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PLANTWIDE CONTROL STRUCTURES DESIGN OF METHYL ACETATE 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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โชคสกุณต์ อารยะศิลป์ธร : การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ของ
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เมทิลอะซิเตตเป็นสารระเหยง่ายซึ่งส่วนมากใช้เป็นสารละลายทางอุตสาหกรรม
สำหรับกระบวนการผลิตเมทิลอะซิเตต เมทานอลจะถูกทำปฏิกิริยาดีไฮเดรชันได้ผลิตภัณฑ์เป็นได
เมทิลอีเทอร์ และหลังจากนั้นจะถูกทำปฏิกิริยากับคาร์บอนมอนอกไซด์เป็นเมทิลอะซิเตต ซึ่ง
กระบวนการนี้เหมาะสำหรับโรงงานที่มีคาร์บอนมอนอกไซด์สำรองอยู่ กระบวนการจะถูกพิจารณา
ออกเป็นสองส่วนคือส่วนของปฏิกิริยาดีไฮเดรชันและคาร์บอนิลเลชัน ซึ่งวิธีการทางการควบคุม
แบบแพลนท์ไวด์จะถูกนำมาใช้กับกระบวนการเมทิลอะซิเตตในทั้งสองส่วนที่กล่าวมา ส่วนการ
ออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์จะถูกประยุกต์เข้ากับวิธีการออกแบบการควบคุม
ของวงศ์ศรีเพื่อให้ได้มาซึ่งเป้าหมายในการควบคุมและการจัดการกับตัวแปรกระบวนการอย่างมี
ประสิทธิภาพ โปรแกรมจำลองจะแสดงผลการควบคุมโดยจำลองกระบวนการทั้งในระบบคงตัว
และระบบไดนามิกส์พร้อมทั้งให้ผลการตอบสนองของตัวแปรที่สำคัญ

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Methyl acetate is a fast-evaporating chemical component with many uses as solvent. For its production, methanol is first dehydrated to dimethyl ether and then carbonylated to methyl acetate. For a plant which carbon monoxide available, this may be workable. The two sections of the plant, dehydration and carbonylation section are separately considered. Therefore, the plantwide control strategy is considered for the entire methyl acetate process including two sections above. The control design methodology, wongsri is applied to the plantwide control structures design for reach the control objectives and effectively operating large disturbances in production rate and fresh feed compositions. A commercial process simulator achieves the dynamics simulation of this research, both of steady-state and dynamics conditions.

Department : Chemical Engineering..... Student's Signature

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CHAPTER I

INTRODUCTION

1.1 Importance and Reasons for Research

Plantwide process control concerns systems and tactics required to control many interconnected unit operations consisted in entire chemical process. There is regularly a complicated process flowsheet composing recycle stream, energy integration, and many different units. Given an integrated process and various classify of equipment, the necessary logic, instrumentation and strategies to reach the design objectives and perform the plant operation safely. The plantwide control's method can be classified into two types, based on heuristic and mathematical approaches. Luyben et al. (1997) submitted the nine steps of the design procedure about the fundamental theory of plantwide control (energy management, production rate, product quality, some constraints, liquid level and gas pressure inventories, makeup of reactants, component balances, and economic or process optimization. The nine-step method is based on the heuristic procedure. It is complicated for less experience user but some generic description and specific guidelines are given. Nonetheless, Wongsri presented the eight-step plantwide control procedure based on heuristics and mathematical approaches. The eight-step method is completely difference from Luyben's method and can be used for inexperienced user. The step is uncomplicated and can be easily acted according to the instructions.

The process of methyl acetate production through dehydration and carbonylation consist of many operating units. There are specific conditions to obtain desired product, which are strictly controlled. It indicates that the process control is important for achieving a good performance operation. The two sections of the plant, dehydration and carbonylation section are separately considered. The first section, dehydration reaction can be conducted in either the vapor or the liquid phases. The reaction is vapor-phase and exothermic. The second section, carbonylation reaction is

also vapor-phase and exothermic. Therefore vapor-phase tubular reactors are used in the both section. The strict controls are used for operating the two sections effectively. Reasonable conceptual designs of these two sections of the plant are developed, including recycle streams and energy integrations for improving the economics. Then plantwide dynamic control of the entire process is considered.

Methyl acetate is a fast-evaporating chemical component with many uses as solvent. There are many alternative productions. Methyl acetate is conventionally made by esterification of acetic acid with methanol. The esterification is complicate because of difficulty in separating acetic acid and water, and the presence of azeotropes either between methyl acetate and methanol or between methyl acetate and water. So there is an alternative way to produce methyl acetate. Methanol is first dehydrated to dimethyl ether and then carbonylated to methyl acetate. For a plant which carbon monoxide existed, this may be workable. Moreover, the price of methanol and acetic acid found on the ICIS.com Web site (2011) is \$26.24/kmol and \$42.6/kmol respectively, which show that methanol dehydration and then carbonylation to methyl acetate possibly make more profits than esterification of acetic acid and methanol.

1.2 Research Objectives

This research aims to design the plantwide process control structures for methyl acetate process via carbonylation of dimethyl ether by using Wongsri design procedure (Wongsri).

1.3 Scopes of Research

The scopes of this research are as follows:

1. The detail of methyl acetate process using carbonylation of dimethyl ether is given by Luyben (2010).

2. The simulations of methyl acetate process using carbonylation of dimethyl ether in steady state and dynamic behavior are achieved via the commercial process simulator.

3. Wongsri design procedure (Wongsri 2012) is considered for obtaining the new control structures of methyl acetate process using carbonylation of dimethyl ether.

1.4 Contribution of Research

The contribution of this research is the effectively control structure of methyl acetate process using carbonylation of dimethyl ether by using Wongsri design procedure (Wongsri 2012).

1.5 Research Procedures

The research procedures are following steps:

1. Study of the plantwide process control structure design methodology, the methyl acetate process using carbonylation of dimethyl ether and the relevant information.

2. Research the Luyben's control structure design of the methyl acetate process using carbonylation of dimethyl ether.

3. Simulate the process in steady state and dynamic behavior by commercial process simulator.

4. Design new control structures using Wongsri design procedure (Wongsri 2009).

5. Simulate the new control structure in dynamic behavior and compare with the base case, Luyben's control structure.

6. Analyze the result of the new design control structure simulation.

7. Summarize the research studied

1.6 Research Framework

This thesis is divided into six parts as follows:

Chapter I: An introduction of research consisting of reasons, objectives, scopes, contributions and procedure of the research.

Chapter II: Review of the earlier researches of plantwide control, control structure design, plantwide control procedure and related researches.

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

Chapter IV: Description of the methyl acetate process using carbonylation of dimethyl ether via the commercial process simulator.

Chapter V: Description of the designed control structures, dynamic simulation results and comparison of the control structures with Luyben's structures.

Chapter VI: Conclusion of this research and Recommendations.

CHAPTER II

LITERATURE REVIEWS

Plantwide control design was studied because most chemical process is complicate. The presence of energy integrations and recycle streams cause disturbances that are not able to simply handle. The researchers are interested in the strategies of the control design for plant scale. This chapter shows reviews of the previous works on the plantwide control design procedure and control structure design theory.

2.1 Plantwide Control

Luyben et al. (1997) presented the procedure of the plantwide control design. This research shows the nine-step procedure. The steps are both in plant scale and unit scale. Five steps of nine deal with plantwide issues that would not be addressed by simply combining the control systems from all of the plant's units. The procedure was applied with three industrial processes, vinyl acetate monomer process, east-man plantwide control process and HDA process. The strategy confirms a workable plantwide control strategy for given process designs. This control strategy can satisfy the plant's design objectives. However, the method is still based on the heuristic approach. In case of non-experience workers, it hard to illustrate the plantwide control design strategy with any process.

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

very useful. There is much-needed link between steady-state optimization and process control. The actual bottom-up design of the control system is done after the control problem has been defined.

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

2.2 Control Structure Design

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

Luyben (1996) illustrated the calculation of the design degrees of freedom and the control degrees of freedom for complex processes. Three considered complex processes are Luyben challenge process (involving three reactors, three columns, two recycles, three fresh feed streams, and six components), Eastman plantwide problem (involving a two-phase reactor, a condenser/separator, a stripper, a gas recycle stream, four fresh feed, and seven components), and vinyl acetate process. There is an easy way to determine the design degrees of freedom. The study presented that the complexity of the phase equilibrium and the physical properties does not affect the degrees of freedom.

Bildea and Dimian (2003) revisited the Luyben's Rule, fixing flow rates in recycle systems. They found that fixing the reactor-outlet flow rate and allowing variable reactor holdup leads to stable controllable plantwide control structure. The inlet of the reactor must be fixed the flow rates. The snowball effect is also avoided and the location ensures stable behavior. In the first-order reaction cases, if the conversion is low, the snowballing occurs when the fresh reactant feed flow to the reactor is set. However, the conventional structure is good at high conversion of the reaction. The second-order reaction with low-conversion, if the recycles are separated, setting inlets on flow control prevents the instability. If the reactants are recycled together, the recommended strategy is to design the plant for high conversion of on reactant, set its feed on flow control, fix the flow of total recycle, and add the make-up of other reactant in the recycle.

Konda et al. (2005) showed the plantwide control methodology with integrated framework of simulation and heuristics. An improved heuristic procedure is suggested by specifying the limitation related to the nine-step heuristic procedure of Luyben et al. More specific and generic guidelines are included. Beginners are supported to understand the alternatives at each stage and choose the better one based on the process knowledge and requirement. The improved heuristic methodology integrated with simulation as the heuristic procedure cannot always be trusted on plantwide control

decisions. The significance of this work is that the control system design cannot be performed just by heuristics without help of rigorous nonlinear simulation tools.

Konda et al. (2006) used simulation-based heuristic approach for designing plantwide control structure. This work is proposed for obtaining both of economic and operational benefits. The approach consists of two stages. The first stage, Alternatives are systematically originated and ranked based on economics. Then, A few top-ranked alternatives are forwarded to the second stage for analysis on their dynamics to define the best process that is economical as well as easy to operate.

Konda et al. (2006) presented the important steps for designing plantwide control through control degrees of freedom. The control degrees of freedom are measured in cases of highly integrated processes. The propose is for giving a maximum number of flows that be able to manipulate simultaneously in a process, and some (or all) of them can be utilized based on process requirement. The procedure is clearly simpler than the conventional approach.

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

Luyben at al. (2010) studied on methyl acetate process using carbonylation of dimethyl ether. The two-step process is used, dehydration of methanol to dimethyl ether and carbonylation to methyl acetate. The objects are to optimize the economics and study its dynamic control. The plantwide control design strategy is considered for developing the entire two-section process to effectively handle large disturbances in production rate and fresh feed compositions.

CHAPTER III

THEORIES

In favor of designing the control system methodology, the unit-based system is generally used to design the entire plant. The highly integrated processes (material and energy) are tightly strict to the environmental regulations, safety and economic conditions. Wherefore, the plantwide process control strategies are used to obtain satisfactory products, process performance and stability.

3.1 Plantwide Control Issues

Most continuous processing plants contain many units, such as reactor, heat exchangers, and distillation columns. The goal of process design is to minimize capital costs while operating with optimum utilization of materials and energy. Unfortunately, achieving lower plant capital costs and higher processing efficiencies inevitably makes the individual units interact more with each other and thus makes them harder to control. The process control engineer deals with these unit-to-unit interactions by designing a control system that counteracts disturbances before they propagate from their source to other units. Therefore, there are general problems a control system is called on to satisfy.

3.1.1 Integrated Process

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

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

These issues are concerned if we have to deal with a complex plantwide control.

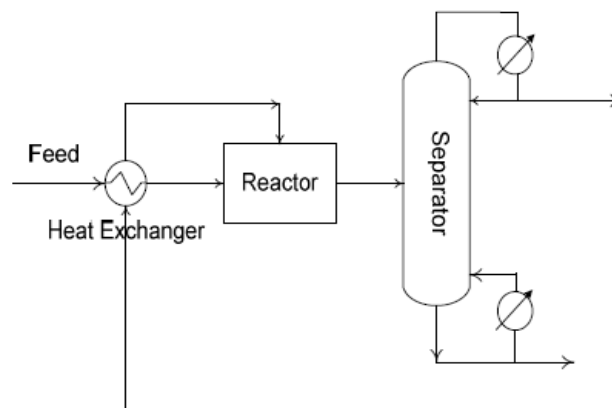


Figure 3.1 Integrated Process Flowsheet

3.1.1.1 Material Recycle

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

1. Increase conversion

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

2. Improve economics

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

3. *Improve yields*

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

4. *Provide thermal sink*

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

5. *Prevent side reactions*

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

6. *Control properties*

In many polymerization reactors, conversion of monomer is limited in order to obtain the desired polymer properties. These include average molecular weight, molecular weight distribution, degree of branching, particle size, etc. Another reason for limiting conversion to polymer is to restraint increase in viscosity that is typical of

polymer solutions. This facilitates reactor agitation and heat removal and allows the material to be further processed.

3.1.1.2 Energy Integration

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

3.1.2 Chemical Component Inventories

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

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

3.2 The Plantwide Control Obstacle

3.2.1 Internal Feedback of Material and Energy

Processes that include recycle systems have an important design requirement—namely, that there must be an exit path for every chemical species. For example, inert components can be kept at reasonable levels by “bleeding off” a small portion of the

recycle stream. However, Luyben (1994) discussed a subtle problem with recycle systems, the snowball effect, which is characterized by a large sensitivity of one or more of the variables in a recycle loop to small changes in a disturbance variable. This problem arises from both a small reactor holdup and a particular control structure.

In particular, if changes in fresh feed composition “load the reactor excessively”- that is, beyond its ability to provide the required conversion-then the separator/recycle system will be called on to make up the deficiency. For the case where extra reactor capacity is available through an increase in the reactor level, the particular choice of level/flow control structure within the recycle loop can radically affect plant gains (sensitivities). In the following, we assume that the reactor design is fixed and its level is set at less than full capacity. The question to be considered is how alternative designs of level and flow loops mitigate the effect of fresh feed flow rate or composition disturbances.

3.2.1.1 Steady-state Behavior: The Snowball Effect

Firstly, an interesting observation that has been made about recycle system is their tendency to exhibit large variations in the magnitude of the recycle flows. Plant operators report extended periods of operation when very small recycle flows occur. It is often difficult to turn the equipment down to such low flow rates. Then, during other periods when feed conditions are not very different, recycle flow rates increase drastically, usually over a considerable period of time. Often the equipment cannot handle such a large load.

This high sensitivity of the recycle flow rates to small disturbances called the snowball effect. It is important to note that this is not a dynamic effect; it is a steady-state phenomenon, it can be analyzed by considering a steady-state model. However, it does have dynamic implications for disturbance propagation and for inventory control. There is nothing to do with closed-loop stability. Furthermore, this does not imply that it is independent of the control structure. On the contrary, the extent of the snowball effect is very strongly dependent upon the control structure used. The large swings in recycle

flow rates 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. Therefore, it is important to select a plantwide control structure that avoids this effect.

