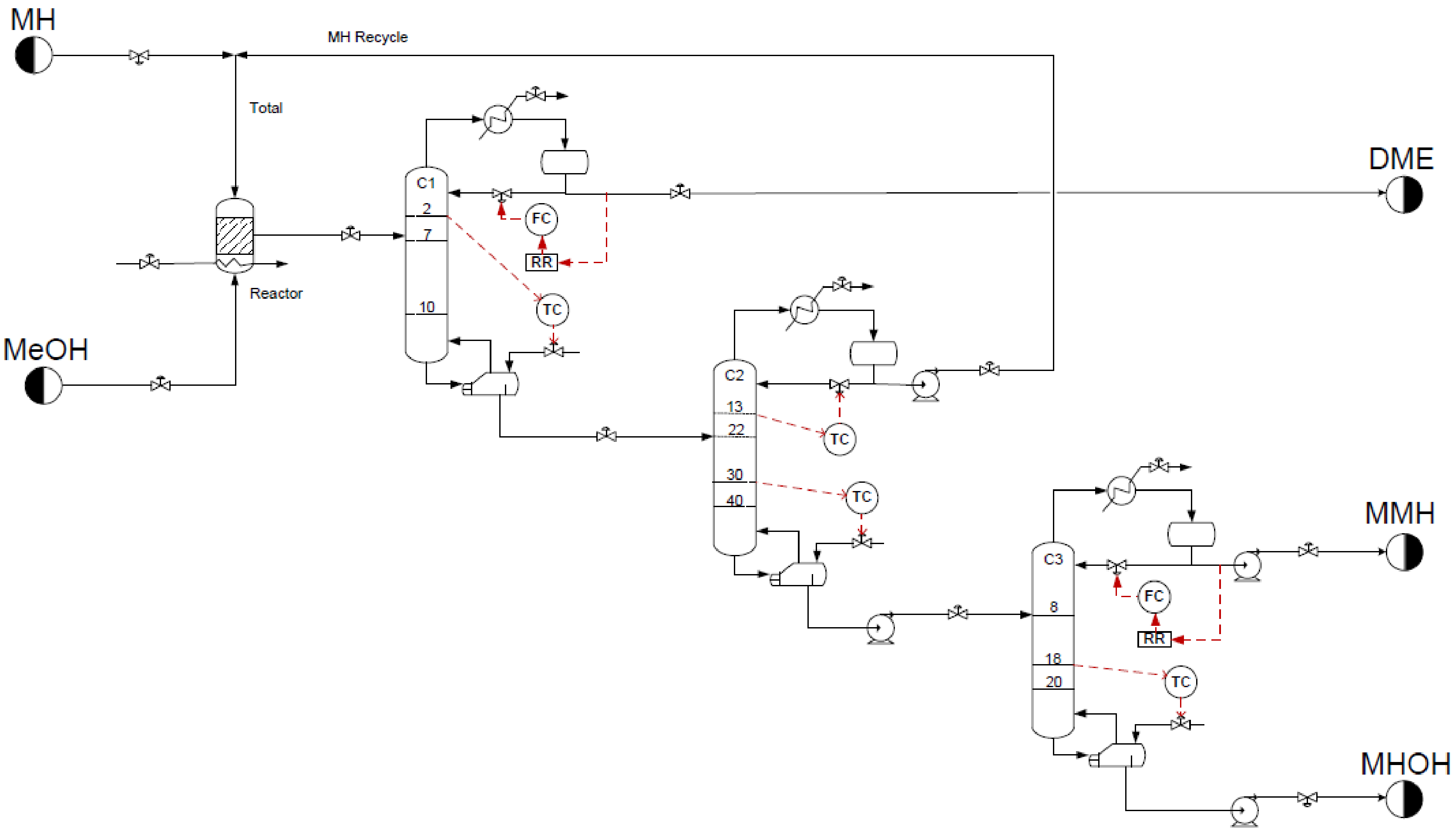


Figure 5.40 Flowsheet with controllers in each column for step 4.2 .

The material disturbances can be generated at reactors and separators, besides coming with feeds and recycle streams. The desired material pathways and the control structures used for managing each material disturbance are given in Figure 5.41-5.47.

Methanol disturbance

There are three options for managing methanol disturbance as follows:

- Option 1: The limiting reactant methanol is flow-controlled into the process. The methanol composition in the reactor effluent is controlled by changing the set point of the reactor temperature controller. In addition, ratio controller is added to accommodate the variation of the fresh methanol, i.e. if there is a change in the methanol fresh feed flowrate, the total MH is also changed, as shown in Figure 5.41.
- Option 2: The limiting reactant methanol is flow-controlled into the process, but the methanol composition in the reactor effluent is controlled by changing the set point of the total flow of MH controller and there is no ratio controller, as shown in Figure 5.42.
- Option 3: The limiting reactant methanol is flow-controlled into the process, but the methanol composition in the reactor effluent is controlled by changing the set point of the ratio controller, as shown in Figure 5.43.

MH disturbance

The total MH (fresh feed plus recycle, which is the distillate from column C2) is flow-controlled into the process by manipulating the fresh feed of MH. The remaining MH is separated by column C2 and recycled back to the process. If there is the extra load of MH, this extra load will be pushed to the recycle stream (according to the desired MH pathway) using Dual-end structure, as discussed earlier. See Figure 5.44 for an illustration.

DME disturbance

DME byproduct is generated at the reactor and separated by column C1 as the distillate product. If there is the extra load of DME, this extra load will be pushed to the to the distillate stream (according to the desired DME pathway) using RR structure, as discussed earlier. Figure 5.45 gives the control structures for DME disturbance management.

MMH and MHOH disturbances

MMH product and MHOH byproduct are generated at the reactor and separated from each other by column C3. The purity of MMH product is focused for this column while the disturbance occurs. As discussed earlier, RR structure is used for MMH and MHOH disturbance managements. See Figures 5.46 and 5.47.

Step 5: Design the rest of the control loops

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

The rest of the inventory loops (pressure and liquid levels) in each unit are designed and listed below with their controlled and manipulated variables. See Figure 5.48 for an illustration.

- Reactor liquid level is controlled by manipulating reactor effluent.
- Pressures in all three columns are controlled by manipulating condenser heat removal.
- The reboiler levels in column C1 and C2 are controlled by manipulating bottoms flow rates.
- The reflux-drum level in column C2 is controlled by manipulating distillate flow rate.

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

No adding enhanced controls in this study, so this step is skipped.

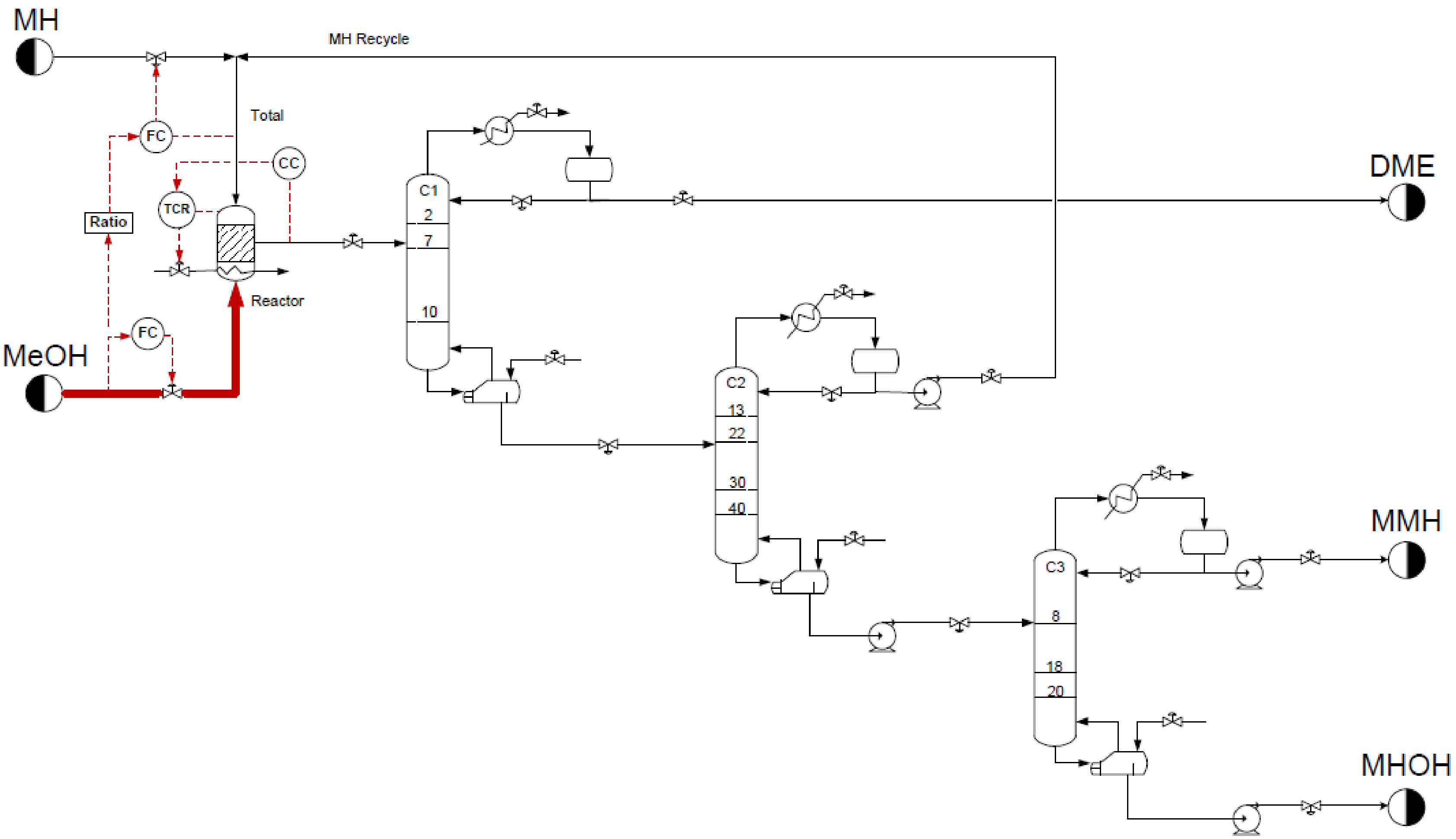


Figure 5.41 Control structures for methanol disturbance management (option 1)

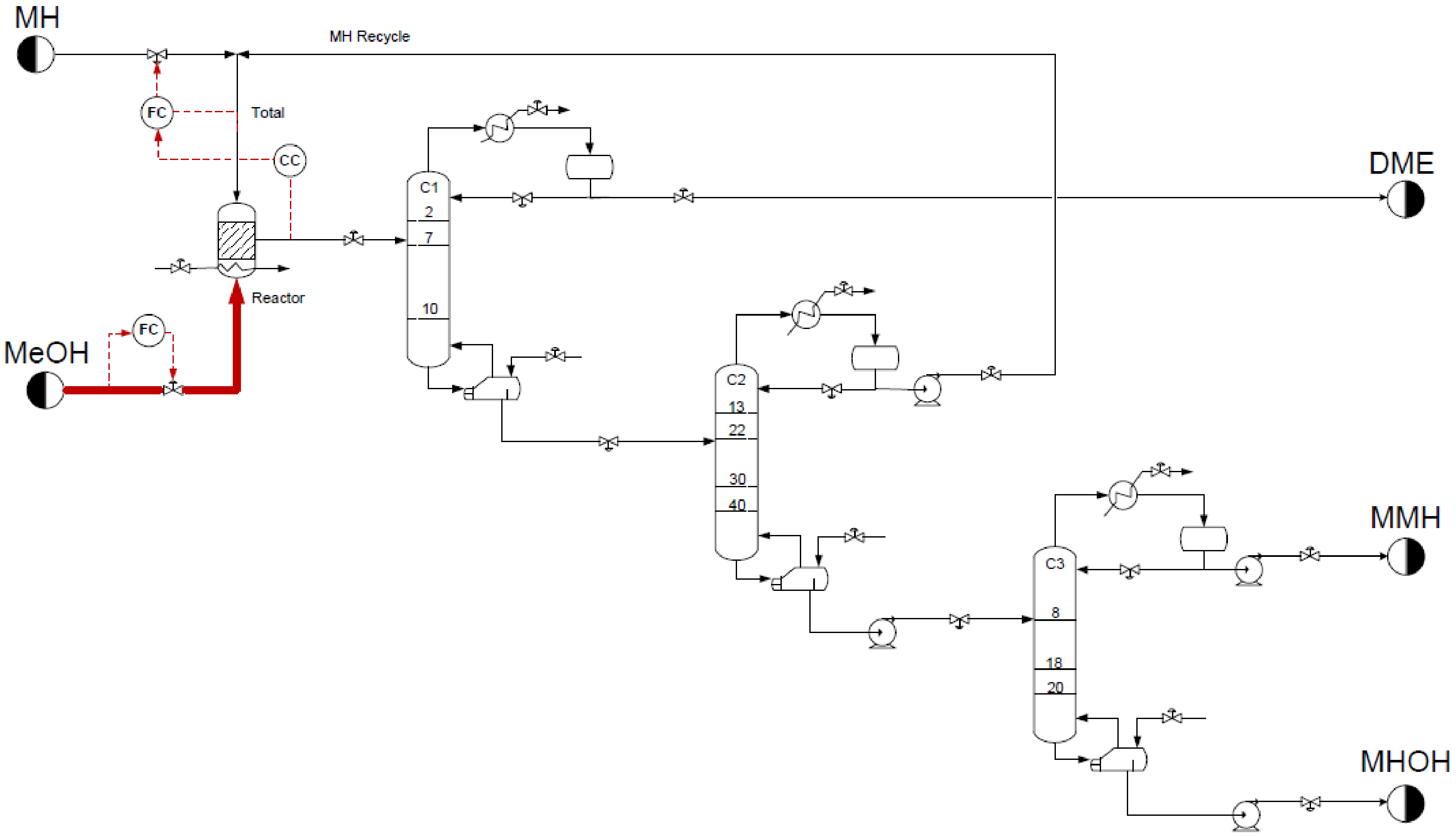


Figure 5.42 Control structures for methanol disturbance management (option 2)

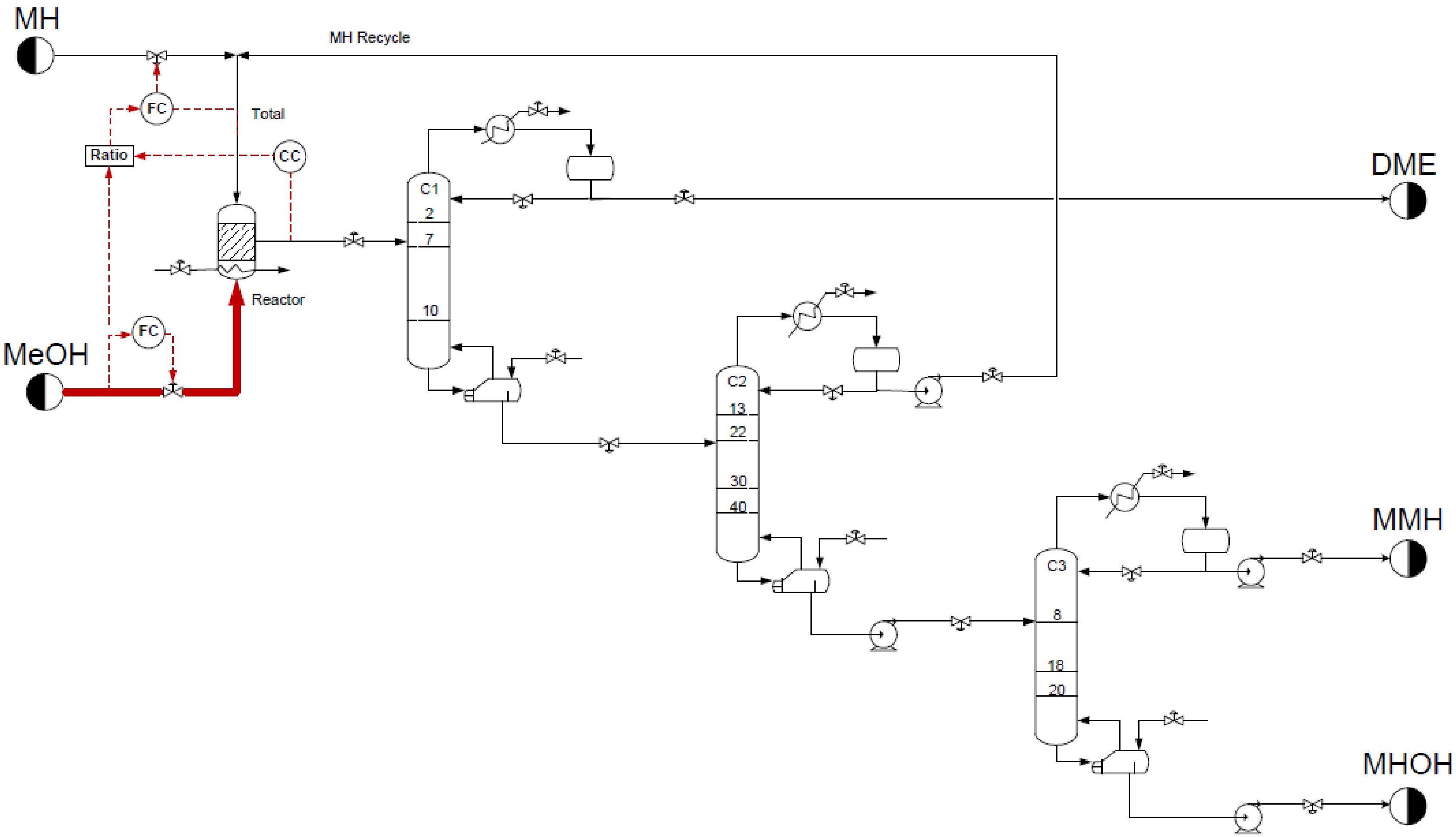


Figure 5.43 Control structures for methanol disturbance management (option 3)

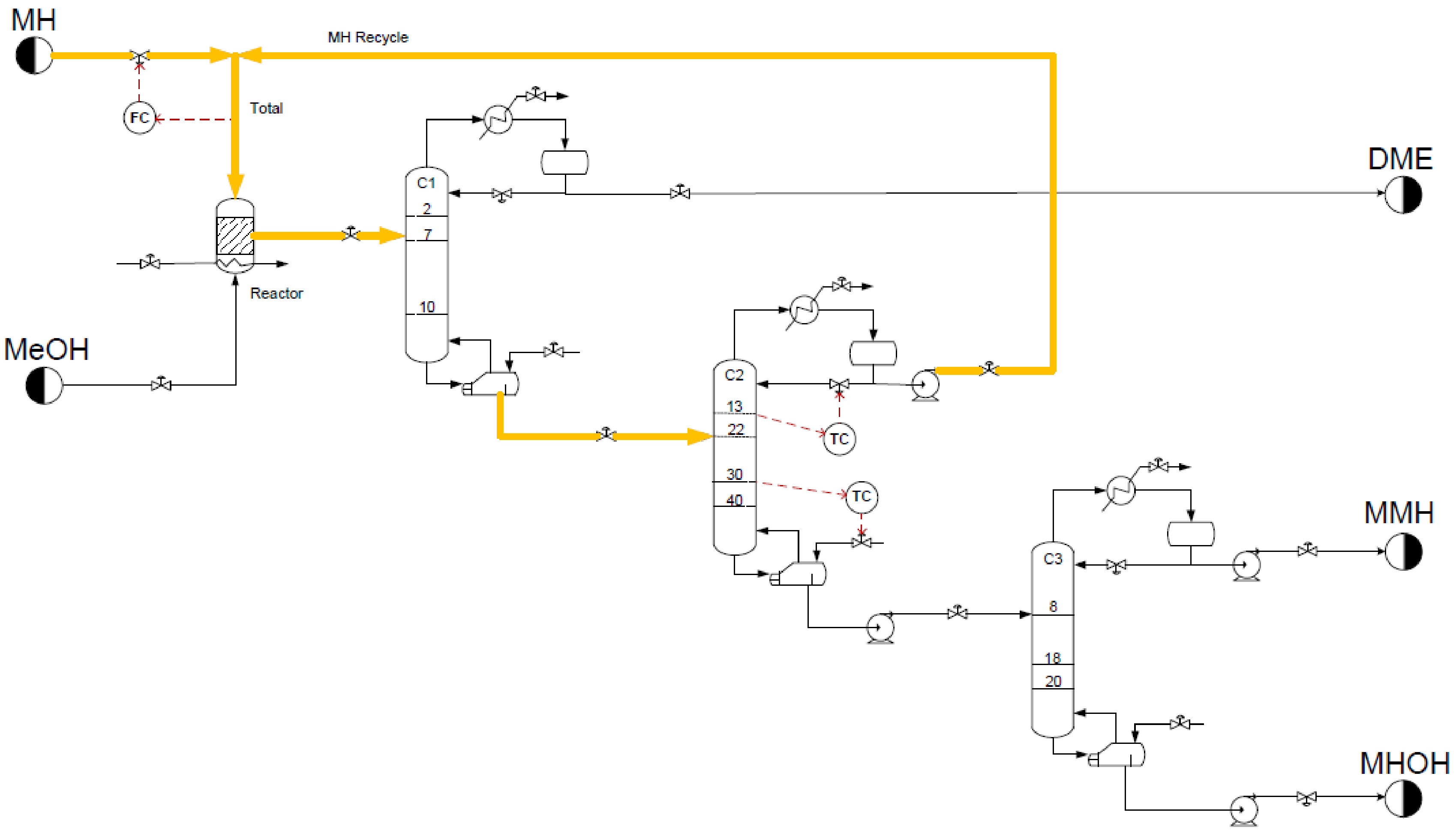


Figure 5.44 Control structures for MH disturbance management

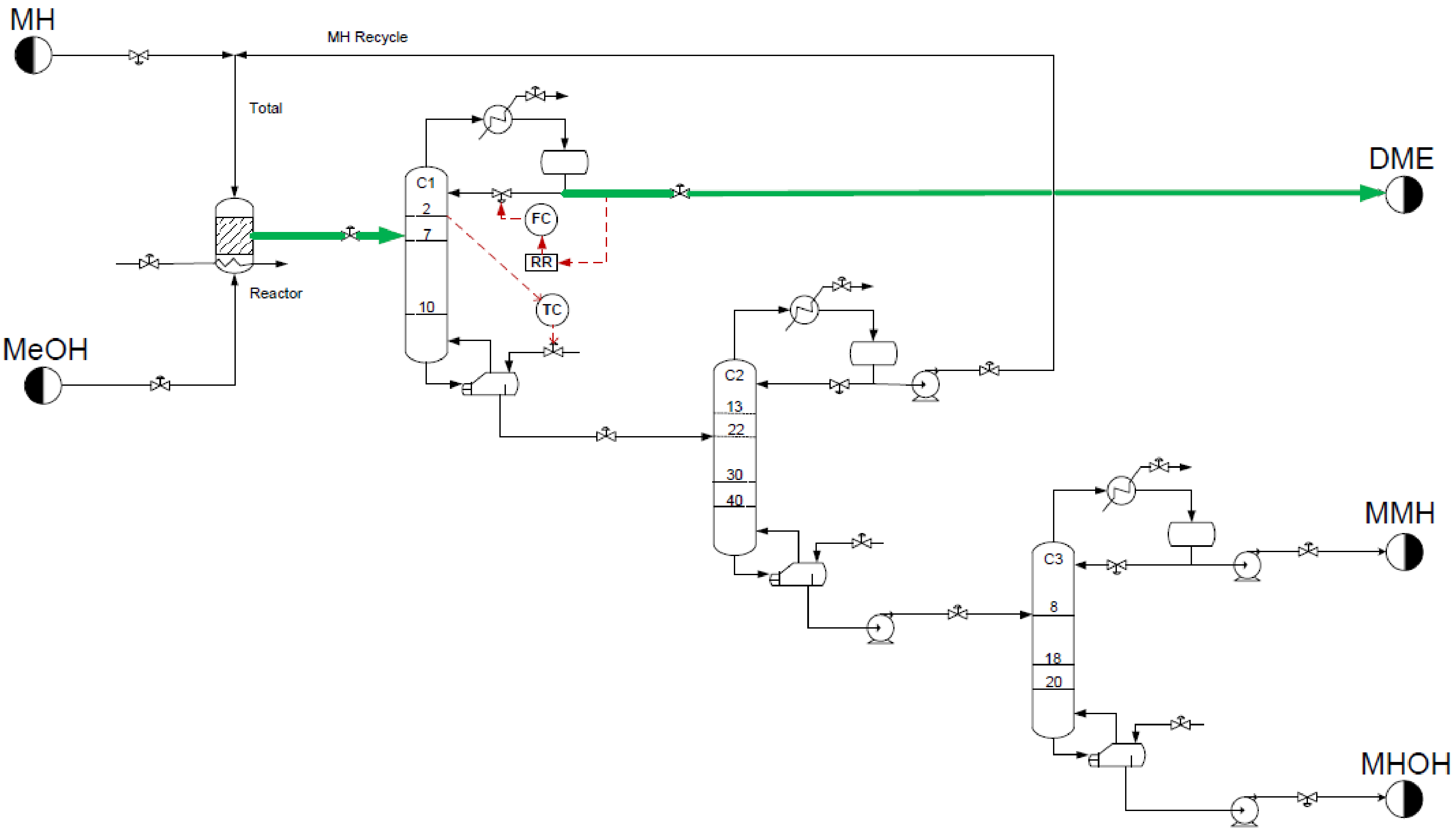


Figure 5.45 Control structures for DME disturbance management

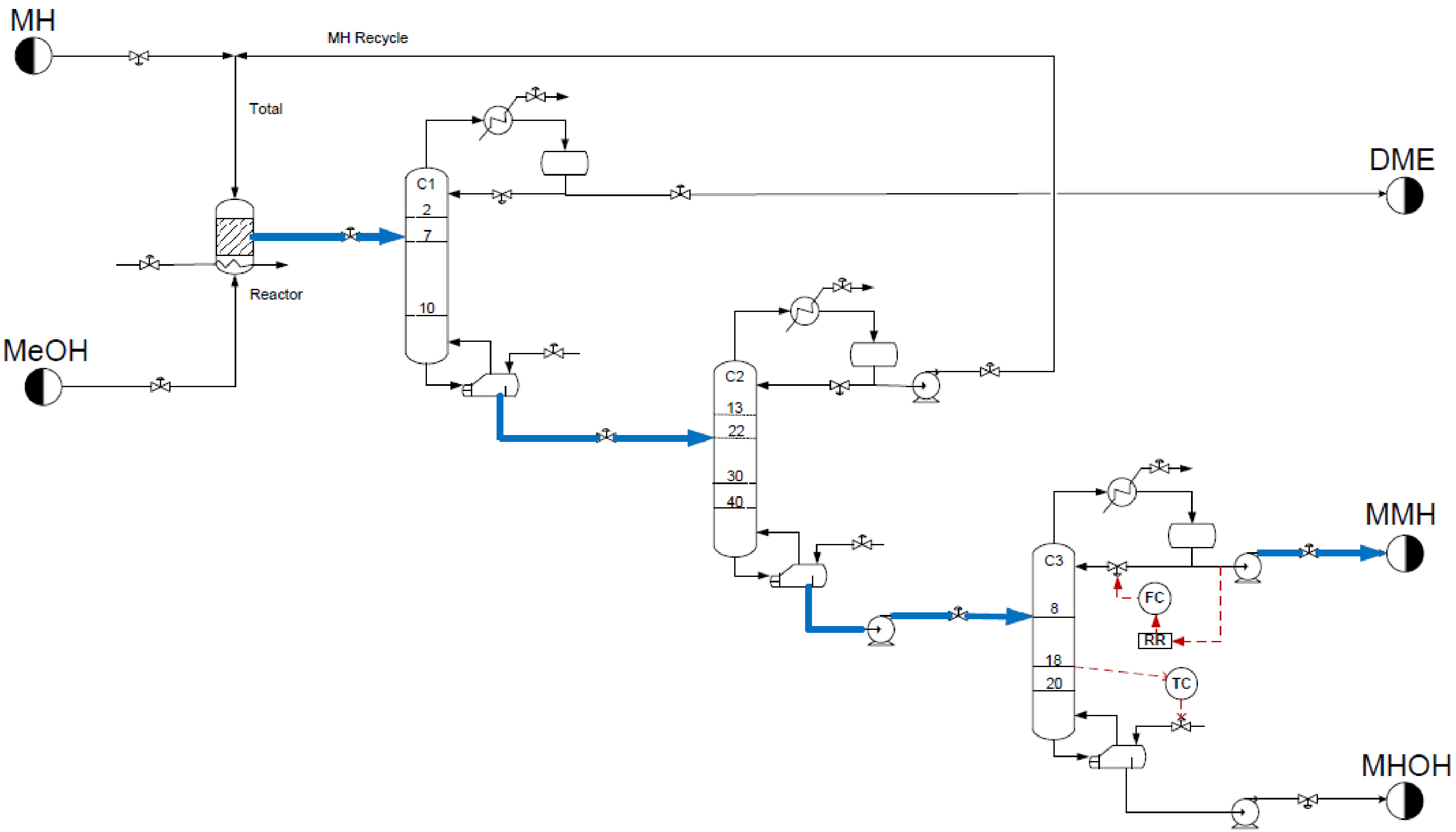


Figure 5.46 Control structures for MMH disturbance management

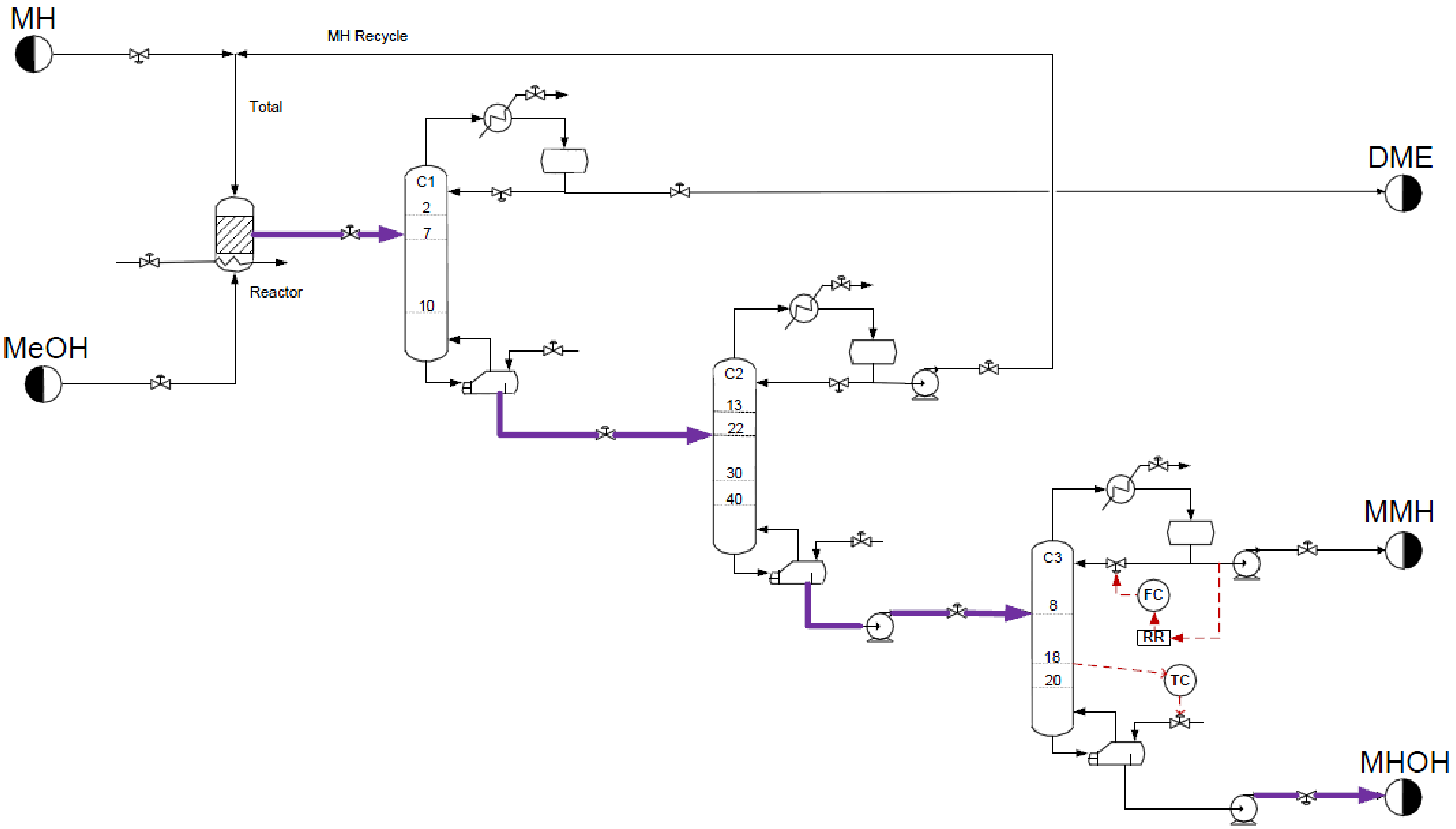


Figure 5.47 Control structures for MHOH disturbance management

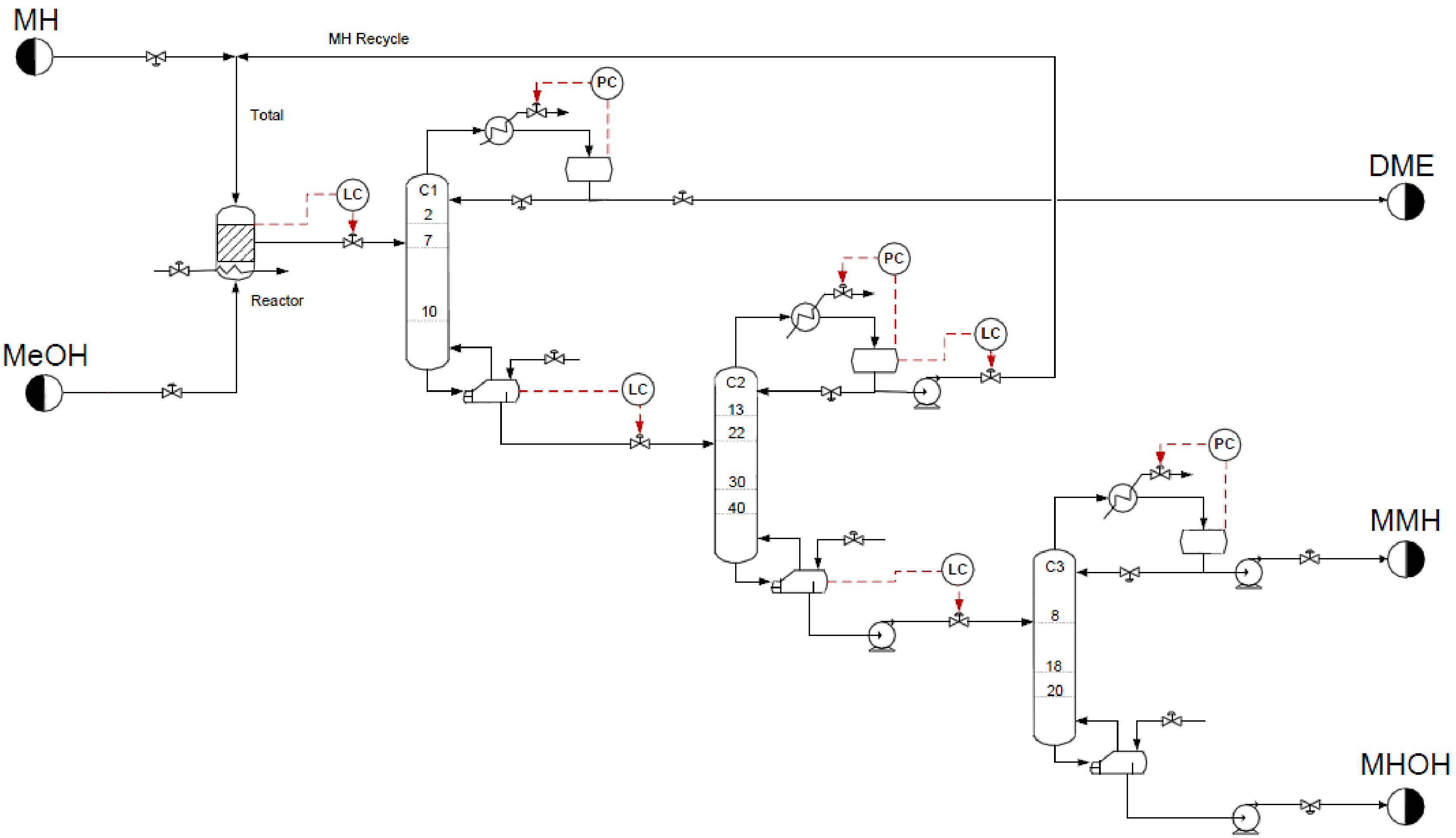


Figure 5.48 Flowsheet with controllers for step 5.1

Step 6: Energy management via heat exchanger networks

Since there are no hot process streams that must be cooled and cold process streams that must be heated in the process, so it is not necessary to design a network of heat exchangers.

Step 7: Optimize economics and/or improve control performance

The economics of the process explored by Luyben (2010a) have already been used as the basis in this study, so this step is skipped.