3.2.1.2 Transient Behavior: The Slowdown in Overall System Dynamics

A second characteristic of using material recycle and/or heat integration is that the plant may respond to disturbances much more slowly than would be anticipated based on the time constants of individual units.

3.2.1.3 Propagation and Recirculation of Disturbances

A third major effect often encountered with recycle and heat integration is the propagation of disturbances from unit to unit, and their recirculation around internal process flow paths. This understanding why this plantwide control issue differs so substantially from single-unit issues.

In a single unit regulation, one desirable effect of using feedback control to attenuate disturbances in a process unit is to transfer these variations to a utility stream. For example, if a reactor temperature is disturbed, the cooling water flow rate will be changed by the temperature controller so as to reduce the effect of the disturbance. Even so, some variation in reactor temperature inevitably will remain, and this will propagate to downstream units as a disturbance.

A minor side effect of these actions is that the supply header temperature itself will change slightly as cooling water demand is raised/ lowered by actions of a reactor temperature controller. Although utility supply systems are built with their own internal controllers, and these are designed to attempt to regulate the utility outputs in the face of process disturbances, it is not possible to attenuate utility disturbances entirely. These propagate directly throughout the plant.

In older plants, surge tanks were used to damp flow variations between units. Material holdup in a surge tank can also serve as a thermal capacitance and thus reduce effluent temperature variations; only reduced flow and temperature variations propagate to downstream units. In today's more highly integrated plants, containing material recycle and/or heat integration but little surge capacity, unattenuated disturbances propagate directly to downstream units, even to adjacent (coupled) units and to upstream units.

3.2.2 Interaction of Plant Design and Control System Design

In the past, when the continuous processing plants were designed to be much less interaction than now, it was possible to complete the plant design before considering control system design. After the proposed plant's flowsheet and equipment specifications were completed, process control engineers were responsible for specifying instruments and controllers. By providing an excess of measurements (instruments) and control valves, plus a feedback controller for every important process variable, the control system designer was reasonably sure that the new plant could be started up and controlled. Continuous processing plants designed or retrofitted today no longer can utilize a sequential design process in which plant design is followed by control system design (Keller and Bryan, 2000), nor can designers specify redundant equipment, except for safety purposes.

Without careful attention to design, highly integrated plants may have too few control degrees of freedom, which makes them difficult to start up and operate safely. For example, in designing the heat exchanger and related equipment for heat integration the heating and cooling loads first must be approximately balanced by the process designer. Then the designer must establish whether the approach temperatures are satisfactory to meet the heat transfer requirements with a reasonably sized heat exchanger; in this step, adjustment of column operating pressures may be required (Seider et al., 2003). Because the energy supply capability in one unit usually will not balance the demand in another unit exactly, a "trim exchanger" (small heat exchanger

sized to make up the difference in heating/cooling capability) generally has to be provided in the steady-state design.

A heat integration scheme also causes two control degrees of freedom to be “lost”: the cooling water flow rate control valve that would have been located in the Column 1 condenser, plus the steam control valve that would have been used in the Column 2 reboiler. If process control engineers are not involved in the plant design process from the beginning, the critical process dynamic and control evaluations may be omitted that would provide such information and an opportunity to resolve any problems (Keller and Bryan, 2000). In short, a suitably sized trim unit must be available to make up for any steady-state heating/cooling deficiency plus lost control degrees of freedom necessary for normal operations. It also can assist in start-up and shutdown operations.

The control system designer must determine whether a proposed plant design will be controllable and operable (Fisher et al., 1988b; Downs and Ogunnaike, 1995). For example, highly integrated distillation columns can cause problems in a number of ways:

1. One or both column products cannot be controlled at the desired set point(s).
2. Disturbances in the Column 1 overhead cannot be prevented from propagating to Column 2.
3. The “lost degrees of freedom” from plant integration need to be restored by the addition of one or two trim heat exchangers operated and controlled using plant utility supplies.
4. The plant cannot be started up easily because of the need to have Column 1 “hot” before Column 2 can be brought into service.

Consequently, there are three main functions of the control system, namely, disturbance rejection. It is the main objective in installing control system. The external disturbance is uncertain so the operator cannot monitor the changing in process. As a result, the control system must be installed to follow the changing of process and

manipulate the process variable to compensate for the disturbance from external factors. Another function is to maintain stability. The stability is necessary for every process. As a result the control system is set to improve the process stability for the guarantee of quality of product, safety to equipment of process and plant. The other is to keep the process performing highest efficiency. Besides rejecting disturbance and maintaining stability, the control system can achieve the great profit because it losses less energy and raw materials during the operating. Moreover, the product will meet the required specification and have high production rate.

3.3 Fundamental Procedures for Plantwide Control

3.3.1 Buckley Basic

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

1. Material balance control
2. Production quality control

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

3.3.2 Douglas doctrines

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

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

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

3.3.3 Drowns drill

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

3.3.4 Luyben laws

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

1. To prevent the snowball effect, all recycle loops should be controlled flow.
2. A fresh feed stream (reactant) cannot be flow controlled unless there is essentially complete one-pass conversion of one of the reactants. This law applies to systems with reaction such as $A+B \rightarrow \text{products}$. In systems with consecutive reactions

such as $A+B \rightarrow M+C$ and $M+B \rightarrow D+C$, the fresh feeds can be flow controlled into the system, because any imbalance in the ratios of reactants is accommodated by a shift in the amounts of the two products (M and D) that are generated. An excess of A will result in the production of more M and less D. An excess of B results in the production of more D and less M.

3. If the final product from process comes out at the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor. Changes in feed flow rate or feed composition have less of a dynamic effect on distillate composition than they do on bottoms composition if the feed is saturated liquid. The reverse is true if the feed is saturated vapor: bottom is less affected than distillate.

3.3.5 Richardson rule

Bob Richardson (1988) proposed the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense because it provides more muscle to achieve the desired control objective. An analogy is that it is much easier to maneuver a large barge with a tugboat than with a life. The point is that the bigger the handle you have to affect a process, the better you can control it. This is why there are often fundamental conflicts between steady-state design and dynamic controllability.

3.3.6 Shinskey schemes

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

3.3.7 Tyreus tuning

The use of P-only controllers for liquid levels, tuning of a P controller is usually trivial: set the controller gain equal to 1.67. This will have the valve wide open when the

level is at 80 percent and the valve shut when the level is at 20 percent. For other control loops, suggest the use of PI controllers. The relay-feedback test is a simple and fast way to obtain the ultimate gain (K_u) and ultimate period (P_u). Then either the Ziegler-Nichols settings or the Tyreus-Luyben (1992) settings can be used:

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

3.4 Step of Plantwide Control Design Procedure

Plantwide control design procedure is importantly satisfying the principles of the overall conservation of energy and mass. Furthermore, economic criterion is essentially taken into account.

Luyben et al., (1997) proposed a nine-step heuristic design procedure for a workable plantwide control strategy. The nine-step of the design procedure essentially concentrate on: energy management; production rate; product quality; operational; environmental and safety constraints; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization.

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. The chosen 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 degree of freedom

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

Step 3: Establish energy management system

Term "energy management" indicates two functions. Firstly, it is necessary that the design is provided 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. The other function, if heat integration does occur between process streams, then this second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

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. To obtain higher production rate, the overall reaction rates must be increased. This can be accomplished by increasing temperature, pressure, reactant concentrations, or reactor holdup.

A variable that has the least effect on the separation section and a rapid and direct effect on reaction rate in the reactor without hitting an operational constraint must be selected.

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. The tight controls of these important quantities are required for economic and operational reasons. Hence, the manipulated variables should be selected 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).

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 with that unit.

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flow in the recycle loop are controlled by levels. 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

Ensure that the overall component balances for each chemical species can be satisfied either through reaction or exit streams by accounting for the composition of a component or inventory at some point in the process.

Component balances can often be quite subtle. Such balances depend upon the specific kinetics and reaction paths in the system and often affect what variable can be used to set production rate or rate in the reactor.

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations. For example a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flow rate to a furnace supplying energy to the reactor. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

Step 9: Optimize economics or improve dynamic controllability

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

Recently, the procedure of Wongsri (2011) presented the eight-step of design procedure which based on heuristics analysis. In this procedure, the precedence of control variables is established. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method (Wongsri, 1990) to cover the material disturbances. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

Step 1: Establishment of control objective

Step 2: Selection of controlled variables

Step 3: Selection of manipulated variables and measurements via DOF analysis

Step 4: Energy management via heat exchanger networks

Step 5: Selection of control configuration using various tools available

Step 6: Completing control structure design by checking the component balance

Step 7: Selection of controller type: single loop or MPC

Step 8: Validation via rigorous dynamic simulation

Fixture Point theorem

The selected controlled variables are ranked using the Fixture point theorem. The step of fixture point theorem analysis is followed below.

1. The process is considered at dynamic mode (the process running until the process responses are at steady state).
2. Controlled variables (CV) can be arranged to follow the most sensibility of the process variable by step change of the manipulated variables (MV) in open loop control (change only one MV, the other should be fixed than alternate to other until complete).
3. Study the magnitude of integral absolute error (IAE) of all process variables that deviates from steady state.
4. Select CV by considering CV that gave the most deviation from steady state (high value score).

3.5 Heat Exchanger and Plantwide Energy Management

Another important issue in process design is energy conservation. Common ways to improve the conservation is to install feed-effluent heat exchangers (FEHs) around reactors and distillation columns where one streams is heated, another must be cooled. For instance, in HDA process, the toluene fresh feed, the makeup hydrogen, the recycle toluene, and the recycle gas stream needed to be heated up to the required reaction temperature. And, the reactor effluent stream must also be cooled to the cooling water temperature to accomplish a phase split. So the energy integration is

required to reduce the utility cost in addition to improve thermodynamic efficiency of the process.

3.5.1 Heat Exchanger Dynamics

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

3.5.2 Heat Pathway

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

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

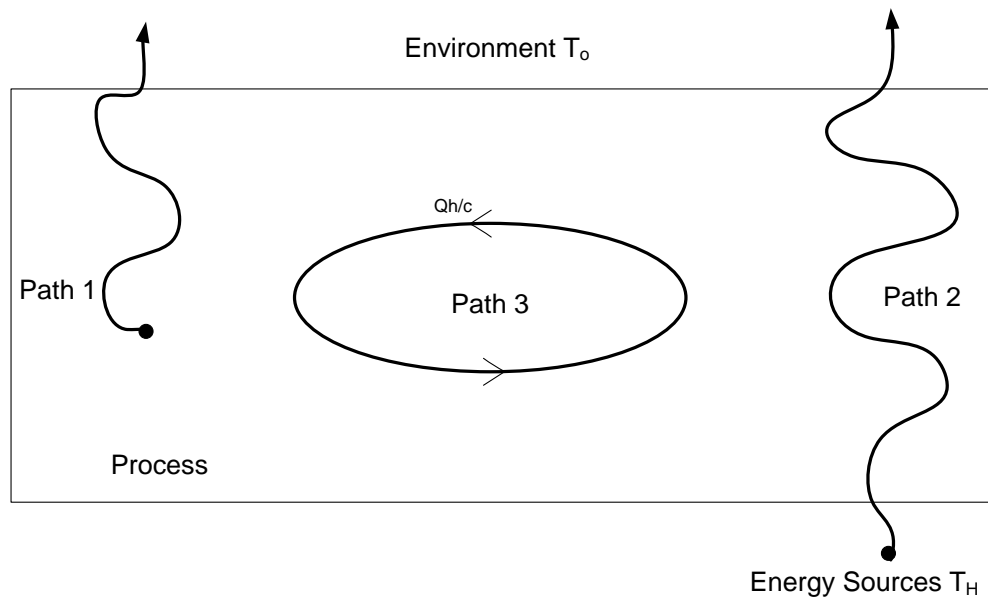


Figure 3.2 Heat Pathways.

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

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

3.5.3 Heat Recovery

The great improvements in the plant's thermal efficiency are made by recycling much of the energy needed for heating and cooling process streams. There is of course a capital expense associated with improved efficiency but it can usually be justified

when the energy savings are accounted for during the lifetime of the project. The current context draws attention on how heat integration affects the dynamics and control of a plant and how energy in plants can be managed with a high degree of heat recovery.

3.6 Control of Process-to-Process Exchangers

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

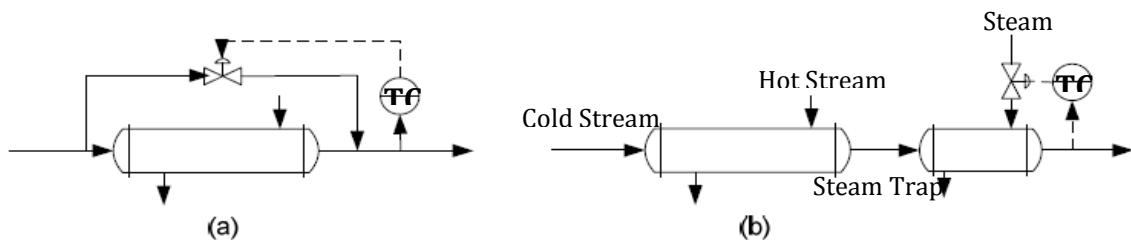


Figure 3.3 Control of P/P heat exchangers; (a) use of bypass; (b) use of auxiliary utility exchanger

3.6.1 Bypass Control

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

service. Cost consideration would also suggest a small bypass flow to minimize the exchanger and control valve sizes.

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

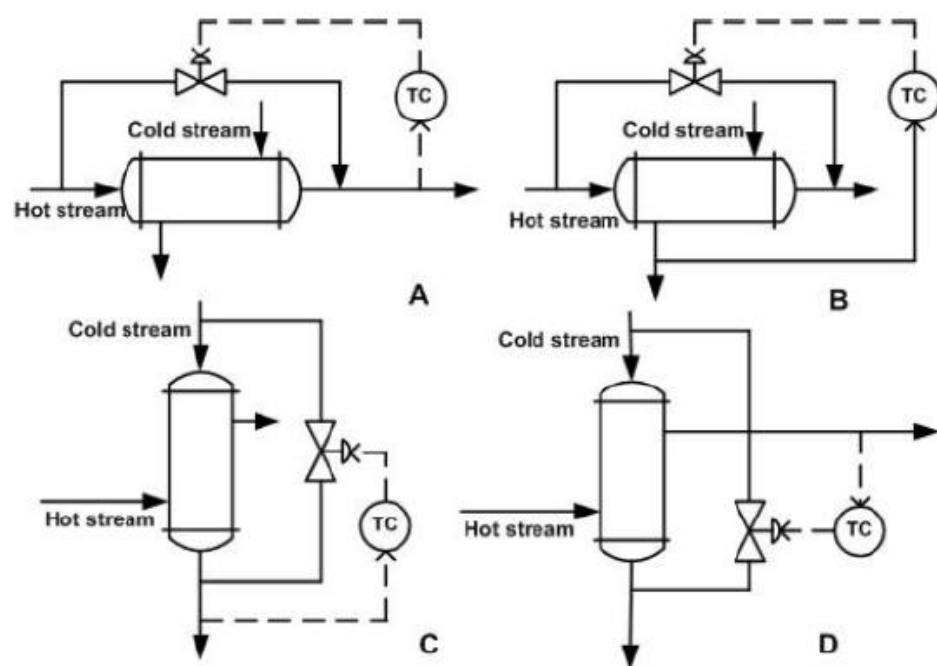


Figure 3.4 Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

3.6.2 Use of auxiliary utility exchangers

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

Though, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control standpoint.