Now, we can conclude that there are four alternative plantwide control structures for this process as follows:

- Control structure of base case (BC): The plantwide control structure proposed Luyben (2010a).
- Control structures 1-3 (CS1-3): The plantwide control structures designed in this study. These plantwide control structures are the same in the separation section, but they are just different in the reaction section.

Figures 5.49 through 5.52 give the control structure of base case and the designed control structures. The control loops with their controlled and manipulated variables for all control structures are given in Table 5.2.

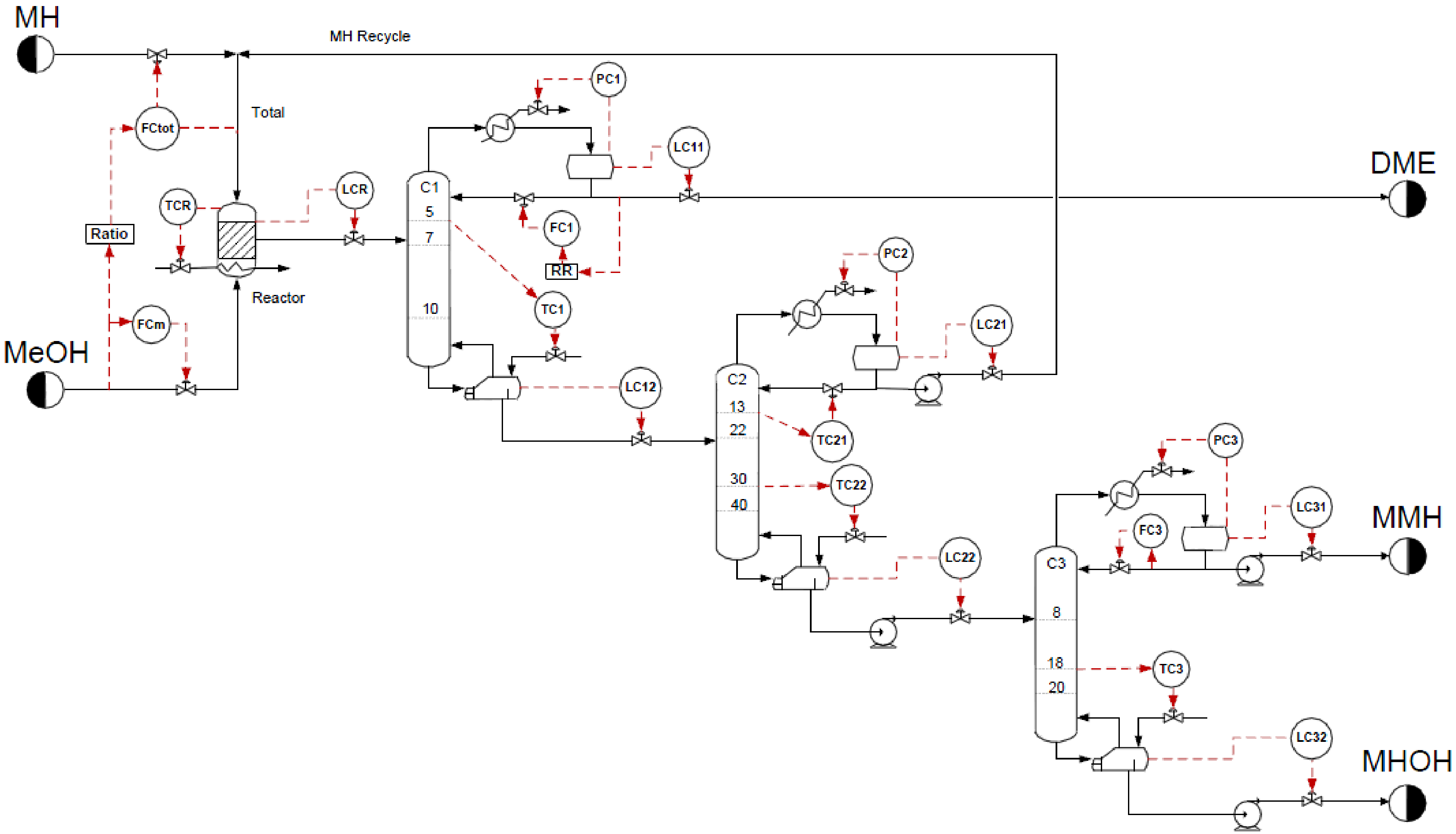


Figure 5.49 Control structure of base case (BC)

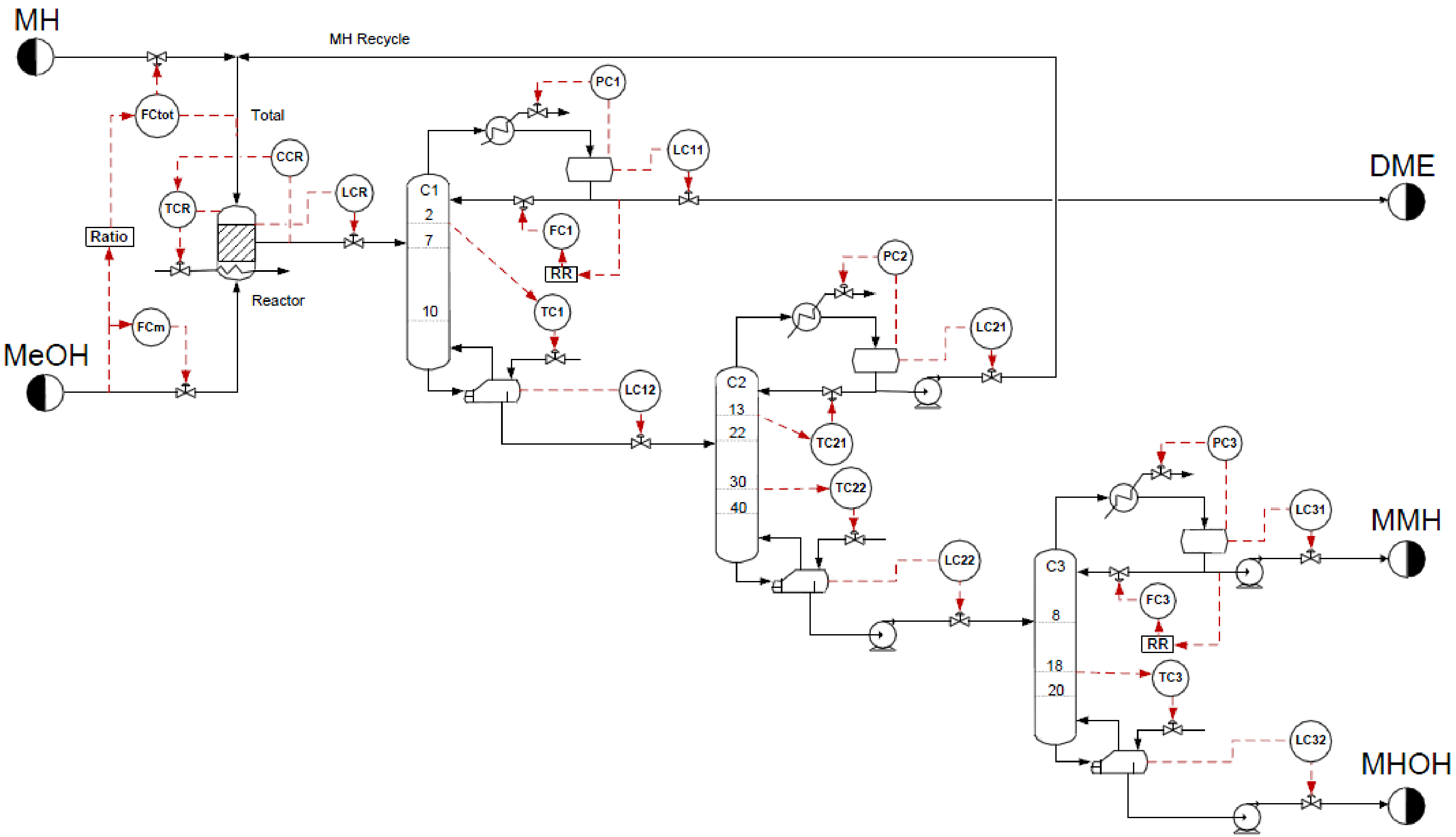


Figure 5.50 Control structure 1 (CS1)

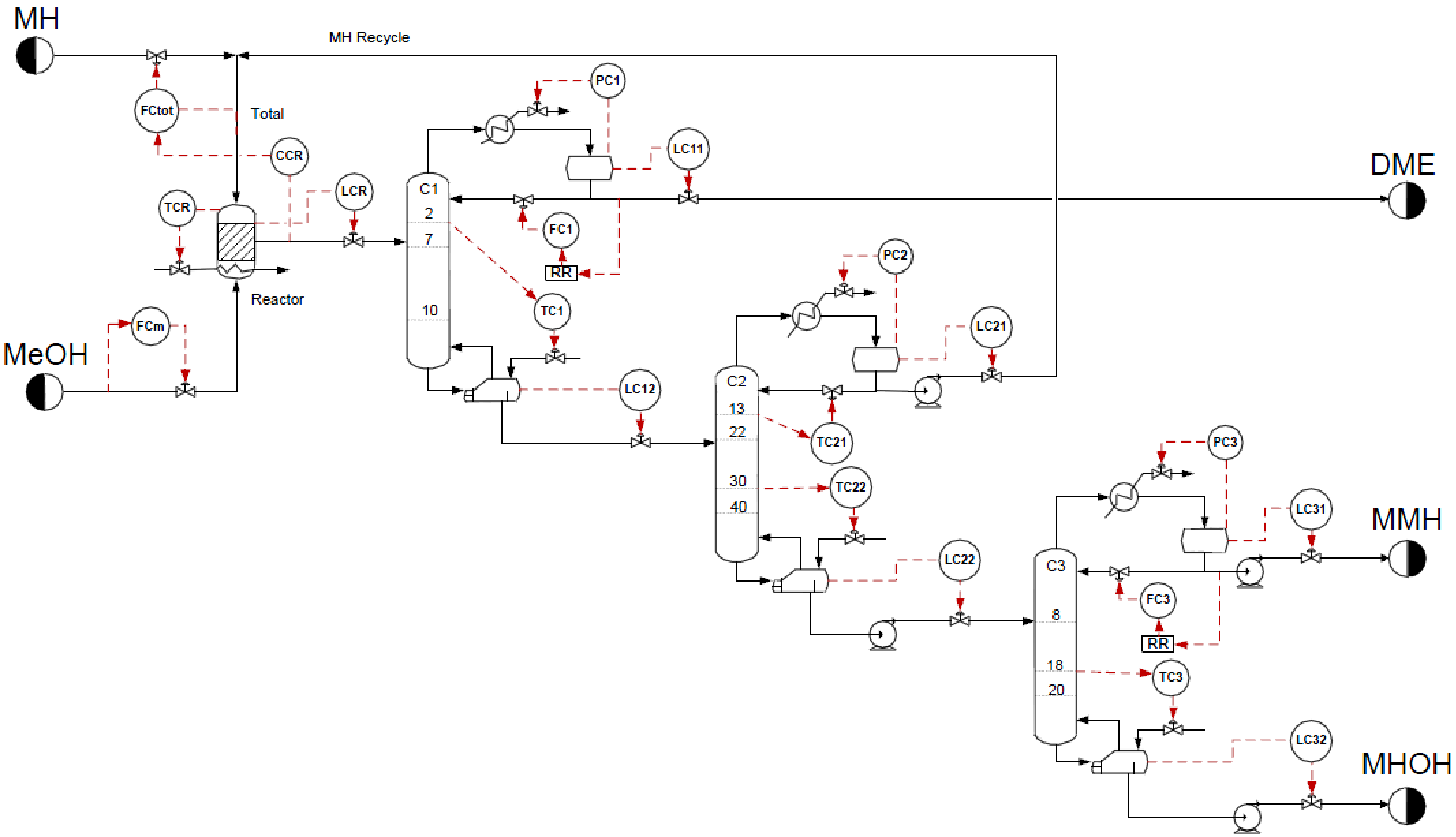


Figure 5.51 Control structure 2 (CS2)

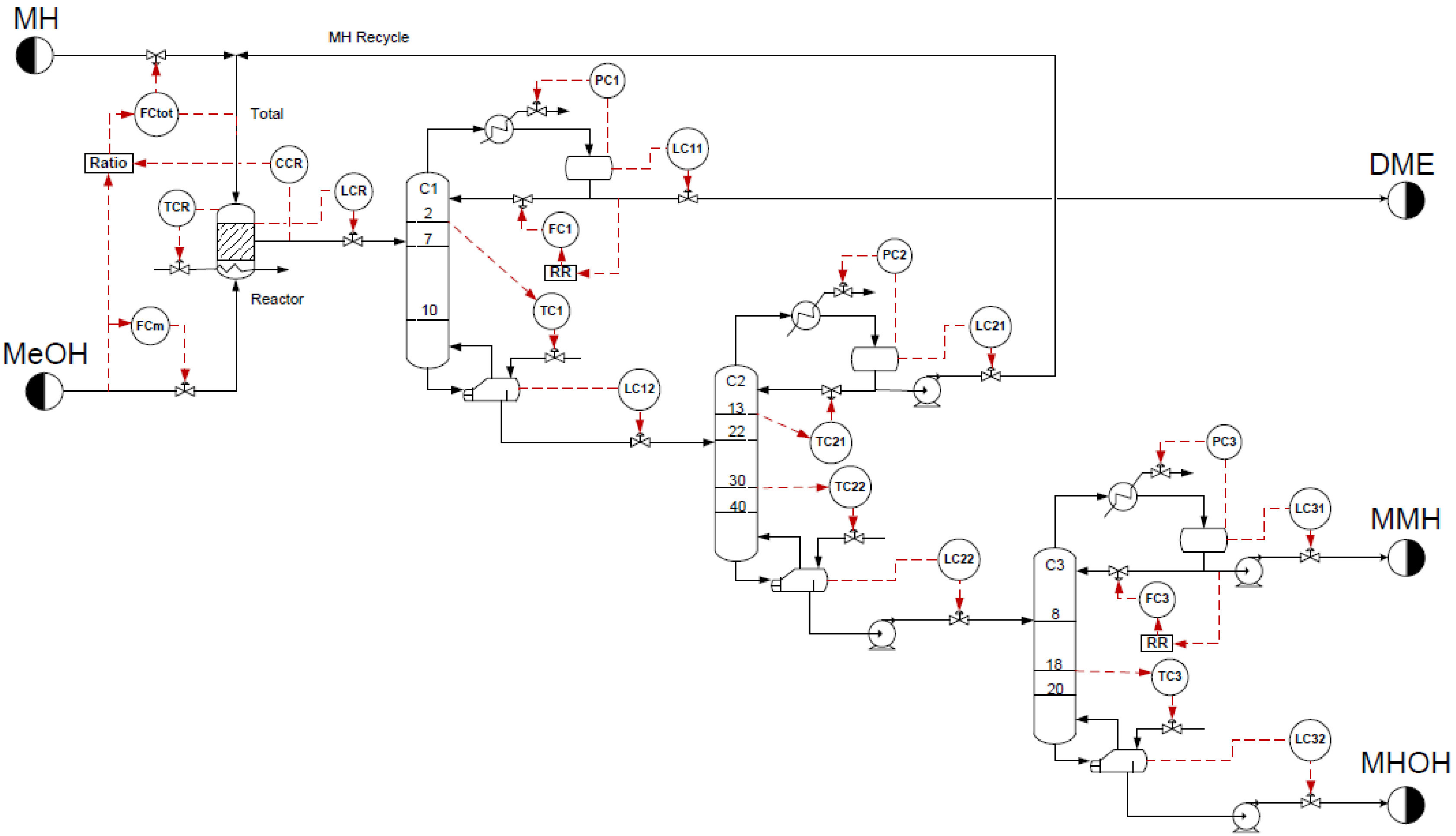


Figure 5.52 Control structure 3 (CS3)

Table 5.2 The control loops with their controlled and manipulated variables for all control structures

Unit	Controller	Variable	BC	CS1	CS2	CS3
Methanol feed	FCm	Controlled variable	Methanol flow rate	Methanol flow rate	Methanol flow rate	Methanol flow rate
		Manipulated variable	Fresh feed of methanol	Fresh feed of methanol	Fresh feed of methanol	Fresh feed of methanol
Total MH	FCtot	Controlled variable	Total flow of MH	Total flow of MH	Total flow of MH	Total flow of MH
		Manipulated variable	Fresh feed of MH	Fresh feed of MH	Fresh feed of MH	Fresh feed of MH
Ratio of feeds	Ratio	Controlled variable	Ratio of feeds	Ratio of feeds	-	Ratio of feeds
		Manipulated variable	Set point of FCtot	Set point of FCtot	-	Set point of FCtot
Reactor	TCR	Controlled variable	Reactor temperature	Reactor temperature	Reactor temperature	Reactor temperature
		Manipulated variable	Coolant flow rate	Coolant flow rate	Coolant flow rate	Coolant flow rate
	LCR	Controlled variable	Reactor liquid level	Reactor liquid level	Reactor liquid level	Reactor liquid level
		Manipulated variable	Reactor effluent	Reactor effluent	Reactor effluent	Reactor effluent
	CCR	Controlled variable	-	Methanol composition	Methanol composition	Methanol composition
		Manipulated variable	-	Set point of TCR	Set point of FCtot	Set point of Ratio
Column C1	FC1	Controlled variable	Reflux ratio	Reflux ratio	Reflux ratio	Reflux ratio
		Manipulated variable	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate
	TC1	Controlled variable	Tray 5 temperature	Tray 2 temperature	Tray 2 temperature	Tray 2 temperature
		Manipulated variable	Reboiler heat input	Reboiler heat input	Reboiler heat input	Reboiler heat input

Table 5.2 (Continued) The control loops with their controlled and manipulated variables for all control structures

Equipment	Controller	Variables	BC	CS1	CS2	CS3
Column C1	PC1	Controlled variable	Condenser pressure	Condenser pressure	Condenser pressure	Condenser pressure
		Manipulated variable	Heat removal	Heat removal	Heat removal	Heat removal
	LC11	Controlled variable	Reflux-drum level	Reflux-drum level	Reflux-drum level	Reflux-drum level
		Manipulated variable	Distillate flow rate	Distillate flow rate	Distillate flow rate	Distillate flow rate
	LC12	Controlled variable	Reboiler level	Reboiler level	Reboiler level	Reboiler level
		Manipulated variable	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate
Column C2	TC21	Controlled variable	Tray 13 temperature	Tray 13 temperature	Tray 13 temperature	Tray 13 temperature
		Manipulated variable	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate
	TC22	Controlled variable	Tray 30 temperature	Tray 30 temperature	Tray 30 temperature	Tray 30 temperature
		Manipulated variable	Reboiler heat input	Reboiler heat input	Reboiler heat input	Reboiler heat input
	PC2	Controlled variable	Condenser pressure	Condenser pressure	Condenser pressure	Condenser pressure
		Manipulated variable	Heat removal	Heat removal	Heat removal	Heat removal
	LC21	Controlled variable	Reflux-drum level	Reflux-drum level	Reflux-drum level	Reflux-drum level
		Manipulated variable	Distillate flow rate	Distillate flow rate	Distillate flow rate	Distillate flow rate
	LC22	Controlled variable	Reboiler level	Reboiler level	Reboiler level	Reboiler level
		Manipulated variable	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate

Table 5.2 (Continued) The control loops with their controlled and manipulated variables for all control structures

Equipment	Controller	Variables	BC	CS1	CS2	CS3
Column C3	FC3	Controlled variable	Reflux flow rate	Reflux ratio	Reflux ratio	Reflux ratio
		Manipulated variable	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate
	TC3	Controlled variable	Tray 18 temperature	Tray 18 temperature	Tray 18 temperature	Tray 18 temperature
		Manipulated variable	Reboiler heat input	Reboiler heat input	Reboiler heat input	Reboiler heat input
	PC3	Controlled variable	Condenser pressure	Condenser pressure	Condenser pressure	Condenser pressure
		Manipulated variable	Heat removal	Heat removal	Heat removal	Heat removal
	LC31	Controlled variable	Reflux-drum level	Reflux-drum level	Reflux-drum level	Reflux-drum level
		Manipulated variable	Distillate flow rate	Distillate flow rate	Distillate flow rate	Distillate flow rate
	LC32	Controlled variable	Reboiler level	Reboiler level	Reboiler level	Reboiler level
		Manipulated variable	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate	Bottoms flow rate

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

Two kinds of disturbances are made to test the ability of Luyben’s control structure (BC) and our control structures (CS1, CS2 and CS3) via HYSYS process simulation software. These compose of methanol feed flowrate disturbances (material disturbances) and methanol feed temperature disturbances (heat disturbances). Conventional PI controllers are used in all loops. All liquid level controllers are proportional only using with Kc = 2, except for the reactor level controller that uses a gain of 5. A higher value of gain is used since reactor level impacts reaction rates. The methodology used for tuning controllers is discussed in appendix B.

1. Methanol feed flowrate disturbances

Table 5.3 shows the responses of the systems for 5% disturbances in the set point of the methanol flow controller at time equal to 1 h. The solid lines are for a 5% increase. The dashed lines are for a 5% decrease. When methanol feed flowrate changes, the methanol composition in the reactor effluent (xMeoH in ROUT) also changes. In cases BC, CS1 and CS3, the set point of the total MH controller is rapidly changed by the ratio multiplier, and as for CS2, it is more slowly changed by the methanol composition controller at the reactor effluent. The reactor temperature (TR) in case CS1 is changed to the new set point to control methanol composition to its set point. The purities of the DME byproduct (xD1) and MMH product (xD3) in cases CS1, CS2 and CS3 are more closely maintained to the desired levels than those in case BC, whereas the purity of the byproduct MHOH changes very little in all cases. MMH product (D3) changes as well as slightly DME byproduct (D1) changes. MHOH byproduct (B3) shows little change. All temperatures are well-controlled. All reboiler heat duties change in the same direction as expected.

Table 5.3 Responses for methanol feed flowrate disturbances

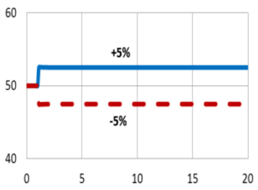
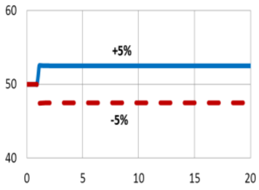
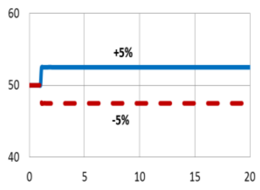
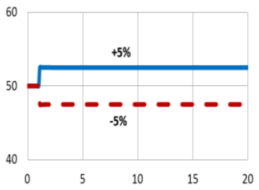
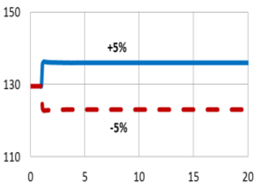
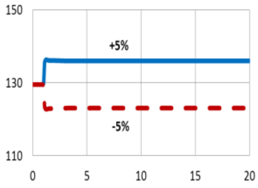
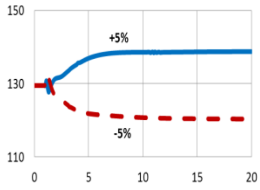
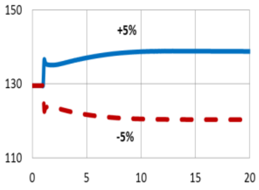
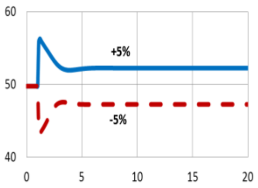
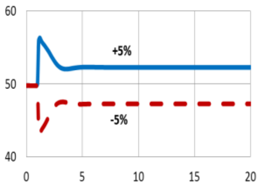
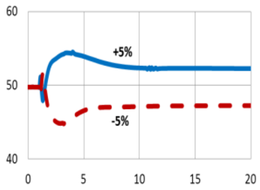
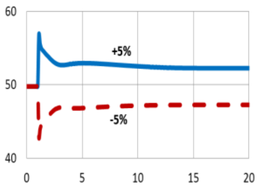
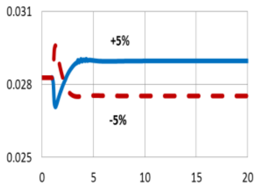
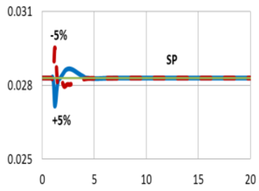
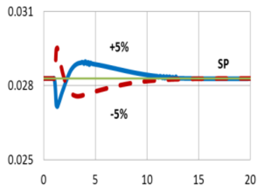
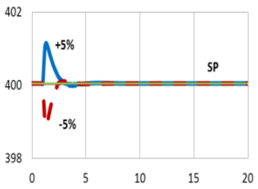
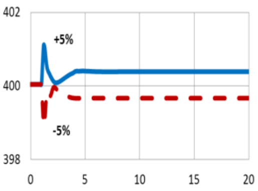
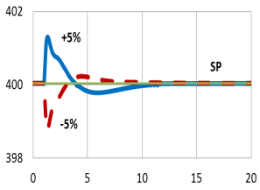
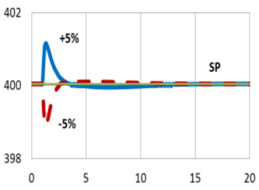
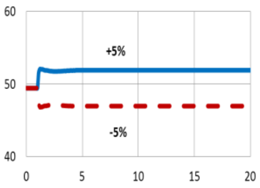
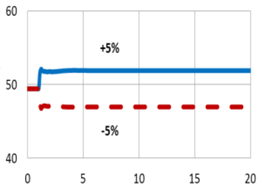
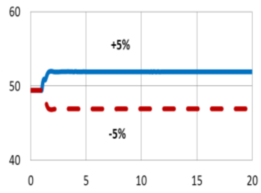
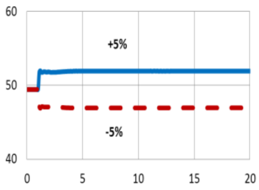
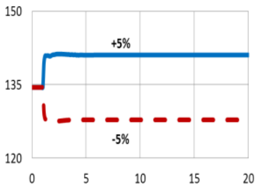
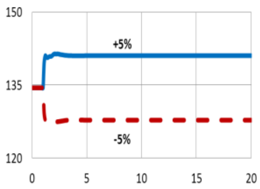
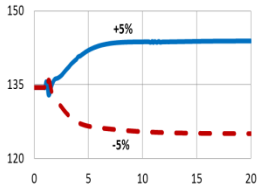
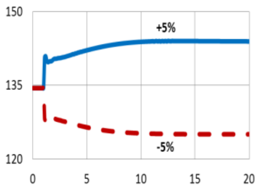
	BC	CS1	CS2	CS3
Methanol (kmol/h)				
Total (kmol/h)				
MH (kmol/h)				
xMeOH in ROUT				
TR (K)				
MMH in ROUT (kmol/h)				
ROUT (kmol/h)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.3 (Continued) Responses for methanol feed flowrate disturbances