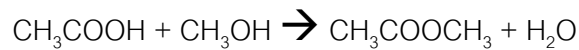
Second, decision on how to combine the utility exchanger with the P/P exchanger must be made. This could be done either in a series or parallel arrangement. Physical implementation issues may dictate this choice but it could affect controllability. Finally, decision on how to control the utility exchanger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

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

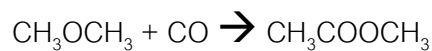
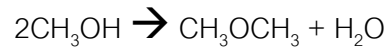
CHAPTER IV
METHYL ACETATE PROCESS AND CONTROL STRUCTURES
DESIGN PROCEDURE

4.1 Introduction

The conventional production of methyl acetate occurs by esterification of acetic acid with methanol over an acid catalyst.



Furthermore, the alternative production, two reaction steps, can be used instead of the esterification. The two reaction steps are dehydration of methanol to form dimethyl ether (DME) and followed by carbonylation with carbon monoxide (CO) to form methyl acetate.



These steps are a feasible option for a CO available plant. For the price of the reactant, methanol and acetic acid are \$26.24/kmol and \$42.6/Kmol respectively, found on the ICIS.com website (2009). Hence, using the two reaction steps are break even.

4.2 Kinetics

The reaction rate was applied by following the rate expression showed in a design project of R. Bertrum Diemer and William L. Luyben. The reactions, dehydration and carbonylation are exothermic. Dehydration, the rate expression is the following form:

$$r_{dehy} = k_{dehy} \left(p_{\text{MeOH}} - \frac{p_{\text{DME}} p_{\text{W}}}{p_{\text{MeOH}} K_{dehy}} \right)$$

$$r_{dehy} = \text{MeOH dehydration rate, kmol/kg}_{\text{catalyst}}/\text{s}$$

$$k_{dehy} = \text{dehydration rate constant, kmol/kg}_{\text{catalyst}}/\text{s}/\text{Pa}$$

K_{dehy} = dehydration equilibrium constant

With:

$$\ln k_{dehy} = -8.00 - 9680/T(K)$$

$$\ln K_{dehy} = -2.8086 + 3061/T(K)$$

And the carbonylation rate expression is as follows:

$$r_{carbonyl} = k_{carbonyl} \left(\frac{p_{CO}}{1 + K_W p_W} \right) \left(\frac{K_{DME} p_{DME}}{1 + K_{DME} p_{DME}} \right)$$

$r_{carbonyl}$ = carbonylation, kmol/kg_{catalyst}/s

$k_{carbonyl}$ = carbonylation rate constant, kmol/kg_{catalyst}/s/Pa

K_W = H₂O adsorption equilibrium constant, Pa⁻¹

K_{DME} = DME pseudo-adsorption equilibrium constant, Pa⁻¹

With:

$$k_{carbonyl} = 8.2 \times 10^{-5} \exp\left(-\frac{8370}{T(K)}\right)$$

$$K_{DME} = 1$$

4.3 Process description

The production of methyl acetate via the two reaction steps can be divided to two sections by the reaction type, dehydration and carbonylation section. The first section, a reactant, methanol is fed to a process by 99 mol% concentration and 1 mol% of water contaminated. A recycle stream at 26.98 kmol/hr is also fed together with the reactant at 500 kmol/hr. The total reactant is preheated in the first heat exchanger before vaporized in a vaporizer. The vaporizer temperature is 423 K and energy consumption is 4.51 MW.

Prior to enter a reactor, the vapor reactant stream is preheated in the second heat exchanger to 628 K. The reactor is a cooled tubular reactor with a constant medium temperature heat-transfer model. The reactor has 300 tubes with 0.0245 m diameter and

10 m length. The cooling medium temperature is 665 K. There is catalyst contained in the reactor in which the density is 2500 kg/m^3 and void fraction is 0.4.

High-pressure steam at 42 atm can be generated by the exothermic heat of reaction on the shell side of the reactor. A used overall heat-transfer coefficient of the reactor is $0.28 \text{ kW K}^{-1} \text{ m}^{-2}$. The conversion of methanol is 94.66%.

The products leave the reactor at 658 K and then are fed to the second heat exchanger to preheat the reactor feed. The product stream is cooled to 467 K. The stream is cooled further in the first heat exchanger that preheats the total methanol feed to 400 K. Before entering to the first distillation column, the product stream enters a water-cooled heat exchanger that is cooled to 351 K.

The first distillation column (C1) is used to separate DME from the unconverted reactant and the water product. Column C1 has 22 stages. Feed stage is on stage 12. The DME quality out of C1 in distillate stream is 99.9 mol% and other is methanol 0.1 mol%. DME flow rate is 247 kmol/hr. The bottom product consisting of the unconverted methanol and the water product is fed to the second distillation column (C2).

Column C2 has 27 stages and is fed on stage 16. In this column, Methanol is distilled from undesired water and recycled back to the process, combined with the fresh feed. A High-purity methanol distillate is 99.97 mol%. The contaminants are water 0.02 mol% and 0.01 mol% of others. The undesired water product leaves the column C2 at 253 kmol/hr.

The DME product from the first section is a reactant of the second section, carbonylation section. CO fresh feed is also a reactant, concentration of 98 mol% contaminated with H_2 2 mol% as an inert. DME must be in vapor phase. Then, DME is fed to vaporizer before entering to the carbonylation section, which operating temperature is 372 K and pressure is 32 atm. The energy consumption in the vaporizer is 1.43 MW. CO fresh feed is fed by using a compressor pumped to 32 atm. The required flow rate of the CO fresh feed is higher than the stoichiometric amount needed

to react with acquired DME from the first section because of loss of CO in purge stream. The DME reactant, CO and recycle streams are combined and then enter to the second reactor for carbonylation reaction.

A reactor with coolant is used in this section for controlling occurred heat of reaction. The reactor has 1000 tubes 0.05 m diameter, and 10 m length. The reactor operates at 475 K temperature and 32 atm pressure. The conversion of DME carbonylation is 88.15%.

Unconverted reactants and products are then partially condensed in a water-cooled heat exchanger. Liquid and vapor phase are separated through a separator operating at 320 K temperature at 30 atm pressure. Most of gas is compressed back to the process at 32 atm. Component in vapor phase stream from separator mostly are CO and hydrogen, 55.61 mol% and 0.4 mol% respectively. There is a purge stream for quality control of 40 mol% hydrogen.

The condensed liquid stream is fed to the third column (C3) for recovering the unconverted reactant. Column C3 has 17 stages and feed stage is on stage 2. Bottom product of the column C3 is main product methyl acetate and flow rate is 246.49 kmol/hr. Concentration of methyl acetate is 99.9% with methanol 0.1 mol% contaminated. The unconverted reactant is then pumped to 32 atm and reentered to the process.

4.4 Control Structures Design Procedure

The wongsri procedure, 8-step procedure is considered in this research. The 8-step procedure is a method for designing plantwide control structures. Performer can follow the method step by step. This procedure could establish effective plantwide control structures. The 8-step procedure is as follows:

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

List all control variables:

- I. An independent stream must have a control valve (1 DOF) you cannot place two control valves on a single stream.
- II. A heater, cooler, pump, or compressor has one degree of freedom (to adjust heat load or duty or work load)
- III. A process to process heat exchanger has one degree of freedom by adding a by-pass line.
- IV. A reactor has zero or one degree of freedom depends on its type. For example, an isothermal reactor need heat input to keep its temperature constant, while an adiabatic reactor has zero degree of freedom.
- V. A flash separator has two degree of freedom.
- VI. A simple distillation column has five degree of freedom.

How to pair manipulated and controlled variables:

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

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

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

3. Establish fixture plant

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

- 3.1 Keep the raw materials entered and reentered fixed
- 3.2 Adjust the flow of exit material streams according to their accumulation (products, by-products, and inert)
- 3.3 Locate the quantifiers for the rest of the components and design the control loops to regulate their inventories in the plant. The material flow in the plant should be fixed. In the case that this cannot be done the change of the material flow must be slow.

4. Handling the disturbances

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

4.1 Heat Disturbances

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

4.2 Material disturbances

The configuration of the control loops depend on the desired material pathways by analyzing the material disturbance tests on changes of composition, total flow, component flow: At reactor, we adjust the reactor inlet temperature in

order to keep the reactor outlet composition or the product component flow fixed. For distillation columns, to control top or bottom temperature depend on the material disturbance rejection policy.

5. Find the most disturbed point and design the control loops to alleviate the effects of disturbances.
6. Design the control loops for the rest of the control variables and/or adding enhanced controls, i.e. cascade, feed forward controls.
7. Optimize economics and/or improve control performance
8. Validate the designed control structures by rigorous dynamic simulation

CHAPTER V

NEW CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION

This research follows the 8-step of Wongsri for designing the control structure of methyl acetate process. Plantwide controls are considered because of complex of the process such as heat integration and recycle streams. The new control structures completed by Wongsri procedure are compared with the structure established by Luyben (2010). The new control structures are accomplished by the following steps:

5.1 New control structures

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

Control Objectives:

1. Capacity of production is about 19,000 tons methyl acetate/year.
2. Product quality of methyl acetate is 99.9 mol%.

Plant information:

1. Outlet temperatures of reactor R1 and R2 are 658K and 477K respectively.
2. Temperature inlet column C1 is 351K controlled by water-cooled heat exchanger.
3. Column C1 operates at 10 atm. Dimethyl ether out of column C1 is 99.9 mol%.
4. Column C2 operates at 1 atm. Purities of methanol and water out of column C2 are both 99 mol%.
5. Separator S1 operates at 320K and 30 atm.
6. Column C2 operates at 5 atm. Concentration of methyl acetate out of column C3 is 99.9 mol%
7. H₂ concentration in the recycle loop leaving from separator S1 is 40 mol% controlled by purge stream.

Control Degrees of Freedom:

Table 5.1 manipulated variable and control degrees of freedom

Unit	Manipulated variable	Number	DOF
Independent streams	Flow rate	2	2
Cooler	Heat flow	2	2
Pump	Work	1	1
Compressor	Work	3	3
Heat exchanger with by-pass	By-bass flow rate	2	2
Reactor with coolant	Heat flow	2	2
Separator	Liquid flow and Vapor flow	1	2
Vaporizer	Vapor flow and Heat flow	2	4
Distillation column	Distillate flow, Bottom flow, Reflux flow, Heat reboiler and Heat condenser	3	15
Total degrees of freedom			35

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

There are heat exchanger networks existing in this process. Exchanger H1, total methanol fresh feed is exchanged heat with the stream out of exchanger H2. The methanol before entering the reactor is preheated by the product of reactor R1 in exchanger h2. The both exchangers have a by-pass line which can be controlled temperature of the outlets.

Step 3: Establish fixture plant

The raw materials entered and reentered the process are fixed and the exit streams are adjusted according to their accumulation. The total methanol feed, fresh

feed mixed with recycle stream, is fixed by measuring the total feed then adjust a valve of the fresh feed to keep the total feed of the reactor R1. CO fresh feed is controlled as a ratio of CO/DME for keeping the concentration of CO in total reactor R2 feed by adjusting the pressure setpoint of the compressor. There are 3 exit streams, by-product water, methyl acetate and purge, adjusted in accordance with their accumulation. The water product is adjusted by controlling level of reboiler in column C2. Methyl acetate is adjusted by controlling level of reboiler in column C3. Purge is used to control the concentration of H₂ in recycle stream at 40 mol%.

The other quantifiers, DME and methanol quantifier are controlled the accumulation by adjust the liquid flow out. The quantifier of DME is at the reflux drum of column C1 and the quantifier of methanol is at the reflux drum of column C2. And the CO quantifier is at the reflux drum of column C3 controlled by adjust a vapor flow out for keeping condenser pressure constant. The control structures of fixture plant are established as following figure 5.1.

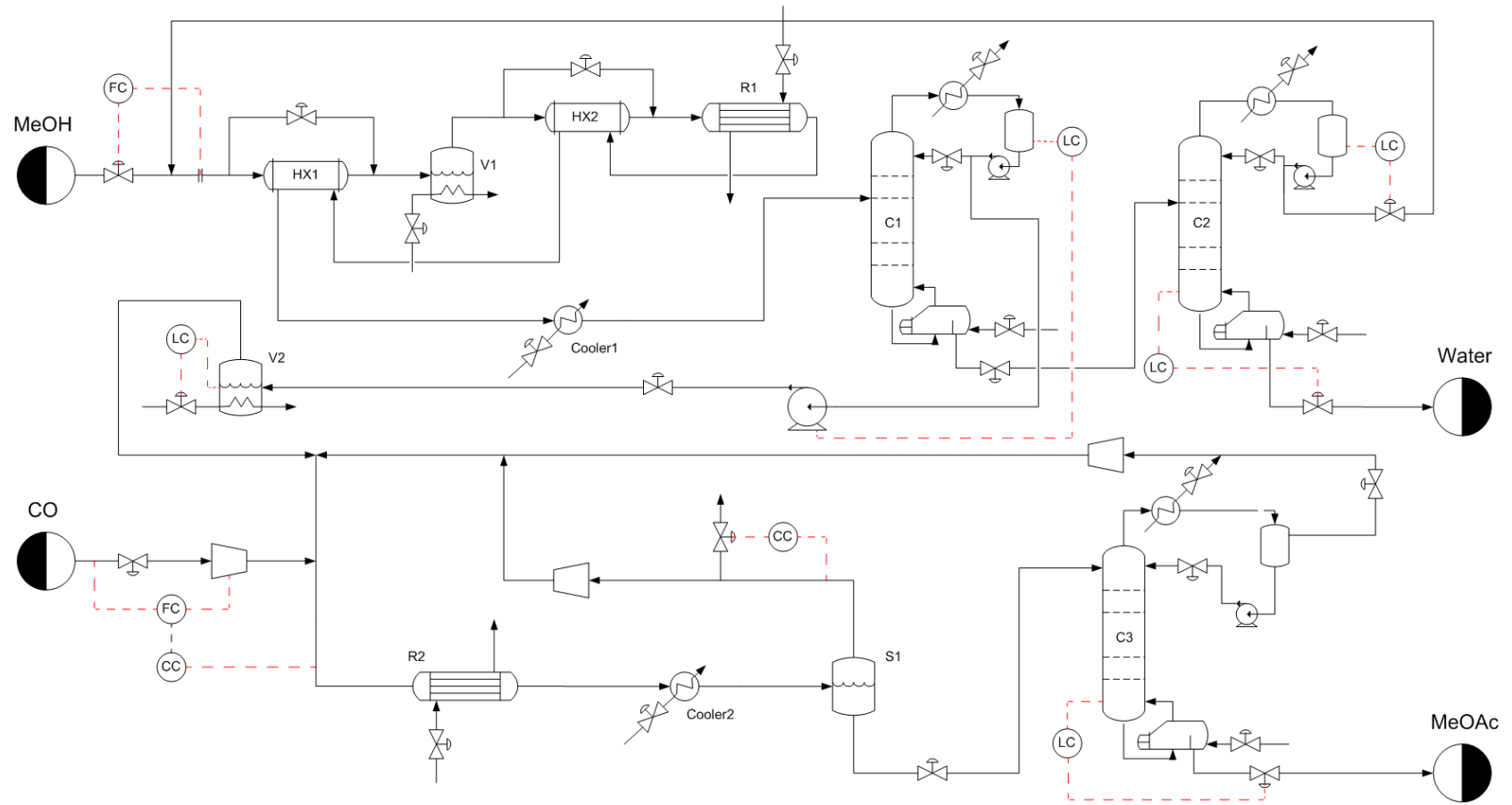


Figure 5.1 the control structures of fixture plant

Step 4: Handling the disturbances

1. Heat disturbances

The heat disturbance can be directed out of the process in four points, at the both vaporizers and the both water coolers. At the heat exchangers, the cool stream out temperatures are controlled by adjust the by-pass streams of the heat exchangers. So the heat disturbances enter the heat exchangers are directed to the hot streams.