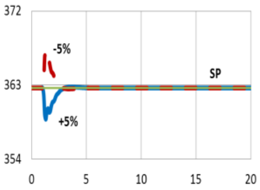
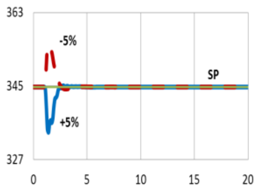
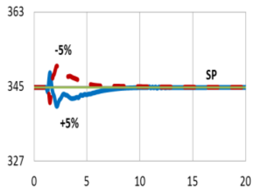
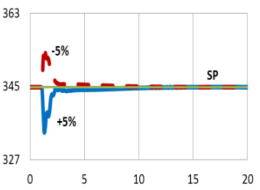
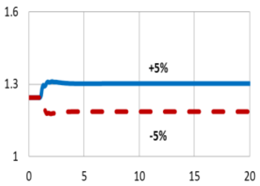
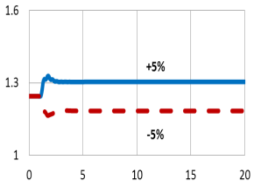
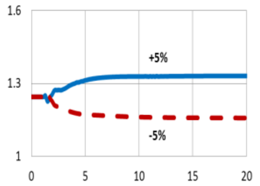
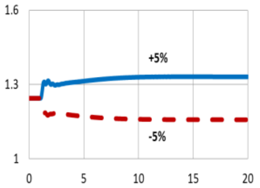
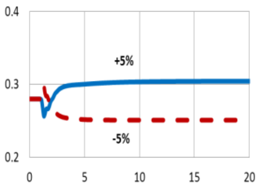
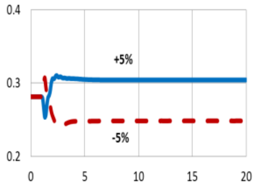
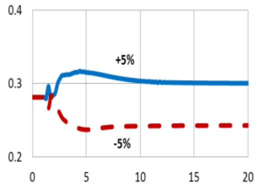
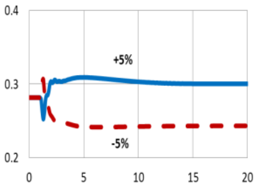
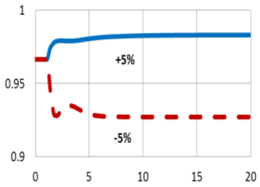
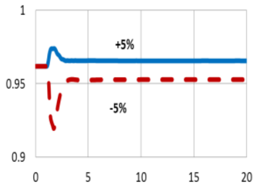
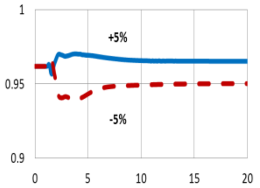
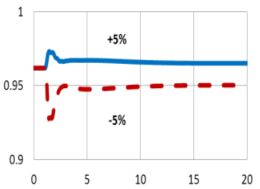
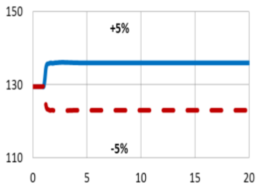
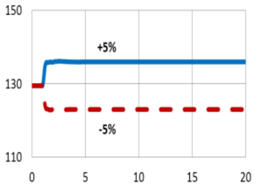
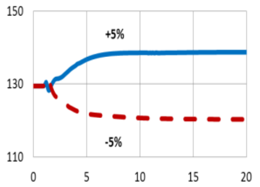
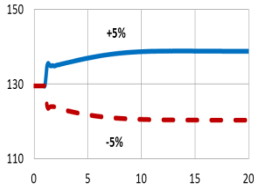
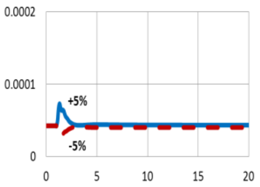
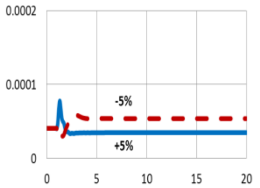
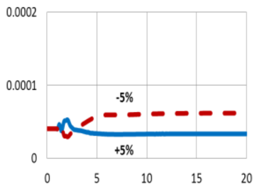
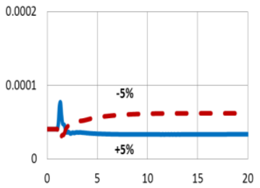
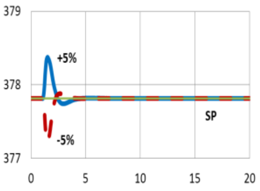
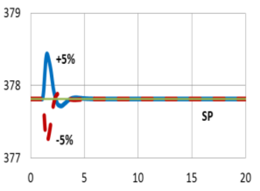
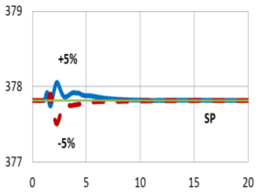
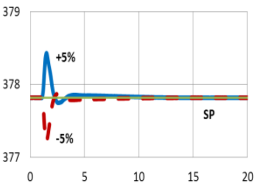
	BC	CS1	CS2	CS3
T1 (K)				
QR1 (MW)				
D1 (kmol/h)				
xD1 (DME)				
B1 (kmol/h)				
xB1 (DME)				
T21 (K)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.3 **(Continued)** Responses for methanol feed flowrate disturbances

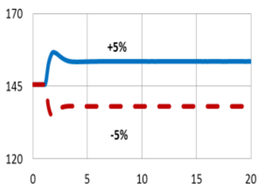
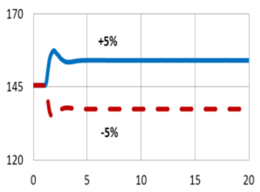
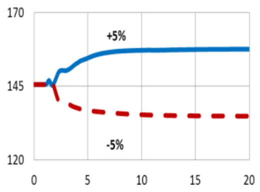
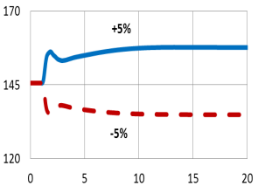
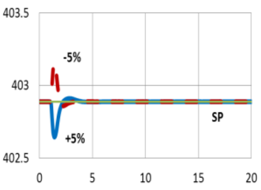
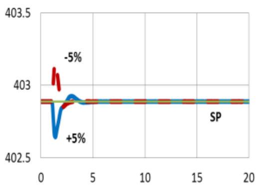
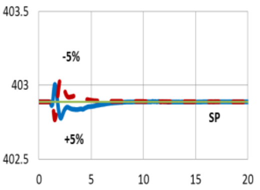
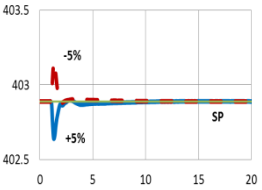
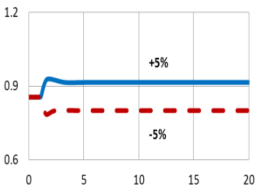
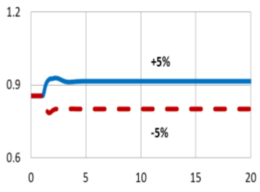
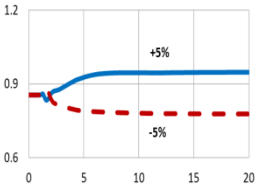
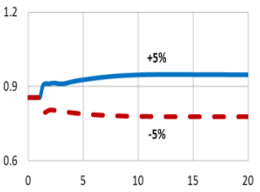
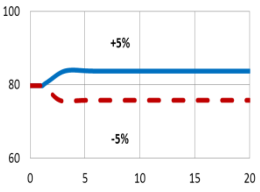
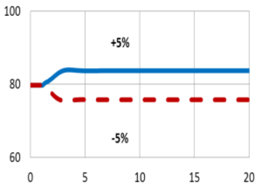
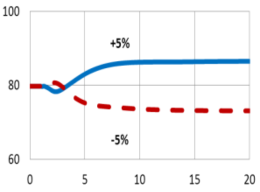
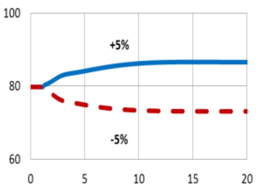
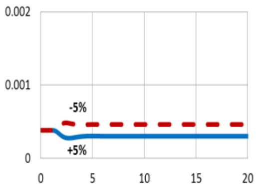
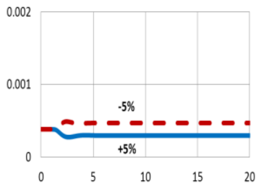
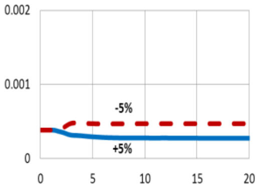
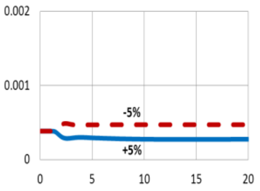
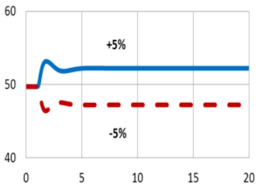
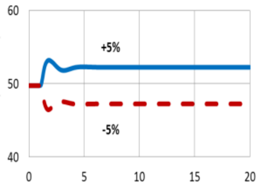
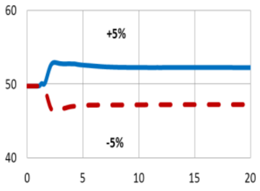
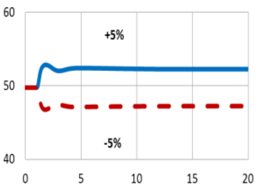
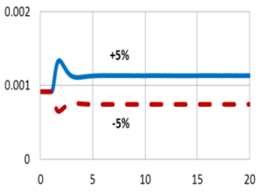
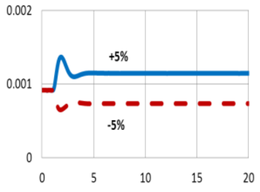
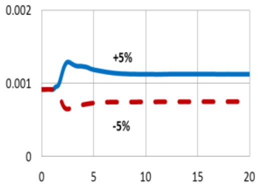
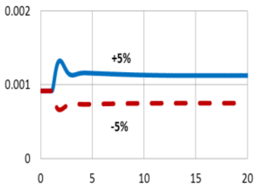
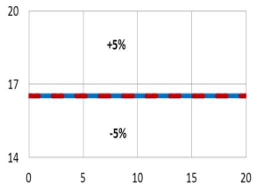
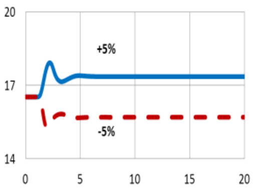
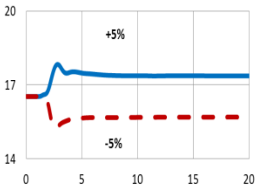
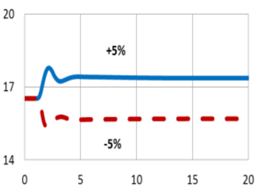
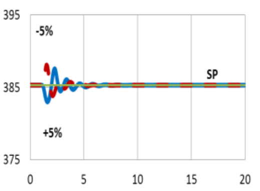
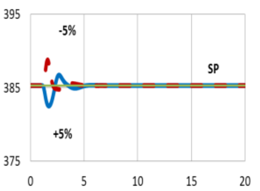
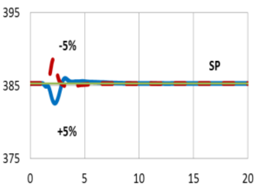
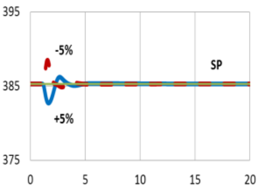
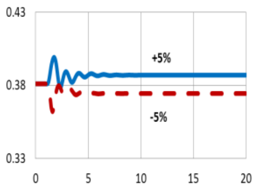
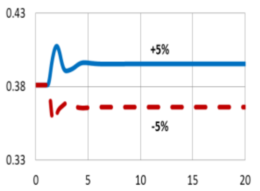
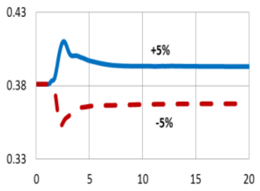
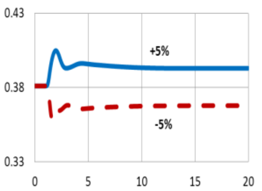
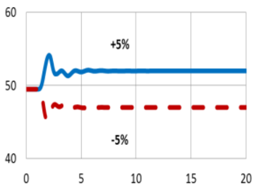
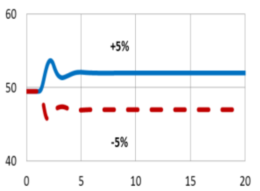
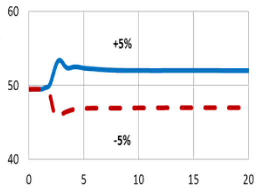
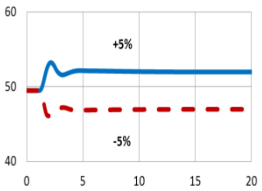
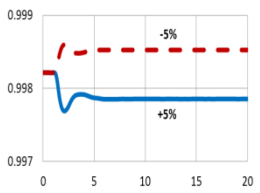
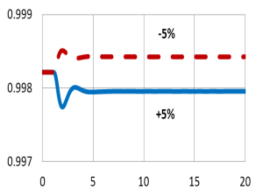
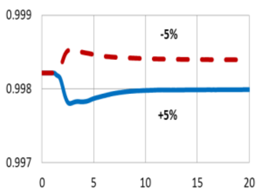
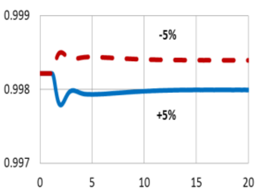
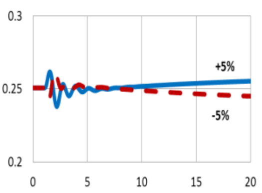
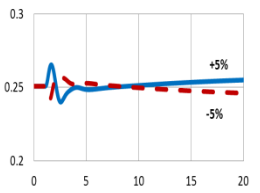
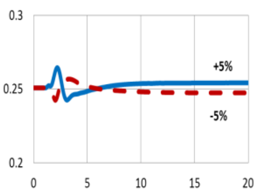
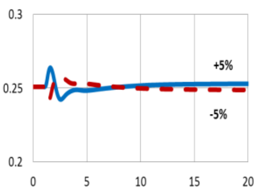
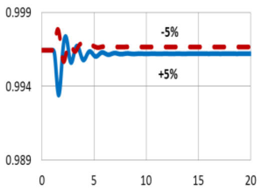
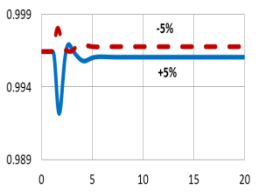
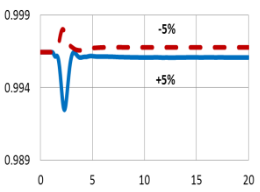
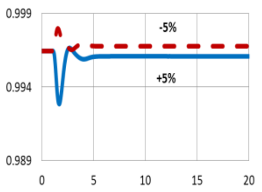
	BC	CS1	CS2	CS3
R2 (kmol/h)				
T22 (K)				
QR2 (MW)				
D2 (kmol/h)				
xD2 (MMH)				
B2 (kmol/h)				
xB2 (MH)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.3 (Continued) Responses for methanol feed flowrate disturbances

	BC	CS1	CS2	CS3
R3 (kmol/h)				
T3 (K)				
QR3 (MW)				
D3 (kmol/h)				
xD3 (MMH)				
B3 (kmol/h)				
xB3 (MHOH)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

2. Methanol feed temperature disturbances

Table 5.4 gives results for 10 K disturbances in temperature of the methanol feed at time equal to 1 h. The solid lines indicate when methanol feed temperature is increased. The feed temperature is changed from 393K to 403K. The dashed lines indicate when methanol feed temperature is decreased. The feed temperature is changed from 393K to 383K. When methanol feed temperature changes, the methanol composition in the reactor effluent (xMeoH in ROUT) also changes. In cases CS2 and CS3, this results in changes in the set point of the total MH controller and then in the reactor effluent flowrate (ROUT). Absolutely, the reactor effluent is the feed stream entering the separation section. If its flowrate changes, it causes the changes in process variables (PV) for all control loops in the separation section as seen in their initial responses. However, all temperatures and the purities of MMH product and DME and MHOH byproducts can be still controlled to their steady state values/set points. As a consequence, cases CS2 and CS3 are certain to be worse than the other cases. The control structures BC and CS1 can handle this disturbance better and their results are quite the same.