The other temperature control loops related with qualities are entered for avoiding the composition disturbance. All quality control loops are outlet temperature controls of reactor R1-R2, and temperature controls of column C1, C2 and C3.

2. Material disturbances

There are path ways of any material showed in figure 5.2-7. The material path ways indicate the control structures to manage each material according to their path ways. Methanol is controlled to react in reactor R1. Unconverted methanol is recycled back to the process combining the fresh methanol feed. DME generated at reactor R2 is distilled at column C1 and sent to the second section for reacting, carbonylation. Partial unconverted DME and CO are separated at separator S1 and the remainder is distilled at column C3 to be recycled back. H₂O product is carried out from the first section at the bottom column C2. Methyl Acetate is carried out as a product from the bottom of column C3. Furthermore, inert H₂ come with CO fresh feed are separate out at the purge stream.

All control structures established from step 4 are shown as following figure 5.8.

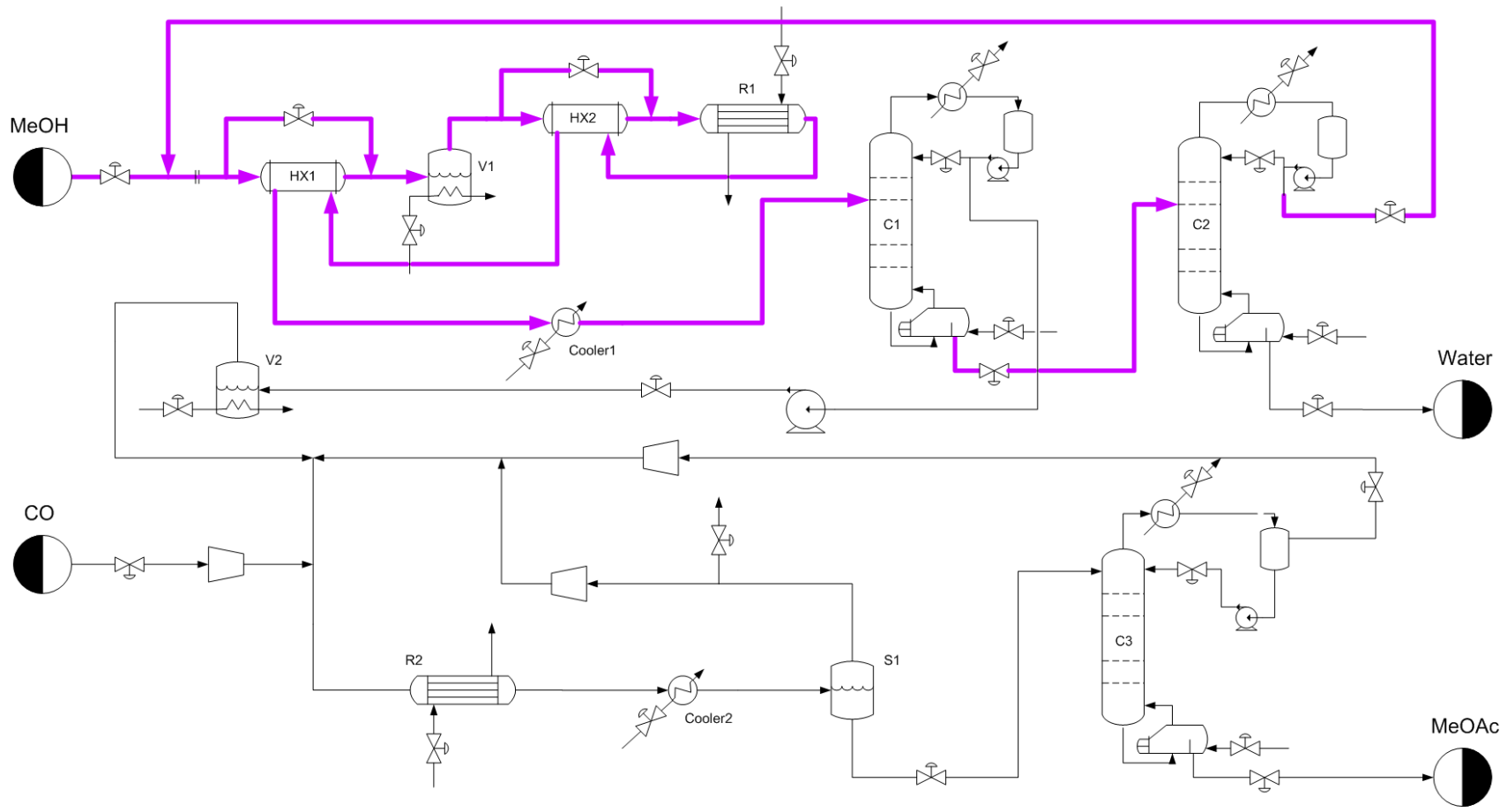


Figure 5.2 Methanol Pathway

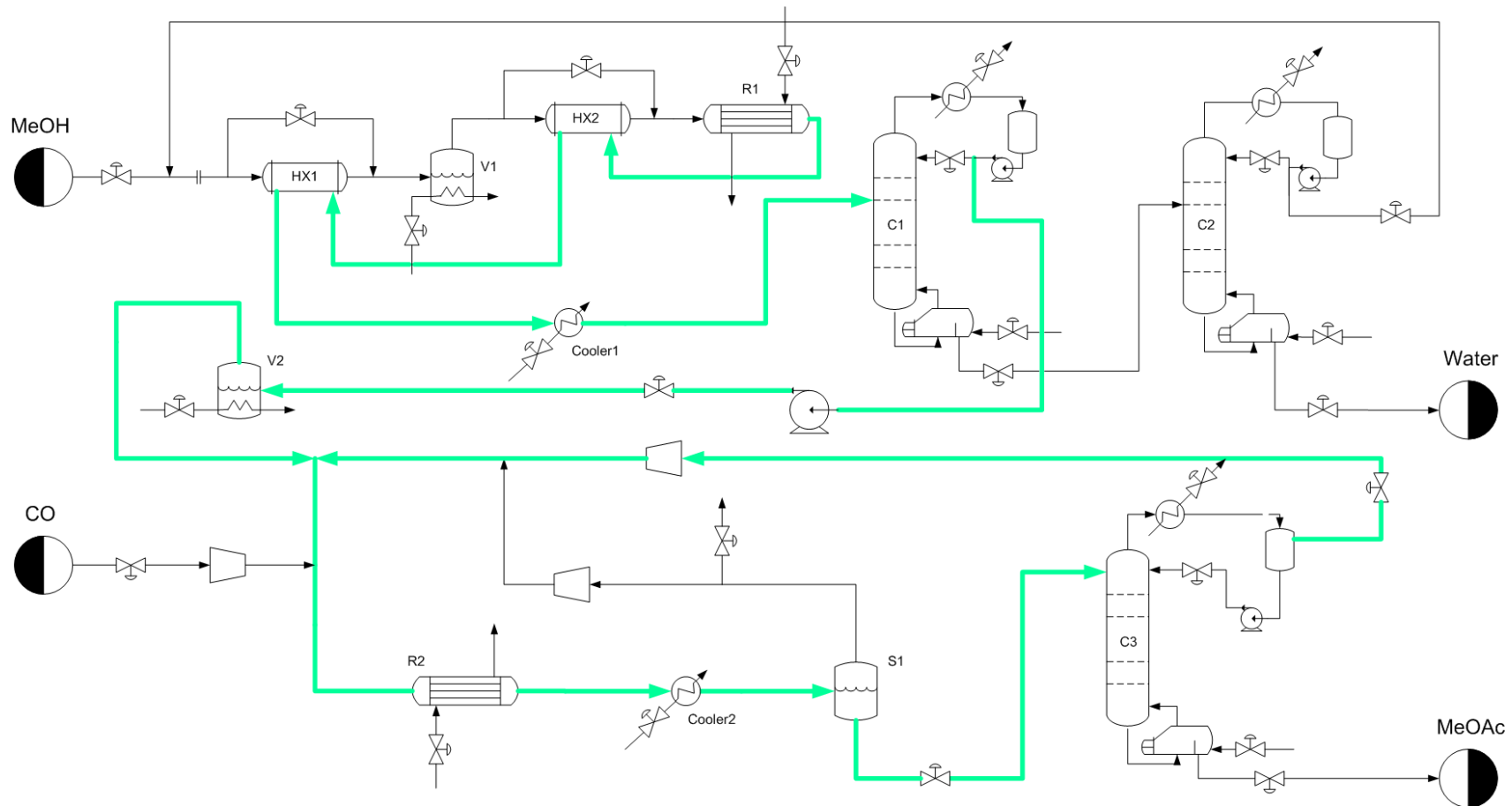


Figure 5.3 Dimethyl Ether Pathway

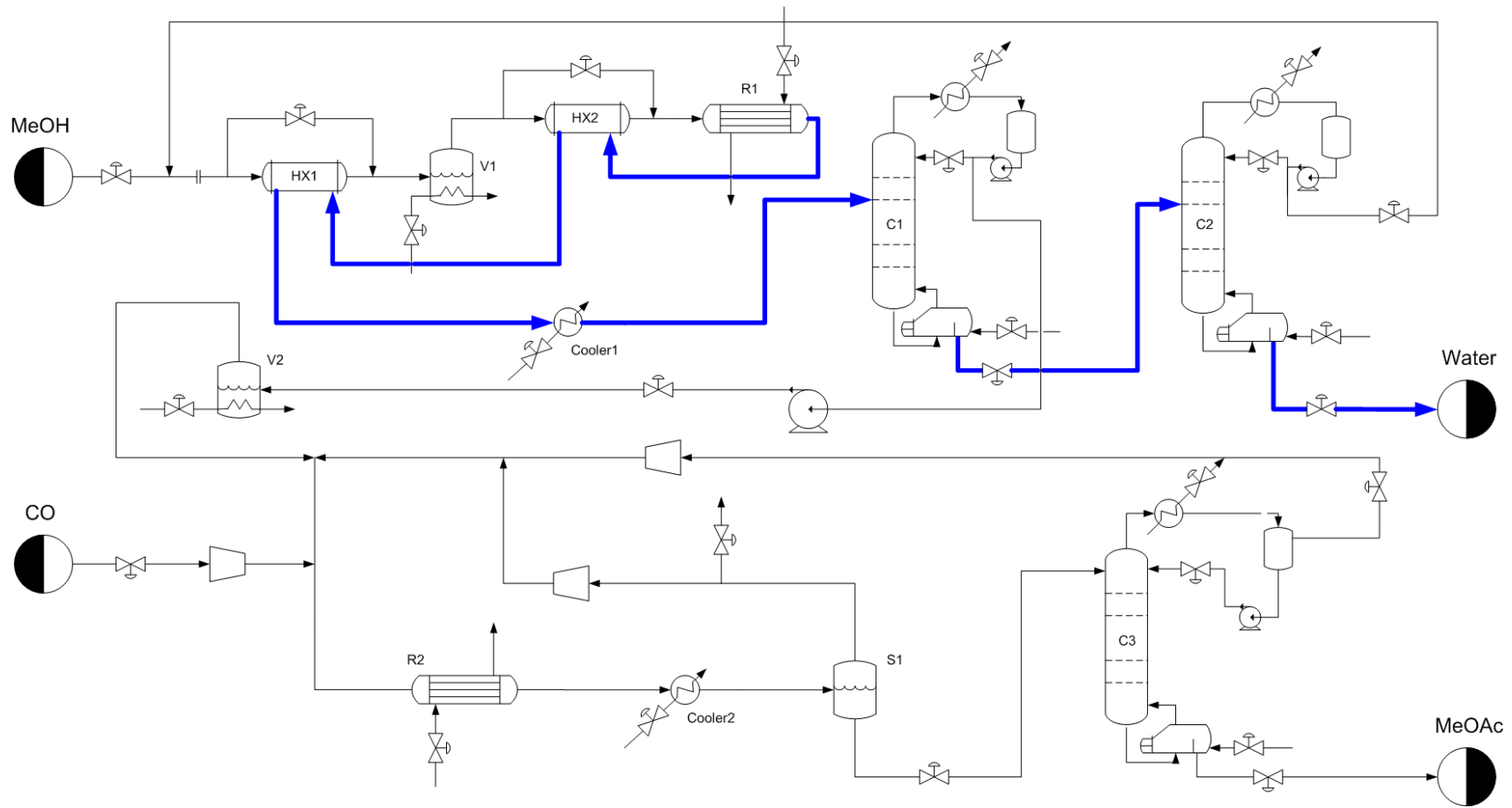


Figure 5.4 Water Pathway

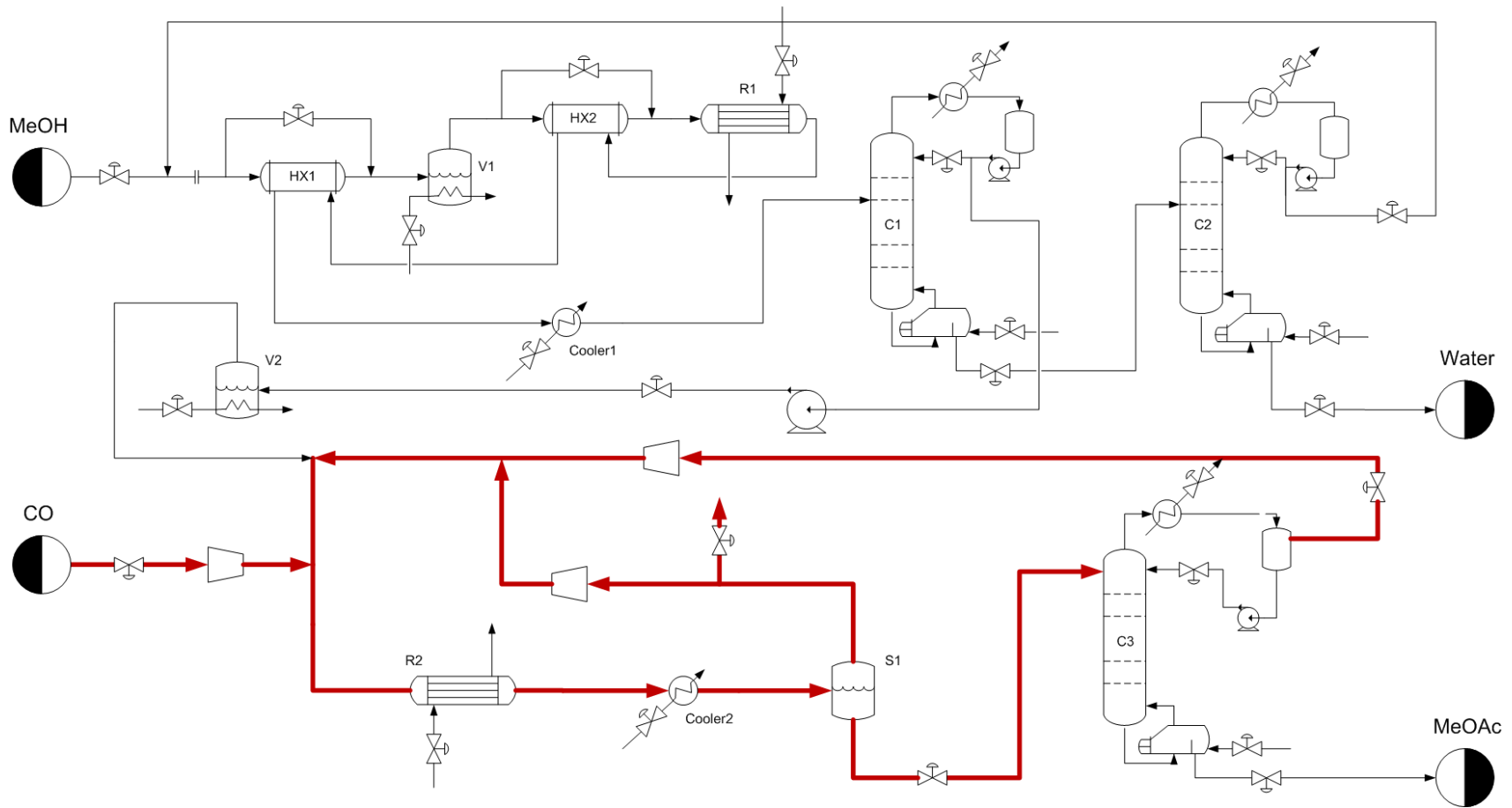


Figure 5.5 Carbon Monoxide Pathway

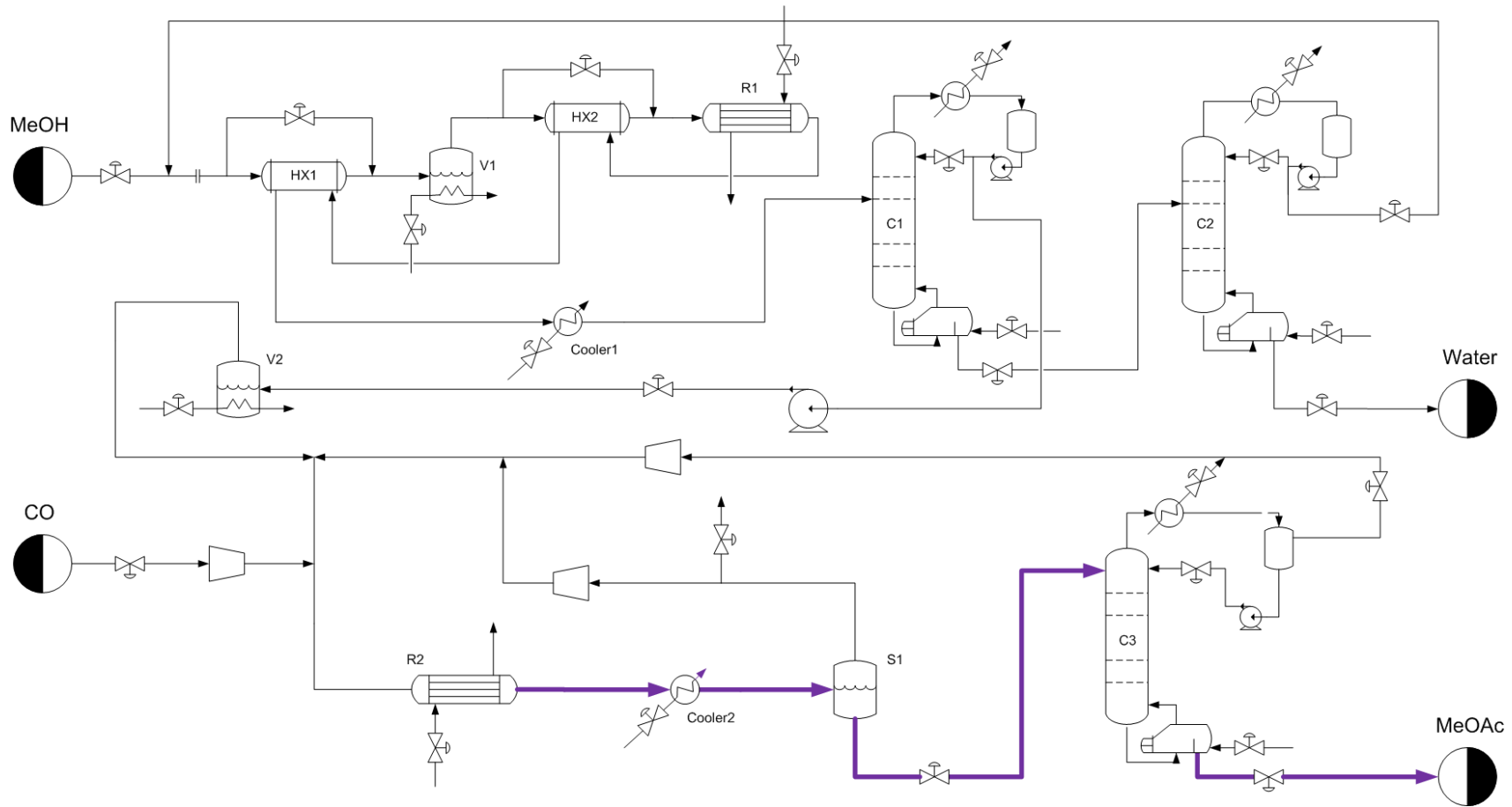


Figure 5.6 Methyl Acetate Pathway

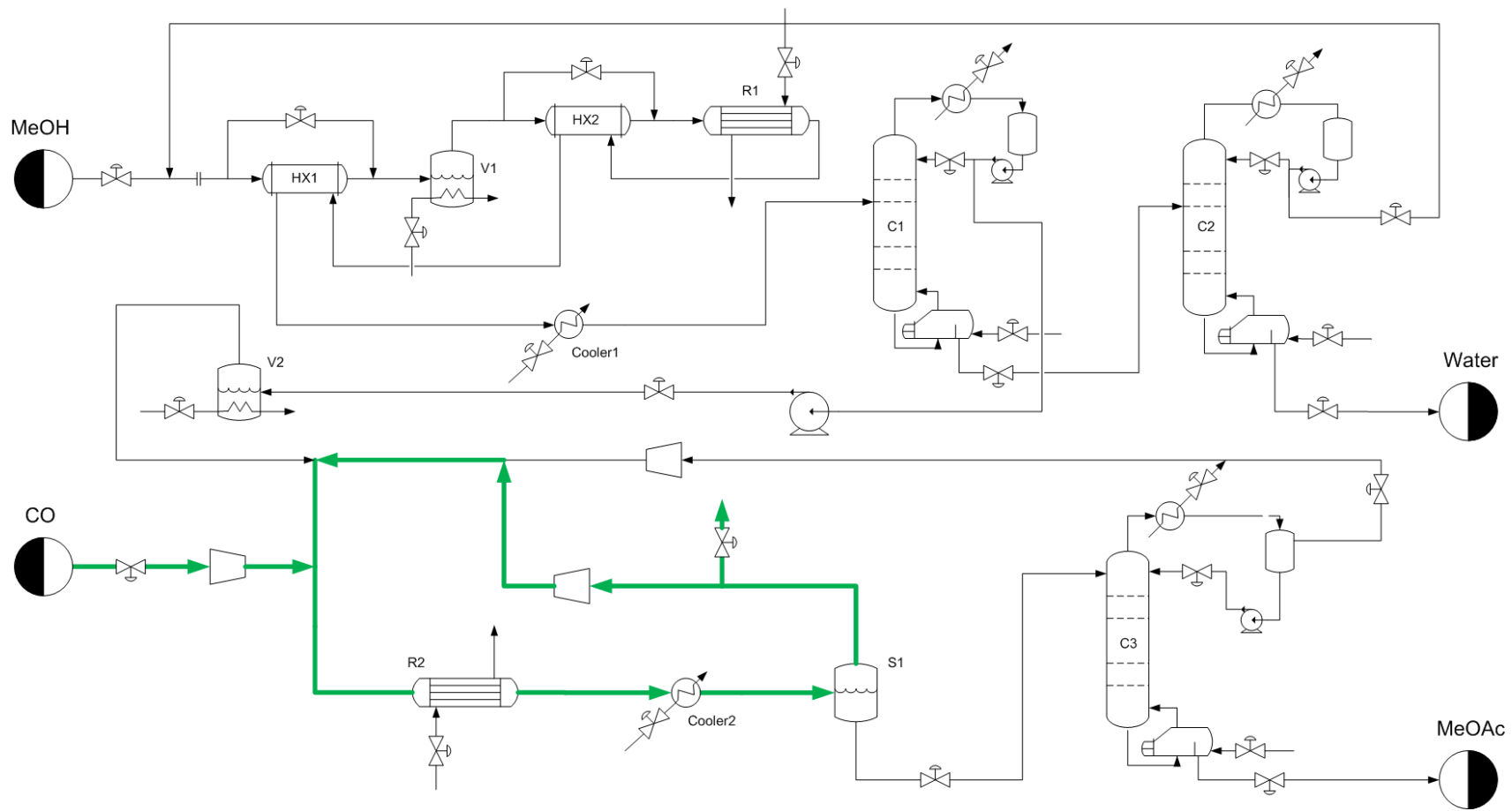


Figure 5.7 Hydrogen Pathway

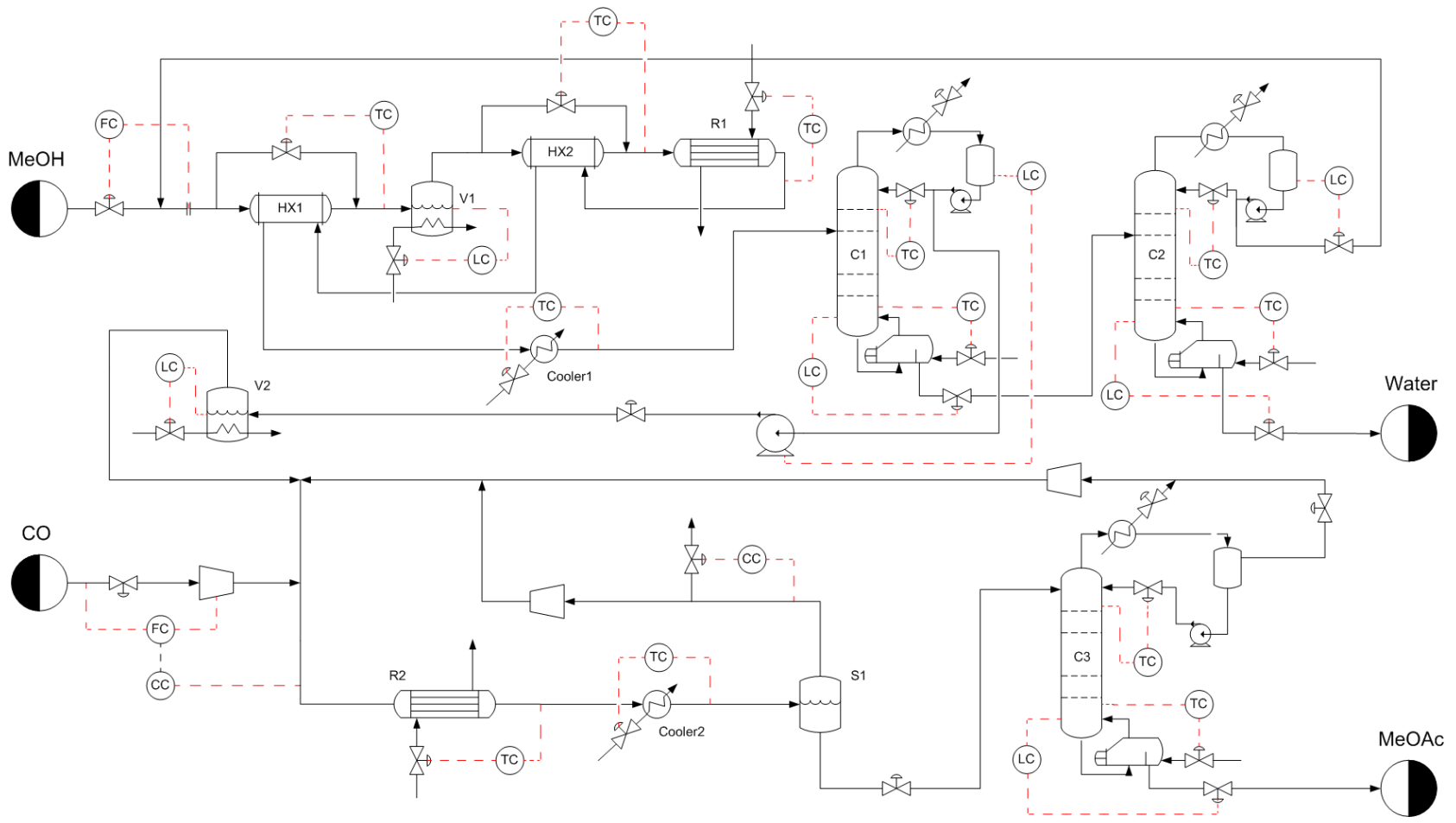


Figure 5.8 control structures (Step 4)

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

The reactors and the columns are considered on disturbances changing. The responses of the variables indicate how strict there are in control. The strictly controls are used for handling the most disturb variables.