Table 5.4 Responses for methanol feed temperature disturbances

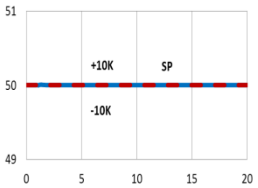
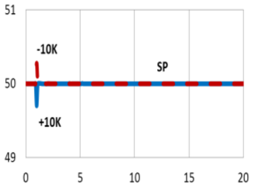
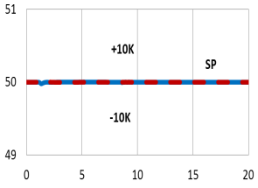
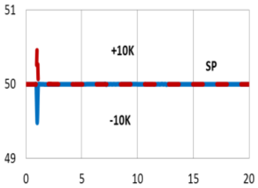
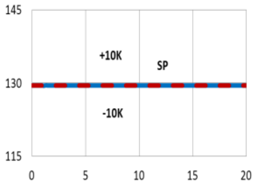
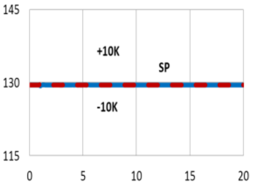
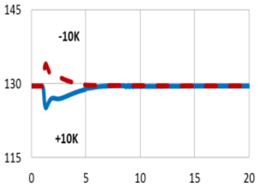
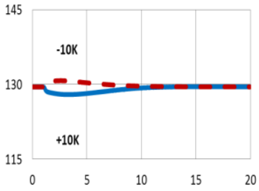
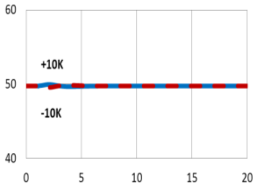
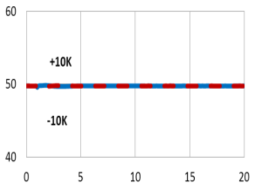
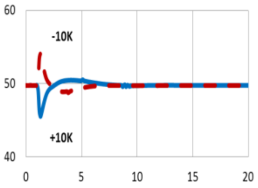
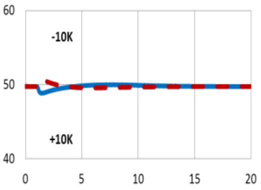
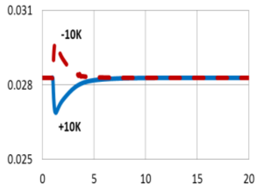
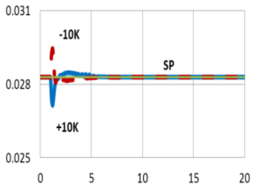
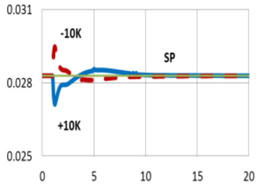
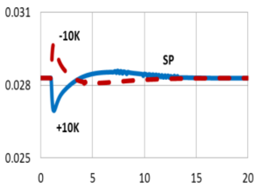
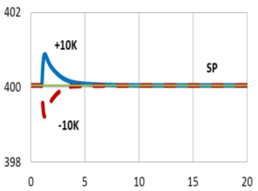
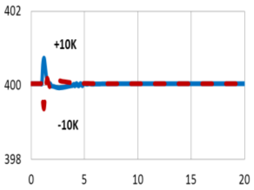
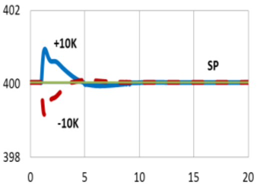
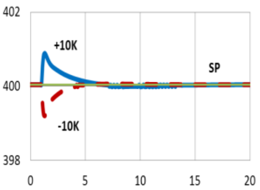
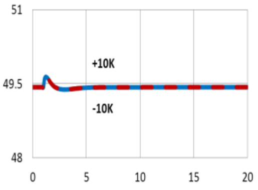
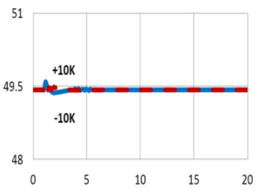
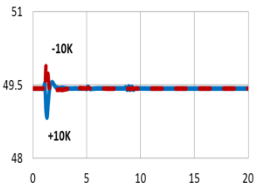
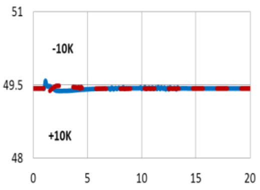
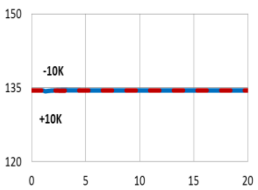
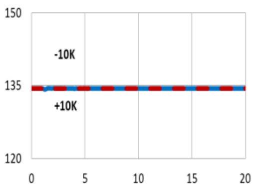
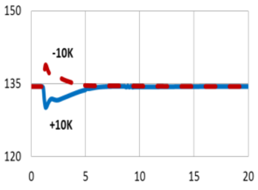
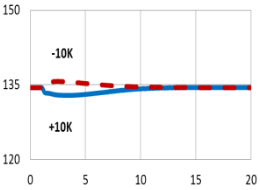
	BC	CS1	CS2	CS3
Methanol (kmol/h)				
Total (kmol/h)				
MH (kmol/h)				
xMeOH in ROUT				
TR (K)				
MMH in ROUT (kmol/h)				
ROUT (kmol/h)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.4 (Continued) Responses for methanol feed temperature disturbances

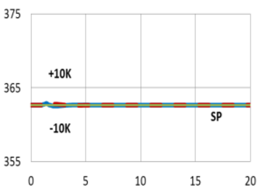
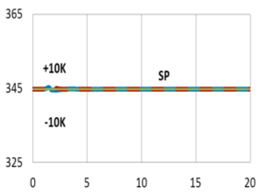
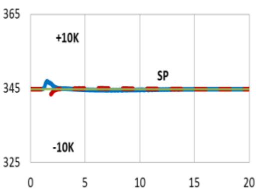
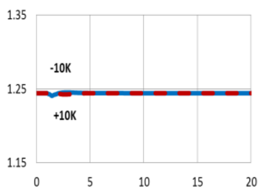
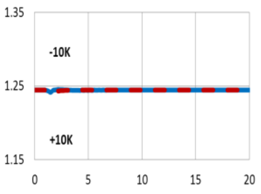
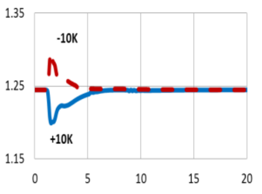
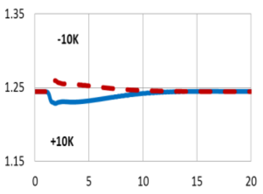
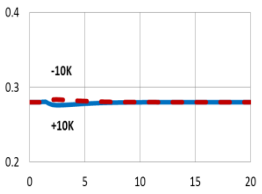
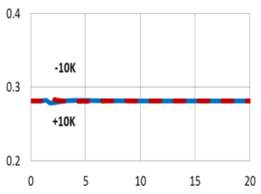
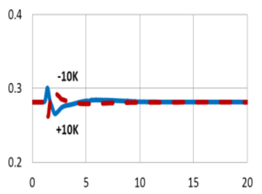
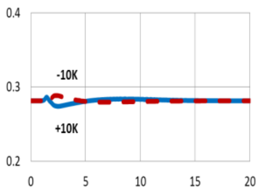
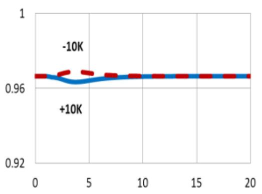
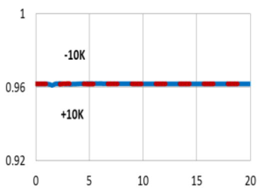
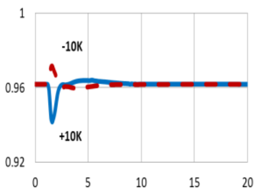
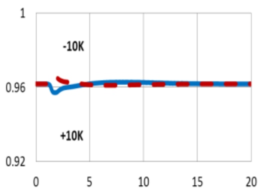
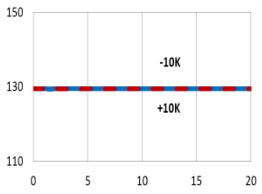
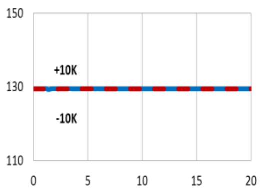
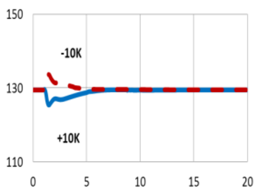
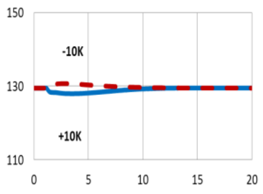
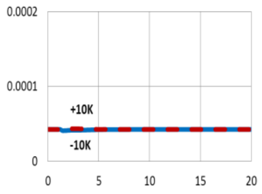
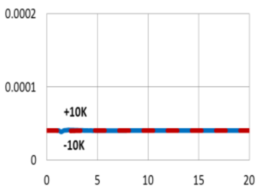
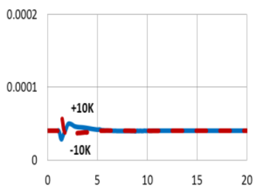
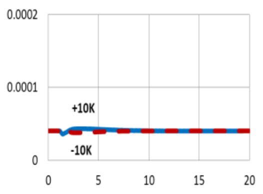
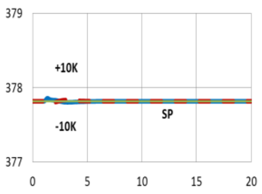
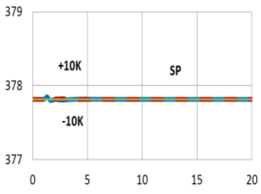
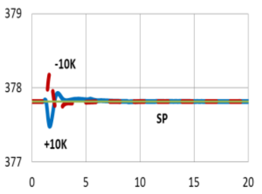
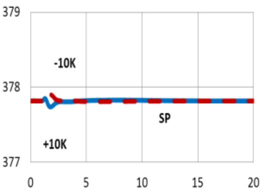
	BC	CS1	CS2	CS3
T1 (K)				
QR1 (MW)				
D1 (kmol/h)				
xD1 (DME)				
B1 (kmol/h)				
xB1 (DME)				
T21 (K)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.4 (Continued) Responses for methanol feed temperature disturbances

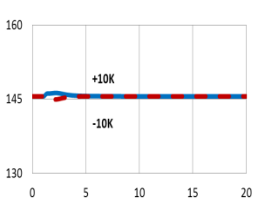
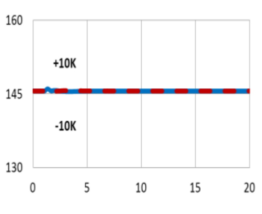
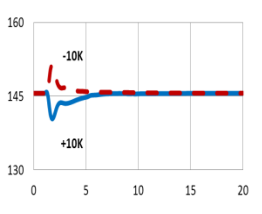
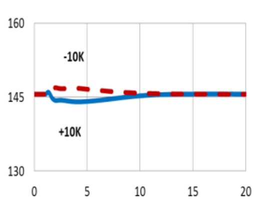
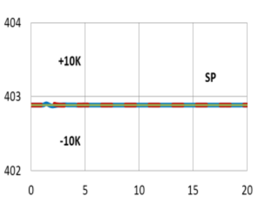
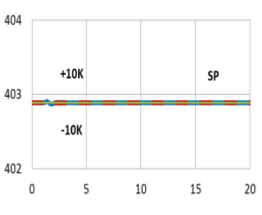
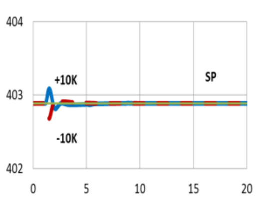
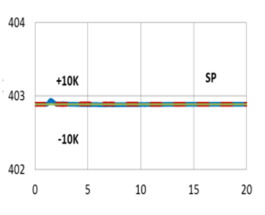
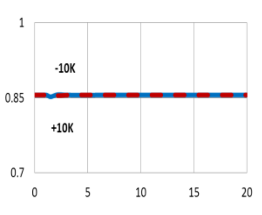
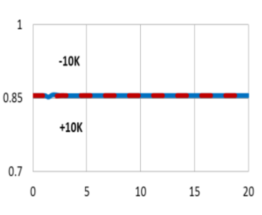
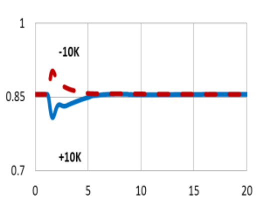
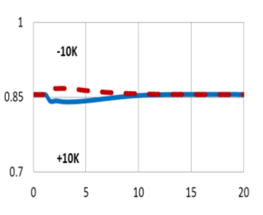
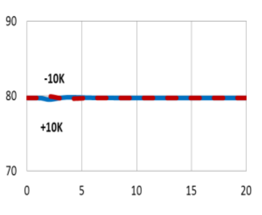
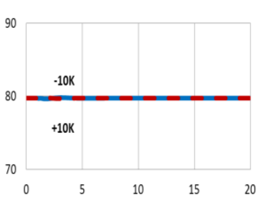
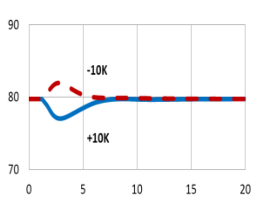
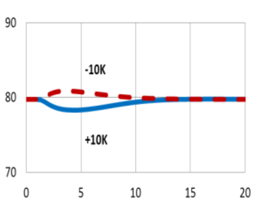
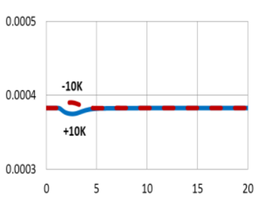
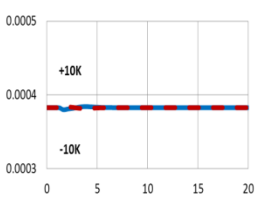
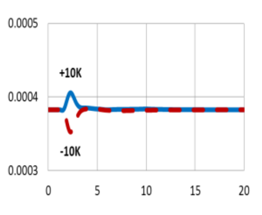
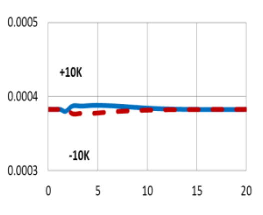
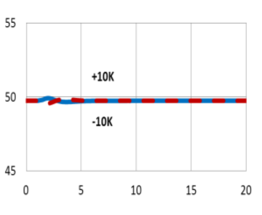
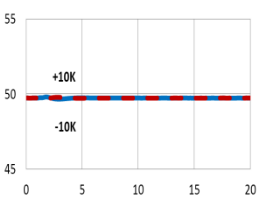
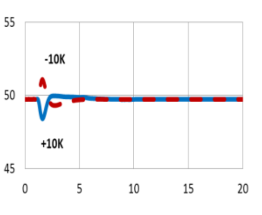
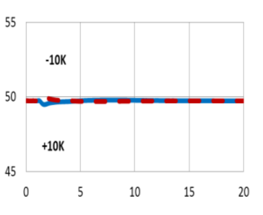
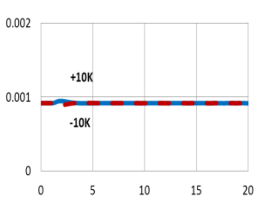
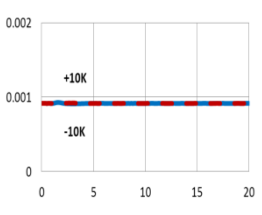
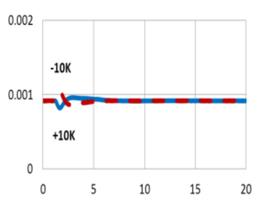
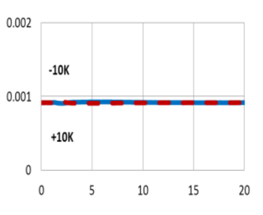
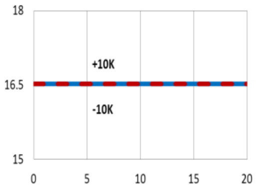
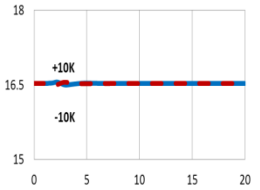
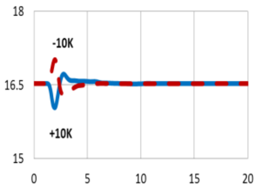
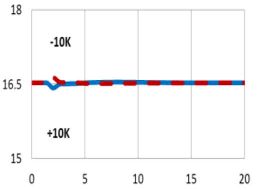
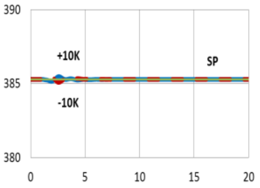
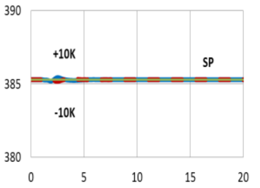
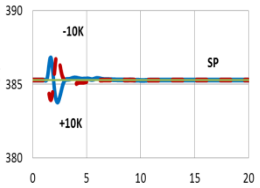
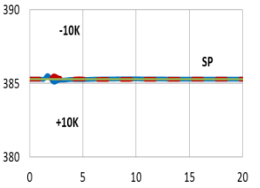
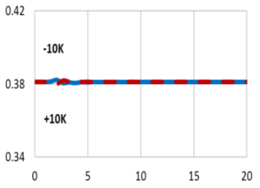
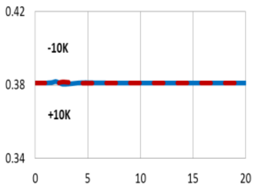
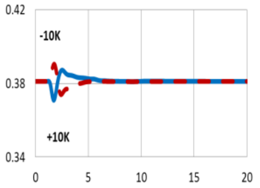
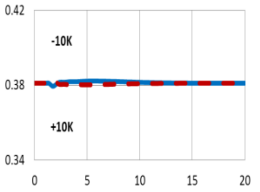
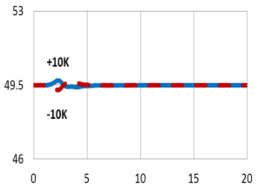
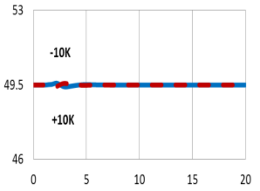
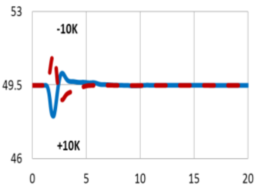
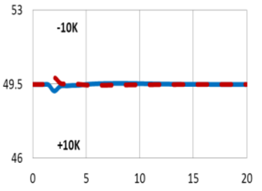
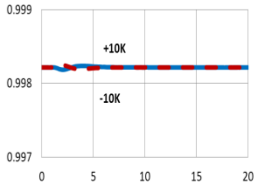
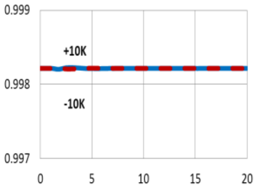
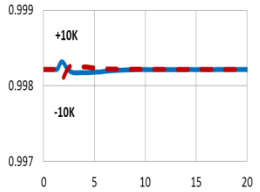
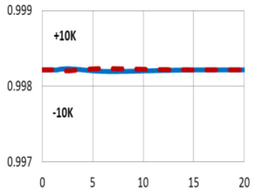
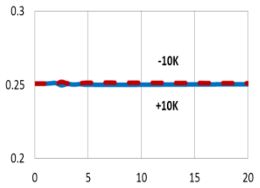
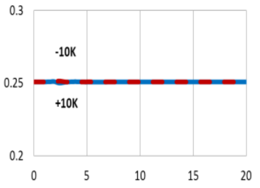
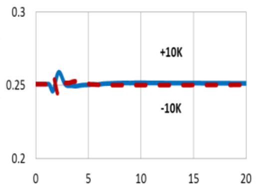
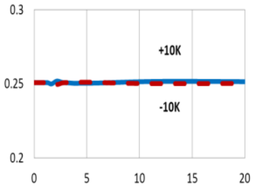
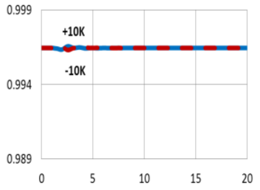
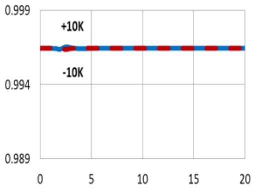
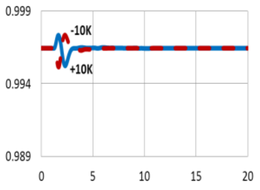
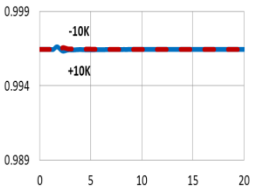
	BC	CS1	CS2	CS3
R2 (kmol/h)				
T22 (K)				
QR2 (MW)				
D2 (kmol/h)				
xD2 (MMH)				
B2 (kmol/h)				
xB2 (MH)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 5.4 (Continued) Responses for methanol feed temperature disturbances

	BC	CS1	CS2	CS3
R3 (kmol/h)				
T3 (K)				
QR3 (MW)				
D3 (kmol/h)				
xD3 (MMH)				
B3 (kmol/h)				
xB3 (MHOH)				
	Time (hr)	Time (hr)	Time (hr)	Time (hr)

5.2 Evaluation of the Dynamic Performance

The achievable dynamic performance of a system is important for the assessment of a current control system in operation. One of the performance measures of a control system used in this study is the IAE value. The IAE performance criterion is defined as

$$\mathrm{IAE} = \int \left| e\left(t\right) \right| dt \tag{5.1}$$

Where e(t) is the error or difference between the controlled variable and its set point. This integral absolute error (IAE) method is used for evaluation of the dynamic performance of four alternative control structures (BC, CS1, CS2 and CS3). In this study, the control loops are divided into 3 categories for IAE determination: composition of product loop (the deviation from the desired value), composition loops (byproducts, and composition loop) and the safety control loops (pressure and temperature loops). The safety control loops are taken into account because those control loops cause the smooth and stable plant operation (Our first control objective).

Table 5.5, 5.6 and 5.7 give the IAE values of each control structure under methanol feed flowrate disturbances, methanol feed temperature disturbances and both disturbances (their summation), respectively. Since there are many loop types (composition, temperature and pressure), we must normalize the IAE values by dividing their spans (the largest expected change in disturbance) of each loop. Then, the IAE values normalized are summed up by weighting the loop types. Weighting factors are estimated values indicating the relative importance of each loop as compared to the other loops. Table 5.8 shows weighting factors for each loop used in this study. The IAE values normalized and their weighted summation of each control structure are given in Table 5.9.

Table 5.5 The process performance in terms of integral absolute value (IAE) under methanol feed flowrate disturbances

	BC	CS1	CS2	CS3
Composition of product	0.012505	0.008949	0.008658	0.008337
Composition	1.085804	0.302920	0.400911	0.382240
Temperature	14.77520	25.69390	36.53670	30.54150
Pressure	0.178942	0.277639	0.269224	0.272502

Table 5.6 The process performance in terms of integral absolute value (IAE) under methanol feed temperature disturbances

	BC	CS1	CS2	CS3
Composition of product	0.000157	0.000054	0.000445	0.000276
Composition	0.032736	0.004806	0.046527	0.038590
Temperature	3.133500	3.526500	21.22970	9.945900
Pressure	0.033914	0.033755	0.231455	0.108830

Table 5.7 The process performance in terms of integral absolute value (IAE) under all disturbances

	BC	CS1	CS2	CS3
Composition of product	0.012662	0.009003	0.009103	0.008613
Composition	1.118540	0.307726	0.447438	0.420830
Temperature	17.90870	29.22040	57.76640	40.48740
Pressure	0.212856	0.311394	0.500679	0.381332

Table 5.8 Weighting factors for each loop

Loops	Weights
Composition of product	1
Composition	0.8
Temperature	0.5
Pressure	0.5

Table 5.9 The IAE values normalized and their weighted summation

	BC	CS1	CS2	CS3
Composition of product	0.025324	0.018006	0.018206	0.017226
Composition	2.237080	0.615452	0.894876	0.841660
Temperature	0.179087	0.292204	0.577664	0.404874
Pressure	0.059796	0.066245	0.115779	0.084061
Summation of IAE	1.934430	0.689592	1.080828	0.935021

As shown in Table 5.9, clearly, CS1 gives the smallest summation of IAE values, so control structure 1 (CS1) gives the best control performance. That is, it not only provides smooth and stable plant operation and rejects the disturbances better than the other control structures, but also maintains the product and byproduct purities effectively.

5.3 Evaluation of utility costs

The costs of utility are calculated from cooling water used in reactor and condensers, steam used in the reboilers, and electricity used at pumps. In the dynamic simulation, pump powers used in BC, CS1, CS2 and CS3 are fixed, so their costs of electricity are the same. The prices of each utility are given as follows:

• Medium-pressure stream (11 bar, 457 K)	$8.22/GJ
• High-pressure stream (42 bar, 527 K)	$9.88/GJ
• Electricity	$16.8/GJ
• Cooling Water	$0.354/GJ

Table 5.10 Utility cost under methanol feed flowrate disturbances

		BC	CS1	CS2	CS3
Medium-pressure stream	GJ/year	39059.92	39068.76	39203.89	39205.80
	$/year	321072.51	321145.25	322255.94	322271.64
High-pressure stream	GJ/year	39240.14	39233.50	39244.38	39245.27
	$/year	387692.58	387626.94	387734.49	387743.28
Cooling water	GJ/year	106117.87	106180.89	109555.82	109653.71
	$/year	37565.73	37588.04	38782.76	38817.41
Electricity	GJ/year	342.12	342.12	342.12	342.12
	$/year	5747.63	5747.63	5747.63	5747.63
Utility cost	$/year	752078.45	752107.86	754520.83	754579.97

Table 5.11 Utility cost under methanol feed temperature disturbances

		BC	CS1	CS2	CS3
Medium-pressure stream	GJ/year	38989.07	38989.94	38990.35	38992.61
	$/year	320490.19	320497.32	320500.65	320519.24
High-pressure stream	GJ/year	39234.42	39247.06	39247.48	39249.65
	$/year	387636.02	387760.96	387765.11	387786.50
Cooling water	GJ/year	104735.16	104755.05	104758.67	104779.21
	$/year	37076.25	37083.29	37084.57	37091.84
Electricity	GJ/year	342.12	342.12	342.12	342.12
	$/year	5747.63	5747.63	5747.63	5747.63
Utility cost	$/year	750950.09	751089.21	751097.96	751145.22

Table 5.10 and 5.11 give the utility costs of each control structure under the disturbances in the methanol feed flowrate and methanol feed temperature, respectively. The results show that the utility costs of each control structure are quite the same. However, the smallest utility cost belongs to Luyben’s control structure (BC) followed by control structure 1 (CS1), control structure 2 (CS2) and control structure 3 (CS3), respectively.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The new plantwide control structures design procedure of Wongsri has been applied to the MMH process. This heuristic-based procedure is systematic and straightforward, and can be followed easily. Specific guidelines are given. Material balance is made by material quantifiers and pathways. The procedure gives three alternative plantwide control structures for this process: control structures 1-3 (CS1-3). The dynamic performance of control structures 1-3 are evaluated and compared with the Luyben's control structure (BC) using the IAE performance criterion under the disturbances in methanol feed flowrate and methanol feed temperature. Furthermore, the utility costs of each control structure are evaluated and compared.

The results show that control structure 1 (CS1) is the best control structure since it gives the best control performance (the smallest summation of IAE values), that is to say, it not only provides smooth and stable plant operation and rejects the disturbances better than the other control structures, but also maintains the product and byproduct purities effectively as compared by integral absolute error (IAE), while the utility costs required are not much different from the other control structures. Composition controllers are not required in the columns since temperature controllers provide adequate product-quality control.

6.2 Recommendation

In this study, we only use simple PI controllers. If a low-performance PI controller works well on the simulation but doesn't work as well in the plant, we still have the flexibility to go to PID control to improve things. In addition, adding enhanced controls, i.e. cascade, feed forward controls may be able to improve the control performance.

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APPENDICES

APPENDIX A
EQUIPMENT DATA AND STREAM CONDITIONS

Table A.1 Equipment data

Units operation	Properties	Value
Reactor	Volume (m^3)	12
Column C1	Number of stages	10
	Inlet stage	7
	Operating pressure (atm)	10
	Reflux ratio	0.43
	Diameter (m)	0.78
	Condenser volume (m^3)	0.02
	Reboiler volume (m^3)	7.82
Column C2	Number of stages	40
	Inlet stage	22
	Operating pressure (atm)	0.4
	Reflux ratio	1.79
	Diameter (m)	2.24
	Condenser volume (m^3)	6.00
	Reboiler volume (m^3)	4.99
Column C3	Number of stages	20
	Inlet stage	8
	Operating pressure (atm)	0.1
	Reflux ratio	0.33
	Diameter (m)	1.98
	Condenser volume (m^3)	2.19
	Reboiler volume (m^3)	1.13

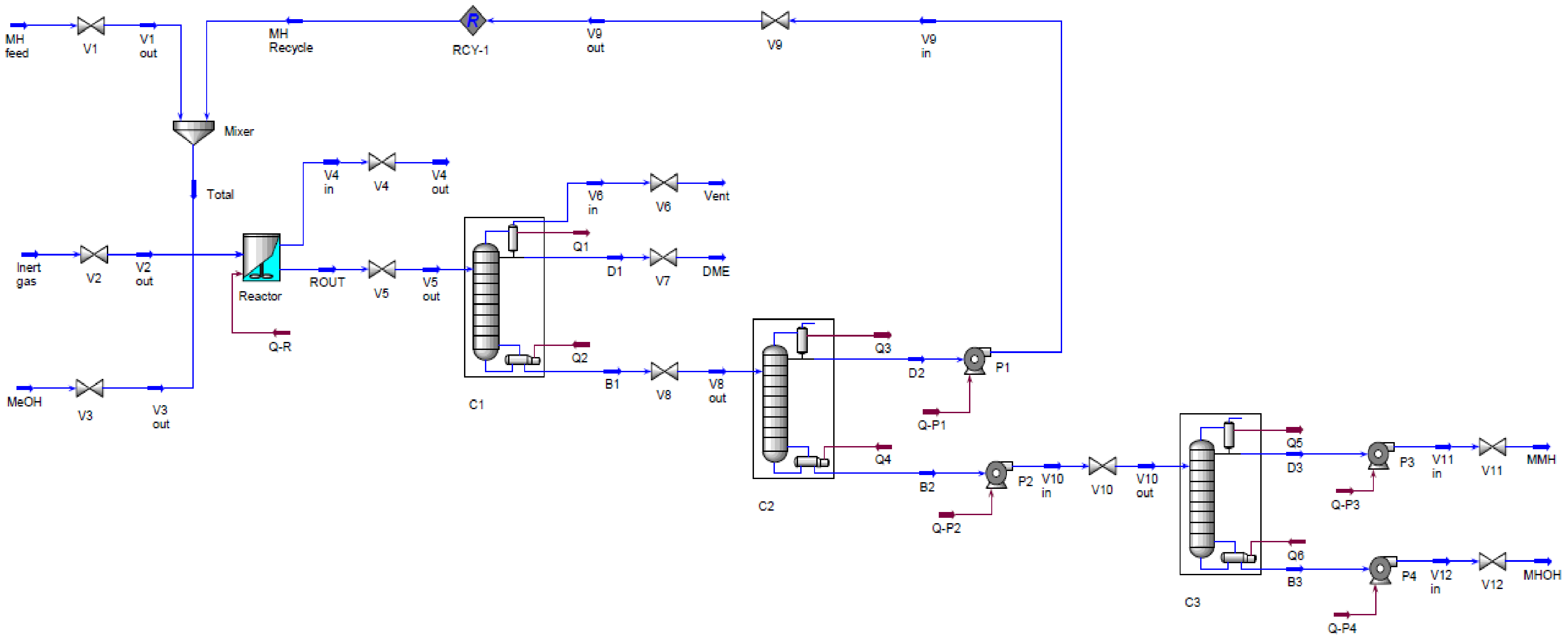

Figure A.1 HYSYS flowsheet

Table A.2 Stream conditions

Stream	MH feed	V1 out	Total	Inert gas	V2 out	MeOH	V3 out	V4 in	V4 out	ROUT
Vapor Fraction	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000
Temperature(K)	393.0	393.0	370.9	393.0	393.0	393.0	393.0	400.0	400.0	400.0
Pressure (atm)	18.00	15.00	15.00	18.00	15.00	18.00	15.00	15.00	12.00	15.00
Flow (kmol/h)	49.51	49.51	129.5	5.000	5.000	50.00	50.00	0.3775	0.3775	134.4
Mole Fraction										
DME	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0079	0.0079	0.0022
MeOH	0.0000	0.0000	0.0295	0.0000	0.0000	1.0000	1.0000	0.0172	0.0172	0.0283
MH	1.0000	1.0000	0.9698	0.0000	0.0000	0.0000	0.0000	0.0488	0.0488	0.5644
MMH	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0137	0.0137	0.3683
MHOH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0022
N_2	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	0.9124	0.9124	0.0346