1. Reactor R1

The disturbances, feed flow and temperature disturbance are tested by step change 10% of the total feed flow or the feed temperature of reactor R1. The conversion of the reactor is collected and compared.

The results (Table 5.2) showed the conversion increase when the total feed decrease. When the materials flow decrease it mean the resident time of the reactor increase which in reaction take longer time. Instead, increasing the feed flow rate makes the conversion decrease.

Table 5.2 conversion of reactor R1 when total feed change.

%Disturbance	%Conversion
+10%	82.72
0%	82.93
-10%	83.10

The temperature changing causes the effect different the feed flow changing (Table 5.3). In generally increase in temperature takes the reaction rate increase causing the conversion increased. Figure 5.9 shows the temperature profiles of the reactor R1. The temperature peaks of the reactor is high when increase the temperature of feed. The higher peak indicates that the conversion of the reactor is higher.

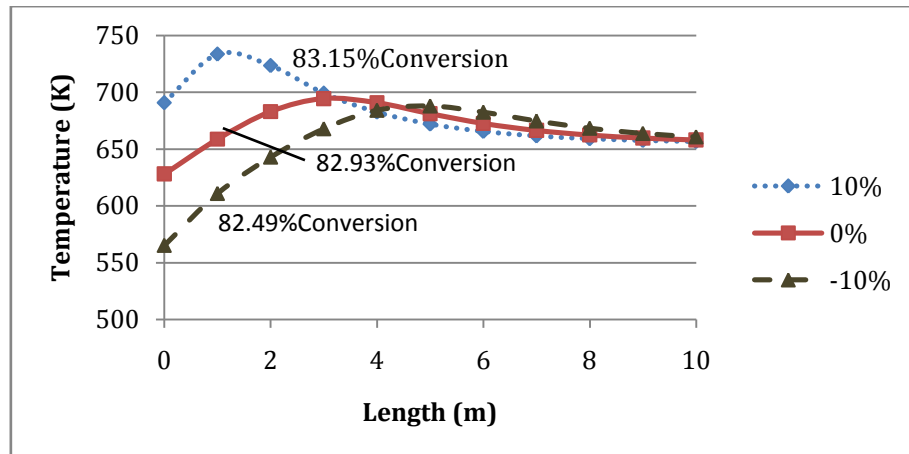


Figure 5.9 temperature profiles of reactor R1 when feed temperature change.

Table 5.3 conversion of reactor R1 when feed temperature change.

%Disturbance	%Conversion
+10%	83.15
0%	82.93
-10%	82.49

However, the temperature peak is controlled to maintain the reactor temperature for safety operation. The control structures are designed for maintain the temperature of the reactor. The possible control structures are shown in figure 5.10. Figure 5.10a showed the temperature outlet control of the reactor by adjusts the flow rate of the coolant. Figure 5.10b showed the temperature peak of the reactor. The temperatures of any length of the reactor are transmitted and the highest is selected for controlling.

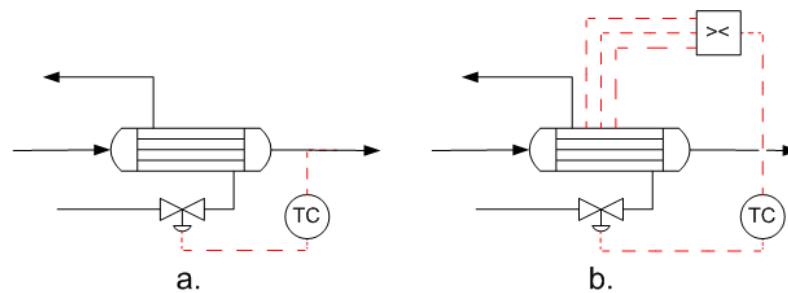


Figure 5.10 the temperature control structures of the reactor a.) Outlet temperature control b.) Temperature peak control

2. Reactor R2

The responses by flow disturbances of the reactor R2 are the same as the responses of the reactor R1. Changing of the total feed flow take the reverse responses, increasing feed flow, the conversion is decreased.

Table 5.4 conversion of reactor R2 when total feed change.

%Disturbance	%Conversion
+10%	57.32
0%	62.41
-10%	68.45

The temperature change does not take significantly differences from the designed conversion. However, the temperature peak (figure 5.11) of the Reactor R2 showed the reaction complete at around 1 m length of the reactor. Then the reactor length could be decreased which be discussed on the step 7. The temperature control is completed by using the control structure as the figure 5.10a.

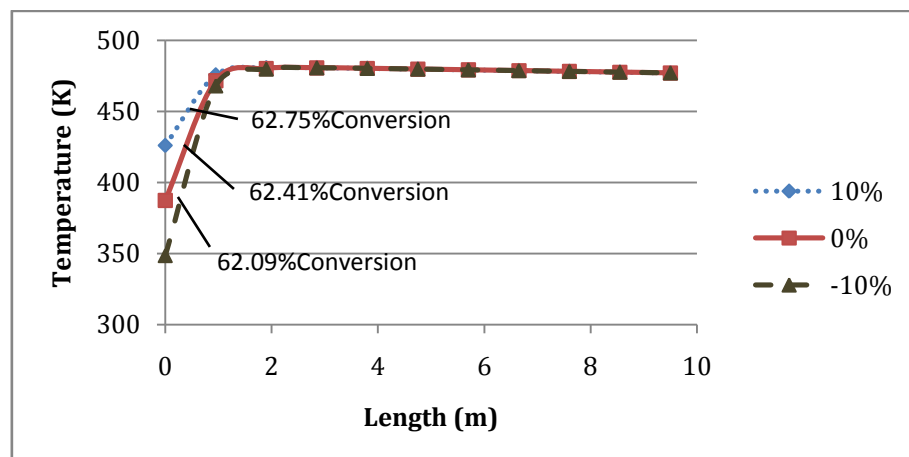


Figure 5.11 temperature profiles of reactor R2 when feed temperature change.

Table 5.5 conversion of reactor R2 when feed temperature change.

%Disturbance	%Conversion
+10%	62.75
0%	62.41
-10%	62.09

3. Column C1

The disturbances testing is accomplished by change the total feed flow or feed temperature. The temperature profiles are considered for responses survey. Any disturbances cause the effect of temperature profiles differently. Controlling the compositions directly require the composition analyzers to measure them. Instead of doing this, it is possible to achieve a good product quality by controlling the temperature at some tray. The typical method to select the temperature controlled tray is to look at the steady-state temperature profile in the column.

The temperature profile of column C1 is shown as figure 5.12. The locations in the column where there are large temperature changes from tray to tray are focused. In figure 5.12, the slope of the temperature profile is steepest from tray 11-15. Tray 13 is selected to control by adjust the reboiler duty for keeping the composition of bottom product constant. The reflux flow rate is controlled by adjusting the flow rate according to feed column C1 flow rate, reflux to feed ratio controller.

Figure 5.13a, changing the total feed of the column C1 effect the temperature profile significantly changes around steep slope showing the strictly control must locate around here. The changing temperature profile when DME feed composition change, figure 5.13b, resembles the changing of the total feed but opposite responses. Figure 5.13c, feed temperature change highly effect the temperature profile. Increase in feed temperature causes the temperature profile increase.

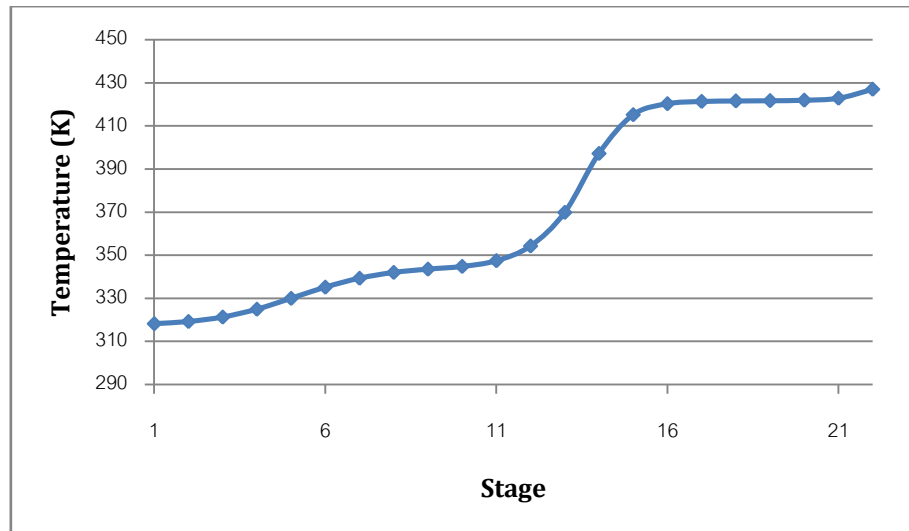


Figure 5.12 temperature profile of column C1

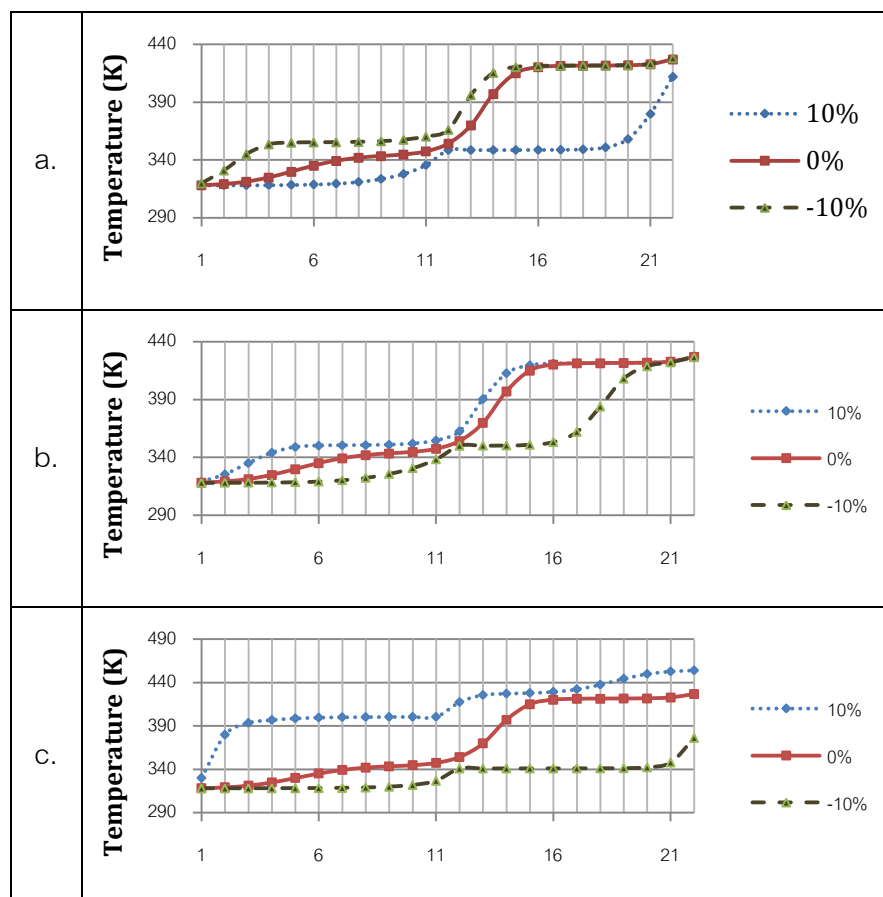


Figure 5.13 temperature profile of column C1 when a.) Total feed, b.) Feed composition and c.) Temperature change

4. Column C2

Figure 5.14, the temperature profile significantly changes with the varied feed flow rate, composition and temperature in both around rectifying and stripping section. It is possible to select the controlled tray at both of section.

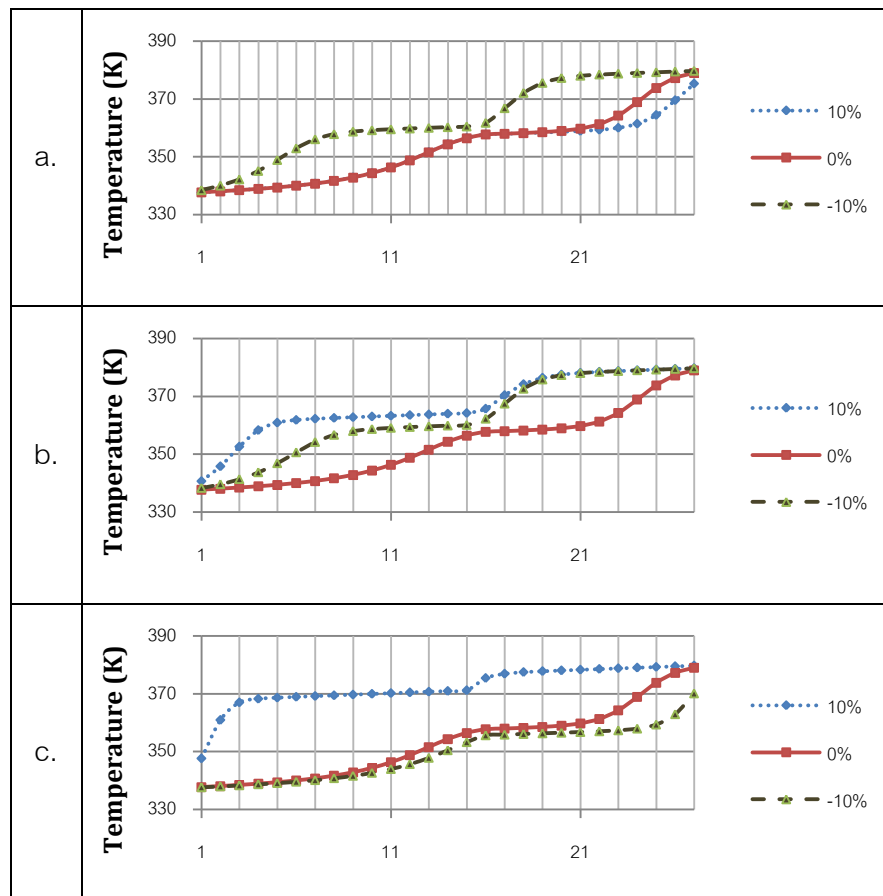


Figure 5.14 temperature profile of column C2 when a.) Total feed, b.) Feed composition and c.) Temperature change

Consider the temperature profile of column C2, figure 5.15, the slopes are steep around tray 6-16 and 21-26. The selected trays are tray 23 and 13 which are controlled by adjust the reboiler duty and reflux flow rate respectively. The two control structures keep the composition of distillate and bottom, methanol and water product constant.