Table A.2 (continue) Stream conditions

Stream	V5 out	V6 in	Vent	D1	DME	B1	V8 out	D2	V9 in	V9 out
Vapor Fraction	0.0148	1.0000	1.0000	0.0000	0.0036	0.0000	1.0000	0.0000	0.0000	0.0000
Temperature(K)	399.8	193.4	193.4	193.4	193.3	501.9	403.7	354.9	356.3	356.3
Pressure (atm)	10.03	10.00	7.000	10.00	7.000	10.05	0.6154	0.4000	18.00	15.00
Flow (kmol/h)	134.4	4.671	4.671	0.2805	0.2805	129.5	129.5	79.71	79.71	79.71
Mole Fraction										
DME	0.0022	0.0040	0.0040	0.9669	0.9669	0.0000	0.0000	0.0001	0.0001	0.0001
MeOH	0.0283	0.0000	0.0000	0.0213	0.0213	0.0293	0.0293	0.0476	0.0476	0.0476
MH	0.5644	0.0000	0.0000	0.0000	0.0000	0.5860	0.5860	0.9513	0.9513	0.9513
MMH	0.3683	0.0000	0.0000	0.0000	0.0000	0.3824	0.3824	0.0010	0.0010	0.0010
MHOH	0.0022	0.0000	0.0000	0.0000	0.0000	0.0023	0.0023	0.0000	0.0000	0.0000
N_2	0.0346	0.9960	0.9960	0.0118	0.0118	0.0000	0.0000	0.0000	0.0000	0.0000

Table A.2 (continue) Stream conditions

Stream	MH Recycle	B2	V10 in	V10 out	D3	V11 in	MMH	B3	V12 in	MHOH
Vapor Fraction	0.0000	0.0000	0.0000	0.5162	0.0000	0.0000	0.0016	0.0000	0.0000	0.0017
Temperature(K)	356.3	416.2	416.5	359.9	352.3	352.6	352.4	418.7	418.9	418.7
Pressure (atm)	15.00	0.8000	3.800	0.1321	0.1000	3.100	0.1002	0.1870	3.187	0.1873
Flow (kmol/h)	79.99	49.74	49.74	49.74	49.47	49.47	49.47	0.2685	0.2685	0.2685
Mole Fraction										
DME	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MeOH	0.0478	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MH	0.9511	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0000	0.0000	0.0000
MMH	0.0010	0.9936	0.9936	0.9936	0.9990	0.9990	0.9990	0.0010	0.0010	0.0010
MHOH	0.0000	0.0059	0.0059	0.0059	0.0005	0.0005	0.0005	0.9990	0.9990	0.9990
N_2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

APPENDIX B
CONTROLLER TUNING

In this appendix, we discuss tuning methodology. As mentioned earlier, PI controllers are used in all loops. You may wonder why more use is not made of PID controllers. In theory, control performance can be improved by the use of derivative action, but in practice the use of derivative has some significant drawbacks:

1. Three tuning constants must be specified.
2. Signal noise is amplified.
3. Several types of PID control algorithms are used, so you must be careful that the right algorithm is used with its matching tuning method.

In addition, it is more conservative to only use PI controllers in the simulation. The simulation is an approximation of the real plant. If high-performance controllers are required to get good dynamics from the simulation, the real plant may not work well. On the other hand, if a low-performance PI controller works well on the simulation but doesn't work as well in the plant, we still have the flexibility to go to PID control to improve things.

B.1 Flow Controllers

The majority of flow control loops feature an orifice-plate sensor, a differential-pressure transmitter, a PI controller and a control valve. The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be turned with a small integral or reset time constant τ_i. A value of τ_i = 0.3 minutes works in most flow controllers. The value of controller gain should be kept modest because flow measurement signal are sometime noisy due to the turbulent flow through the orifice plate. A value of controller gain of K_C = 0.5 is often used. Derivative action should not be used.

B.2 Level Controllers

Most level controllers should use proportional-only action with a gain of 1 to 2. This provides the maximum amount of flow smoothing. Proportional control means there will be steady-state offset (the level will not be returned to its setpoint value). However, maintaining a liquid level at a certain value is often not necessary when the liquid capacity is simply being used as surge volume. So the recommended tuning of a level controller is $K_C = 2$. There are several exceptions to this recommended tuning of level controllers, for example, reactor level control in this study because level impacts reaction rates. However, proportional-only level control can still be applied in reactors if a higher value of gain is used ($K_c = 5$).

B.3 Pressure Controllers

Most pressure controllers can be fairly easily tuned. The process time constant is estimated by dividing the gas volume of the system by the volumetric flowrate of gas flowing through the system. Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Of cause the gain used depends on the span of the pressure transmitter. Some simple step tests can be used to find the value of controller gain that yields satisfactory pressure control. Typical pressure controller tuning constants for columns and tanks are $K_C = 2$ and $\tau_i = 10$ minutes.

B.4 Temperature and Composition Controllers

Temperature and composition loops have significant dynamic lags and/or deadtimes, so arbitrarily tight tuning is not physically possible. Temperature controllers should use 1-min deadtimes. Composition controllers should use 3- to 5-min deadtimes. Failure to insert these dynamic lags or deadtimes will result in a prediction of controller performance that is unrealistically better than what is attainable in the real plant in which these dynamic elements are always present due to measurement and valve dynamics.

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

The method consists of merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the height of the relay, h. This height is typically 5 to 10 percent of the controller output scale. The loop starts to oscillate around the setpoint, with the controller output switching every time the process variable (PV) signal crosses the setpoint. Relay feedback testing is built right into the controller module in HYSYS, so it is much more conveniently done by simple clicking the Start Autotuning button in Autotuning page. Figure B.1 shows the PV and OP signals from a typical relay-feedback test.

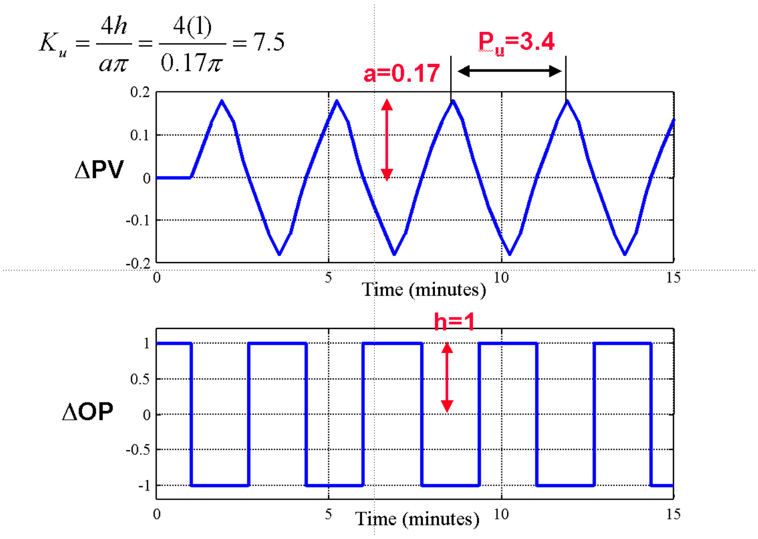

Figure B.1 Input and output from relay-feedback test (Luyben, 2002)

The maximum amplitude (a) of the PV signal is used to calculate the ultimate gain, K_U from the equation:

$$K_u = \frac{4h}{a\pi} \tag{B.1}$$

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

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

1. Only one parameter has to be specified (relay height).
2. The time it takes to run the test is short.
3. The test is closed loop, so the process is not driven away from the setpoint.
4. The information obtained is very accurate in the frequency range that is important for the design of a feedback controller.
5. The impact of load changes that occur during the test can be detected by a change to asymmetric pulses in the manipulated variable. These entire features make relay-feedback testing a useful identification tool.

Knowing the ultimate gain, K_U and the ultimate period, P_U permits us to calculate controller settings. There are several methods that require only these two parameters, e.g., Ziegler-Nichols, Tyreus-Luyben, etc. In this study, we select the Tyreus-Luyben tuning method since it provides more conservative settings with increased robustness. The TL equations for a PI controller are:

$$K_c = K_u/3.2 \tag{B.2}$$

$$\tau_i = 2.2Pu \tag{B.3}$$

Furthermore, there are many other tuning methods, but many of these require more information about the process.

Tables B1, B2, and B3 give controller tuning parameters for all controllers of base case, control structure 1, and control structure 2, respectively.

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

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Methanol feed	FCm	Methanol flow rate	Fresh feed of methanol	PI	Reverse	50 kmol/h	0-100 kmol/h	0.50	0.3
Total MH	FCtot	Total flow of MH	Fresh feed of MH	PI	Reverse	129.5 kmol/h	0-260 kmol/h	0.50	0.3
Ratio multiplier	Ratio	Ratio of feeds	Set point of FCtot	-	-	2.59	-	-	-
Reactor	TCR	Reactor temperature	Coolant flow rate	PI	Direct	400 K	350-450 K	2.60	25.0
	LCR	Reactor liquid level	Reactor effluent	P	Direct	50 %	0-100 %	5.00	-
Column C1	FC1	Reflux ratio	Reflux flow rate	PI	Reverse	2.123 kmol/h	0-4.2 kmol/h	0.50	0.3
	TC1	Tray 5 temperature	Reboiler heat input	PI	Reverse	362.6 K	310-410 K	0.43	30.0
	PC1	Condenser pressure	Heat removal	PI	Direct	10 atm	5-15 atm	2.00	10.0
	LC11	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC12	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C2	TC21	Tray 13 temperature	Reflux flow rate	PI	Direct	377.8 K	320-420 K	3.30	22.0
	TC22	Tray 30 temperature	Reboiler heat input	PI	Reverse	402.9 K	350-450 K	7.10	13.6
	PC2	Condenser pressure	Heat removal	PI	Direct	0.4 atm	0-0.8 atm	2.00	10.0

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

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Column C2	LC21	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC22	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C3	FC3	Reflux flow rate	Reflux flow rate	PI	Reverse	16.52 kmol/h	0-32 kmol/h	0.50	0.3
	TC3	Tray 18 temperature	Reboiler heat input	PI	Reverse	385.3 K	330-430 K	0.55	24.0
	PC3	Condenser pressure	Heat removal	PI	Direct	0.1 atm	0-0.2 atm	2.00	10.0
	LC31	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC32	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-

Table B.2 Type of controllers and tuning parameters of control structure 1

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Methanol feed	FCm	Methanol flow rate	Fresh feed of methanol	PI	Reverse	50 kmol/h	0-100 kmol/h	0.50	0.3
Total MH	FCtot	Total flow of MH	Fresh feed of MH	PI	Reverse	129.5 kmol/h	0-260 kmol/h	0.50	0.3
Ratio of feeds	Ratio	Ratio of feeds	Set point of FCtot	-	-	2.59	-	-	-
Reactor	TCR	Reactor temperature	Coolant flow rate	PI	Direct	400 K	350-450 K	2.60	25.0
	LCR	Reactor liquid level	Reactor effluent	P	Direct	50 %	0-100 %	5.00	-
	CCR	Methanol composition	Set point of TCR	PI	Direct	0.0283	0-0.05	0.69	57.6
Column C1	FC1	Reflux ratio	Reflux flow rate	PI	Reverse	2.125 kmol/h	0-4.2 kmol/h	0.50	0.3
	TC1	Tray 2 temperature	Reboiler heat input	PI	Reverse	344.8K	300-400 K	0.20	35.0
	PC1	Condenser pressure	Heat removal	PI	Direct	10 atm	5-15 atm	2.00	10.0
	LC11	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC12	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C2	TC21	Tray 13 temperature	Reflux flow rate	PI	Direct	377.8 K	320-420 K	3.30	22.0
	TC22	Tray 30 temperature	Reboiler heat input	PI	Reverse	402.9 K	350-450 K	7.10	13.6

Table B.2 (Continued) Type of controllers and tuning parameters of control structure 1

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Column C2	PC2	Condenser pressure	Heat removal	PI	Direct	0.4 atm	0-0.8 atm	2.00	10.0
	LC21	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC22	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C3	FC3	Reflux ratio	Reflux flow rate	PI	Reverse	16.53 kmol/h	0-34 kmol/h	0.50	0.3
	TC3	Tray 18 temperature	Reboiler heat input	PI	Reverse	385.3 K	330-430 K	0.55	24.0
	PC3	Condenser pressure	Heat removal	PI	Direct	0.1 atm	0-0.2 atm	2.00	10.0
	LC31	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC32	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-

Table B.3 Type of controllers and tuning parameters of control structure 2

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Methanol feed	FCm	Methanol flow rate	Fresh feed of methanol	PI	Reverse	50 kmol/h	0-100 kmol/h	0.50	0.3
Total MH	FCtot	Total flow of MH	Fresh feed of MH	PI	Reverse	129.5 kmol/h	0-260 kmol/h	0.50	0.3
Reactor	TCR	Reactor temperature	Coolant flow rate	PI	Direct	400 K	350-450 K	2.60	25.0
	LCR	Reactor liquid level	Reactor effluent	P	Direct	50 %	0-100 %	5.00	-
	CCR	Methanol composition	Set point of FCtot	PI	Direct	0.0283	0-0.05	0.68	130.0
Column C1	FC1	Reflux ratio	Reflux flow rate	PI	Reverse	2.125 kmol/h	0-4.2 kmol/h	0.50	0.3
	TC1	Tray 2 temperature	Reboiler heat input	PI	Reverse	344.8K	300-400 K	0.20	35.0
	PC1	Condenser pressure	Heat removal	PI	Direct	10 atm	5-15 atm	2.00	10.0
	LC11	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC12	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C2	TC21	Tray 13 temperature	Reflux flow rate	PI	Direct	377.8 K	320-420 K	3.30	22.0
	TC22	Tray 30 temperature	Reboiler heat input	PI	Reverse	402.9 K	350-450 K	7.10	13.6
	PC2	Condenser pressure	Heat removal	PI	Direct	0.4 atm	0-0.8 atm	2.00	10.0

Table B.3 (Continued) Type of controllers and tuning parameters of control structure 2

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Column C2	LC21	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC22	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C3	FC3	Reflux ratio	Reflux flow rate	PI	Reverse	16.53 kmol/h	0-34 kmol/h	0.50	0.3
	TC3	Tray 18 temperature	Reboiler heat input	PI	Reverse	385.3 K	330-430 K	0.55	24.0
	PC3	Condenser pressure	Heat removal	PI	Direct	0.1 atm	0-0.2 atm	2.00	10.0
	LC31	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC32	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-

Table B.4 Type of controllers and tuning parameters of control structure 3

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Methanol feed	FCm	Methanol flow rate	Fresh feed of methanol	PI	Reverse	50 kmol/h	0-100 kmol/h	0.50	0.3
Total MH	FCtot	Total flow of MH	Fresh feed of MH	PI	Reverse	129.5 kmol/h	0-260 kmol/h	0.50	0.3
Ratio of feeds	Ratio	Ratio of feeds	Set point of FCtot	PI	Reverse	2.59	0-5	0.50	0.3
Reactor	TCR	Reactor temperature	Coolant flow rate	PI	Direct	400 K	350-450 K	2.60	25.0
	LCR	Reactor liquid level	Reactor effluent	P	Direct	50 %	0-100 %	5.00	-
	CCR	Methanol composition	Set point of Ratio	PI	Direct	0.0283	0-0.05	0.10	29.6
Column C1	FC1	Reflux ratio	Reflux flow rate	PI	Reverse	2.125 kmol/h	0-4.2 kmol/h	0.50	0.3
	TC1	Tray 2 temperature	Reboiler heat input	PI	Reverse	344.8K	300-400 K	0.20	35.0
	PC1	Condenser pressure	Heat removal	PI	Direct	10 atm	5-15 atm	2.00	10.0
	LC11	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC12	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C2	TC21	Tray 13 temperature	Reflux flow rate	PI	Direct	377.8 K	320-420 K	3.30	22.0
	TC22	Tray 30 temperature	Reboiler heat input	PI	Reverse	402.9 K	350-450 K	7.10	13.6

Table B.4 (Continued) Type of controllers and tuning parameters of control structure 3

Unit	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Column C2	PC2	Condenser pressure	Heat removal	PI	Direct	0.4 atm	0-0.8 atm	2.00	10.0
	LC21	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC22	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-
Column C3	FC3	Reflux ratio	Reflux flow rate	PI	Reverse	16.53 kmol/h	0-34 kmol/h	0.50	0.3
	TC3	Tray 18 temperature	Reboiler heat input	PI	Reverse	385.3 K	330-430 K	0.55	24.0
	PC3	Condenser pressure	Heat removal	PI	Direct	0.1 atm	0-0.2 atm	2.00	10.0
	LC31	Reflux-drum level	Distillate flow rate	P	Direct	50 %	0-100 %	2.00	-
	LC32	Reboiler level	Bottoms flow rate	P	Direct	50 %	0-100 %	2.00	-

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