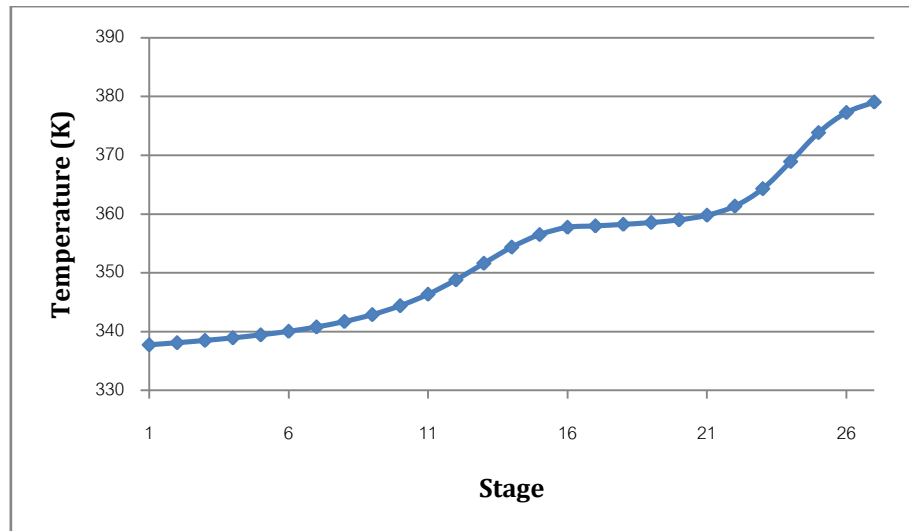


Figure 5.15 temperature profile of column C2

5. Column C3

Column C3 is the special type, small amount of components that is much more volatile than the main component. So the distillate product is a small fraction of the feed stream. It is removed from the reflux drum as a vapor to hold column pressure. Reflux flow is fixed, and reflux drum level is controlled by manipulating condenser coolant.

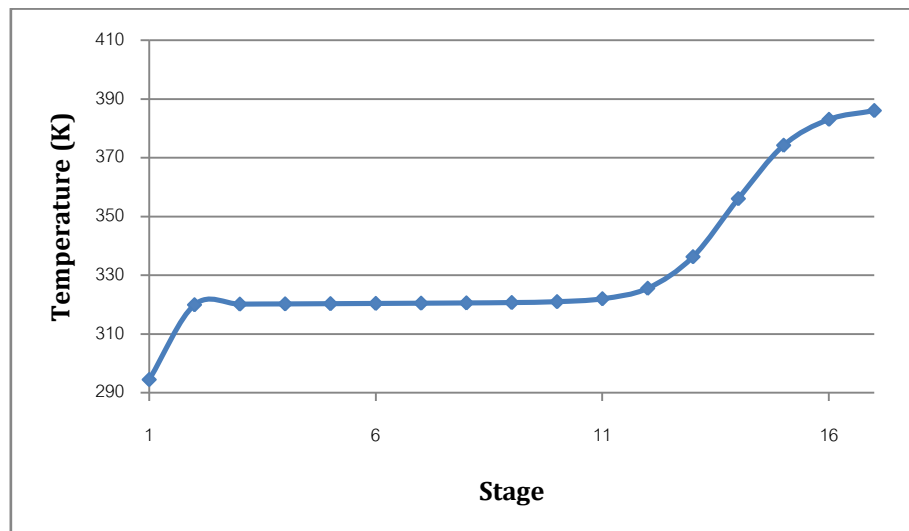


Figure 5.16 temperature profile of column C3

The temperature at the first stage is controlled by adjust the reboiler duty. Changing of the temperature profiles of column C3 by vary the feed flow, composition and temperature shown in figure 5.17. The profiles in picture indicate that temperature

control at the first stage could hold the composition of the bottom product, methyl acetate.

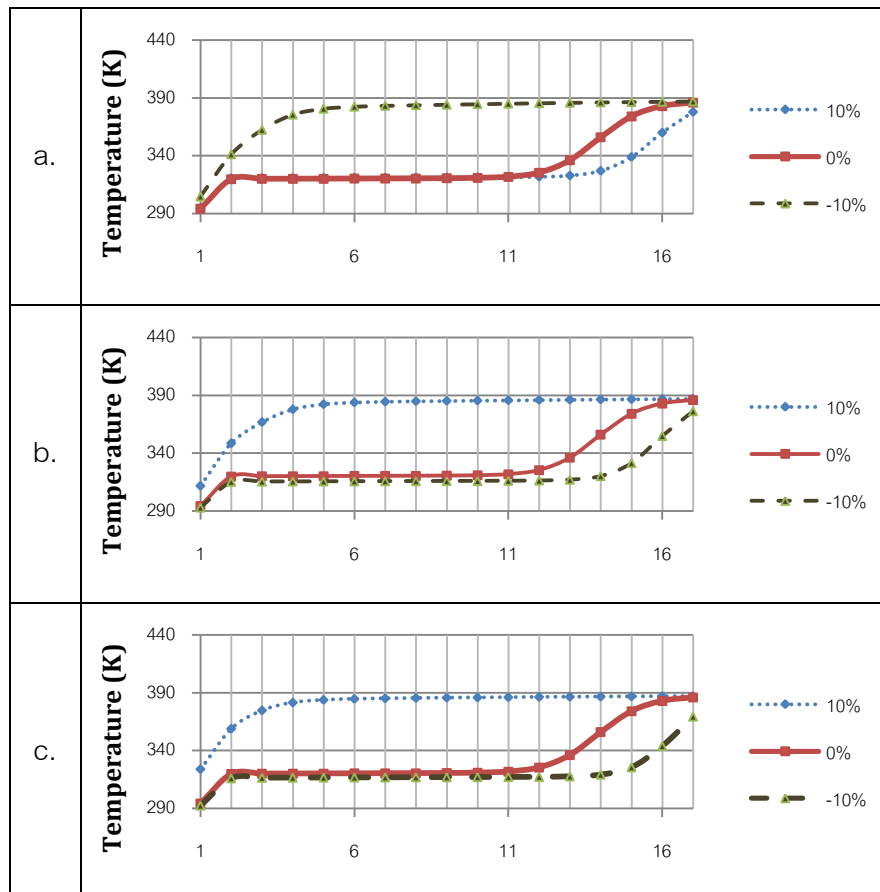


Figure 5.17 temperature profile of column C3 when a.) Total feed, b.) Feed composition and c.) Temperature change

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

The rest control loops are added in this step including pressure controls and level controls of the vessels. Furthermore, we could modify the control loop by enhanced controls. Reactor R1 get the two control structures as figure 5.10. The two control structures are considered in dynamics mode by using the commercial process simulator. The other control structure is no controlling of the temperature exchanger control, HX1 and HX2, for studying the effect of controlling the exchanger outlet temperature.

Nonetheless, the PID controllers are used in case CS4. Control structures of case CS4 are the same as case CS2 but the both reactor temperature controllers are PID controllers, temperature and concentration controls of three columns are also PID controllers. All control structures are established in figure 5.18-21, control structure presented by Luyben (Base case), control structure 1-4 (CS1-4).

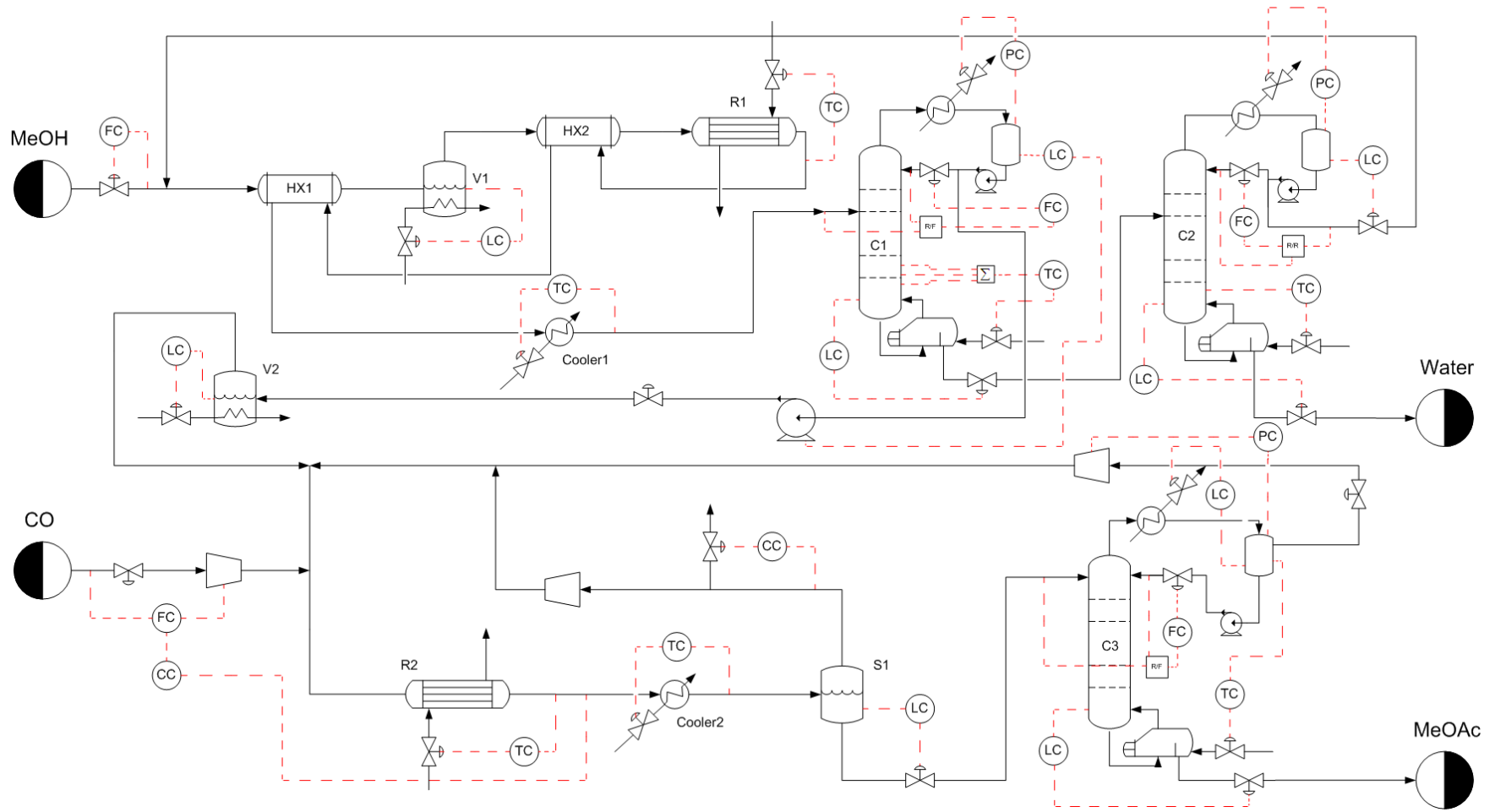


Figure 5.18 Control structures of base case

Table 5.6 Control structure lists of base case

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE*
Methanol feed	FC	Flow rate	Feed flow rate	PI	Reverse	✓	
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	✓	
Reactor (R1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse		✓
Column (C1)	TC	Temperature tray 11-15	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Pump work	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	✓	
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct		
CO feed	CC	Composition R2 out	Set point of FC	PI	Reverse	✓	
	FC	Flow rate	Compressor work	PI	Reverse	✓	
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Separator (S1)	LC	Level	Liquid flow out	P	Direct		
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	✓	
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Condenser duty	P	Direct		
	PC	Condenser pressure	Compressor work	PI	Reverse	✓	✓

*Use for IAE determination.

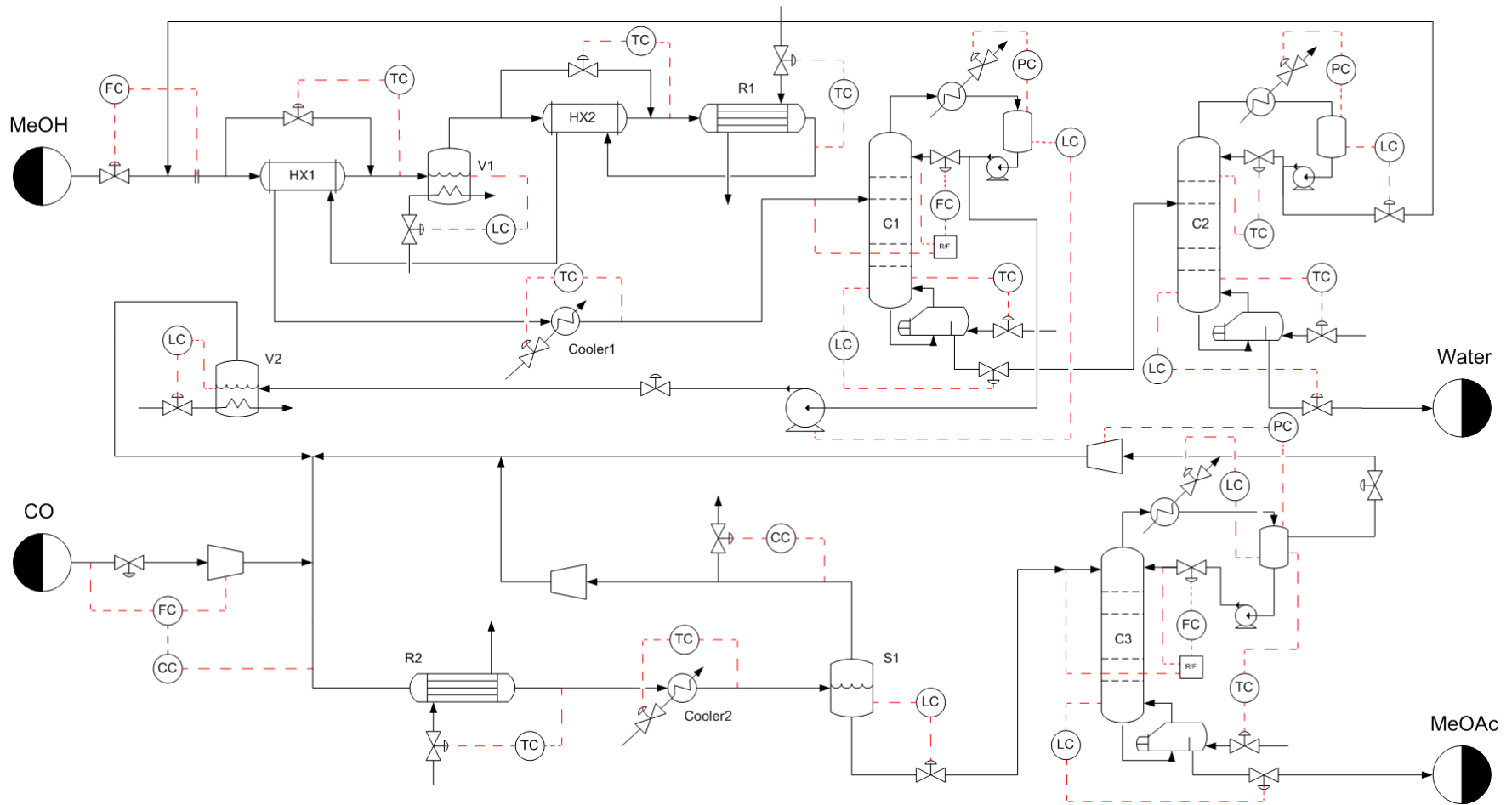


Figure 5.19 Control structures of CS1

Table 5.7 Control structure lists of case CS1

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE*
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	✓	
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct		
Reactor (R1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Pump work	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	✓	
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct		
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	✓	
	FC	Flow rate	Compressor work	PI	Reverse	✓	
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Separator (S1)	LC	Level	Liquid flow out	P	Direct	✓	
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	✓	
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Condenser duty	P	Direct		
	PC	Condenser pressure	Compressor work	PI	Reverse	✓	✓

*Use for IAE determination.

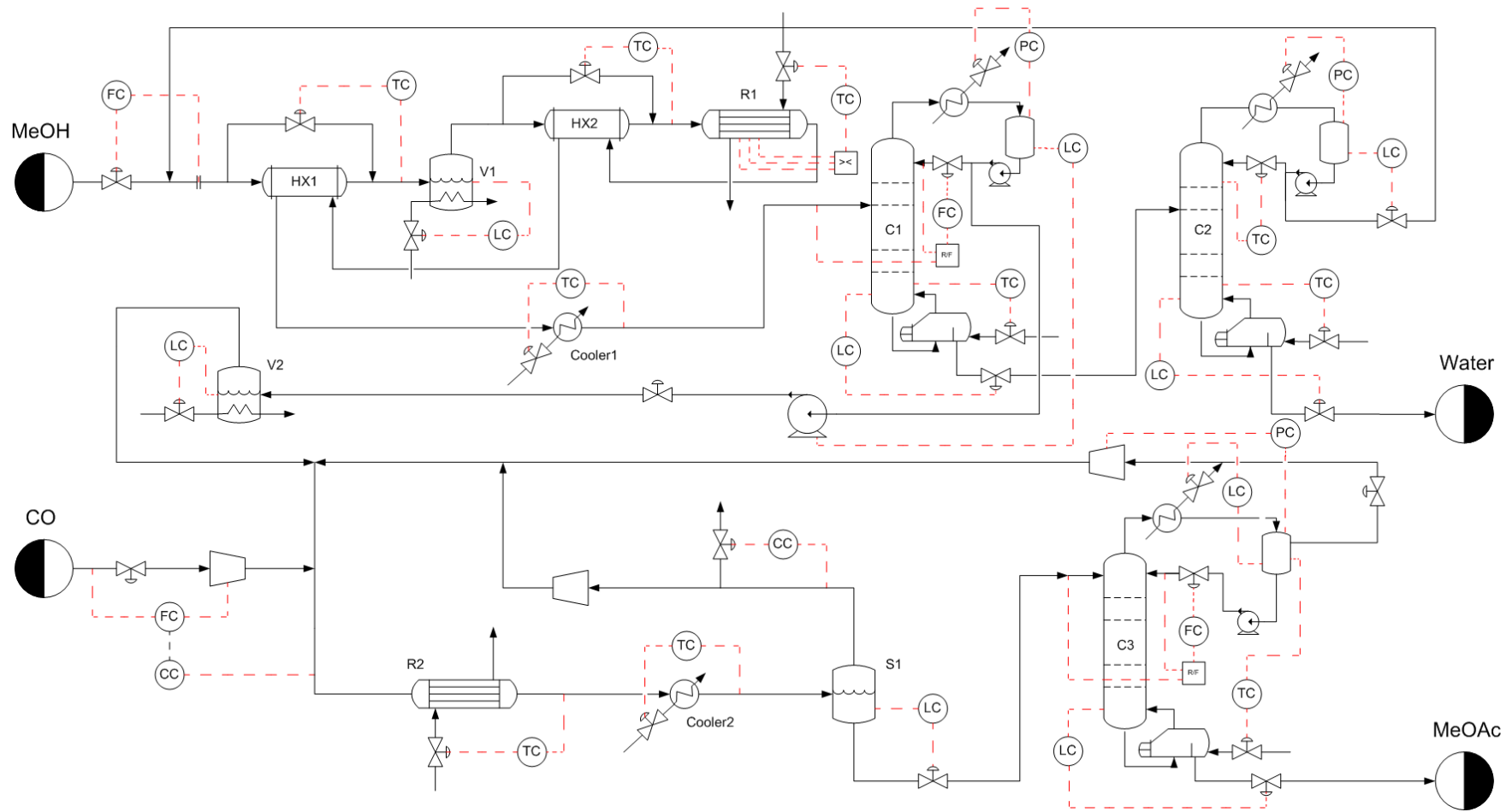


Figure 5.20 Control structures of CS2 and CS4

Table 5.8 Control structure lists of case CS2

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE*
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	✓	
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct		
Reactor (R1)	TC	Temperature peak	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Pump work	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	✓	
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct		
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	✓	
	FC	Flow rate	Compressor work	PI	Reverse	✓	
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Separator (S1)	LC	Level	Liquid flow out	P	Direct	✓	
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	✓	
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Condenser duty	P	Direct		
	PC	Condenser pressure	Compressor work	PI	Reverse	✓	✓

*Use for IAE determination.

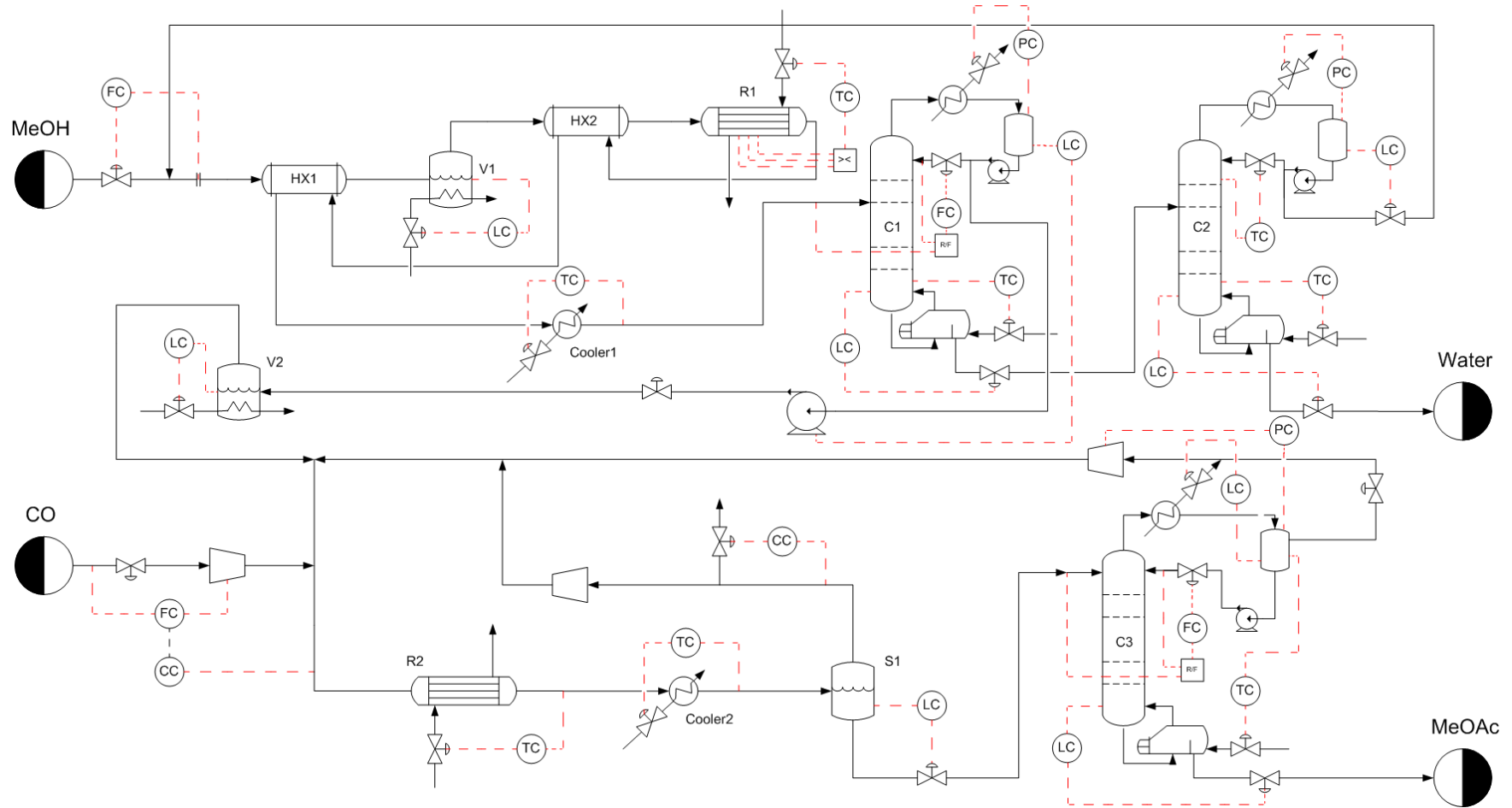


Figure 5.21 Control structures of CS3

Table 5.9 Control structure lists of case CS3

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE*
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	✓	✓
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct		
Reactor (R1)	TC	Temperature peak	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Pump work	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	✓	
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct		
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	✓	
	FC	Flow rate	Compressor work	PI	Reverse	✓	
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Separator (S1)	LC	Level	Liquid flow out	P	Direct		
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	✓	
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Condenser duty	P	Direct		
	PC	Condenser pressure	Compressor work	PI	Reverse	✓	✓

*Use for IAE determination.

Table 5.10 Control structure lists of case CS4

Equipment	Control	Controlled variable	Manipulated variable	Type	Action	SP	IAE*
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	✓	
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	✓	✓
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct		
Reactor (R1)	TC	Temperature peak	Duty flow rate	PID	Reverse	✓	✓
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Column (C1)	TC	Temperature tray 13	Reboiler duty	PID	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Pump work	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Column (C2)	TC	Temperature tray 23	Reboiler duty	PID	Reverse	✓	
	TC	Temperature tray 13	Reflux flow rate	PID	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Distillate flow rate	P	Direct		
	PC	Condenser pressure	Condenser duty	PI	Reverse	✓	✓
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct		
CO feed	CC	Feed R2 composition	Set point of FC	PID	Reverse	✓	
	FC	Flow rate	Compressor work	PI	Reverse	✓	
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PID	Reverse	✓	✓
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	✓	✓
Separator (S1)	LC	Level	Liquid flow out	P	Direct	✓	
Purge stream	CC	Hydrogen composition	Purge flow rate	PID	Direct	✓	
Column (C3)	TC	Temperature tray 1	Reboiler duty	PID	Reverse	✓	
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	✓	
	LC	Reboiler level	Bottom flow rate	P	Direct		
	LC	Reflux drum level	Condenser duty	P	Direct		
	PC	Condenser pressure	Compressor work	PI	Reverse	✓	✓

*Use for IAE determination.

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

The process structure established by Luyben has been optimized. The reactor temperature has been selected from basic kinetic considerations to be at its maximum, the remaining dominant design optimization variables are pressure, reactor size, and purge composition.

The result shown in the paper, 1500-tube reactor is used because very high recycle flow rates and low purge compositions are needed at the low system pressures.

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

The commercial process simulator is used for obtaining the responses of the variables when the disturbances occur, methanol feed flow, feed temperature and composition change. The responses are collected and plotted as graph versus time.

1. Total methanol feed flow change

The methanol fresh feed is varied by change the set point value of the fresh feed controller. For control structures CS1-4, the step change is difficult. The fresh feed of control structures CS1-4 are varied by change the total feed set point for giving the total feed same as the total feed of base case.

Table 5.6 shows responses of variables disturbed by total feed changing. The fresh methanol feed flows (MeOHFeed) in case C1, CS2, CS3 and CS4 gradually increased but the fresh feed of base case rapidly changes because of the higher flow control time constant of case CS1, CS2, CS3 and CS4. Time constant of the total feed control is 10 minutes which higher than the fresh feed control of base case, 0.3 minutes. The higher time constant is used for handle the flow disturbance from the recycle loop. Change of the recycle flow (Recycle) of base case and CS1 are not different but there is a small oscillation at the first period of base case. Case CS2, CS3 and CS4, there are shorter deviation of recycle flow because the temperature peak control of reactor R1 is

used. Using the temperature peak control give the reactor conversion limited, smaller change of the conversion than the temperature outlet control.

Case CS1, CS2 and CS4, the temperature outlet of heat exchanger HX1 and HX2 (THx1, THx2) are controlled causing both temperature outlets converge to the ordinary value. Comparison of base case and CS3, deviation of the temperature outlet of exchanger HX2 in case CS3 is smaller than base case because the temperature out of reactor R1 is not controlled. The higher R1 outlet temperature gives the smaller decreasing of the temperature out of HX2. Temperatures out of water cooler Cool1 are not significantly different in each case (base case, CS1, CS2, CS3 and CS4).

The Feed oscillation at first period of base case causes an impurity of dimethyl ether (XdDMEC1). Methanol purity (XdMeOHC2) at distillate of column C2 shown in the table cannot be controlled by reflux ratio controller in base case. In case CS1, CS2, CS3 and CS4, column C2 controlled by temperature control, tray 13, in which manipulated variable is a reflux flow rate, can handle the concentration of methanol in distillate. From figure 5.14, the significantly change of temperature profile in rectifying section indicates that temperature above feed should be control.

Product flow (DistillateC1) from the first section, dehydration section, of case CS1, CS2, CS3 and CS4, gradually change related to the methanol feed and in base case changes with oscillation of the feed in first period. In all five cases, the CO feed changes (COfeed) with the same direction. Decreasing of methanol fresh feed causes the CO feed flow gradually decrease but higher decreasing at around 7 hours because of amount of hydrogen concentration in recycle loop. The temperature deviation of cooler Cool2 outlet (TCool2) is about 0.1 K. By the way, hydrogen concentration change in the recycle loop causes the temperature out of Reactor R2 (TR2Out) suddenly decreases at 7 hours when the methanol fresh feed decreases. In case CS4, the decreasing peak is smallest compared which case CS1, CS2 and CS3 because of the PID controller effecting the deviation smaller.

Hydrogen in recycle loop can be controlled when concentration decreases by close the purge stream valve but when the concentration of hydrogen in recycle loop decreases there is hard to control because of releasing of both hydrogen and carbon monoxide in purge stream. So the concentration of hydrogen in recycle (H_2Comp) gradually increases when the feed is increased. Methyl acetate product concentration ($X_{bMeOAcC3}$) is disturbed when increases in feed. The methyl acetate composition deviation is about 0.02. By the way, decreasing of methyl acetate concentration in bottom product of case CS4 is smallest.

Table 5.6 Dynamic responses with total fresh methanol feed change.

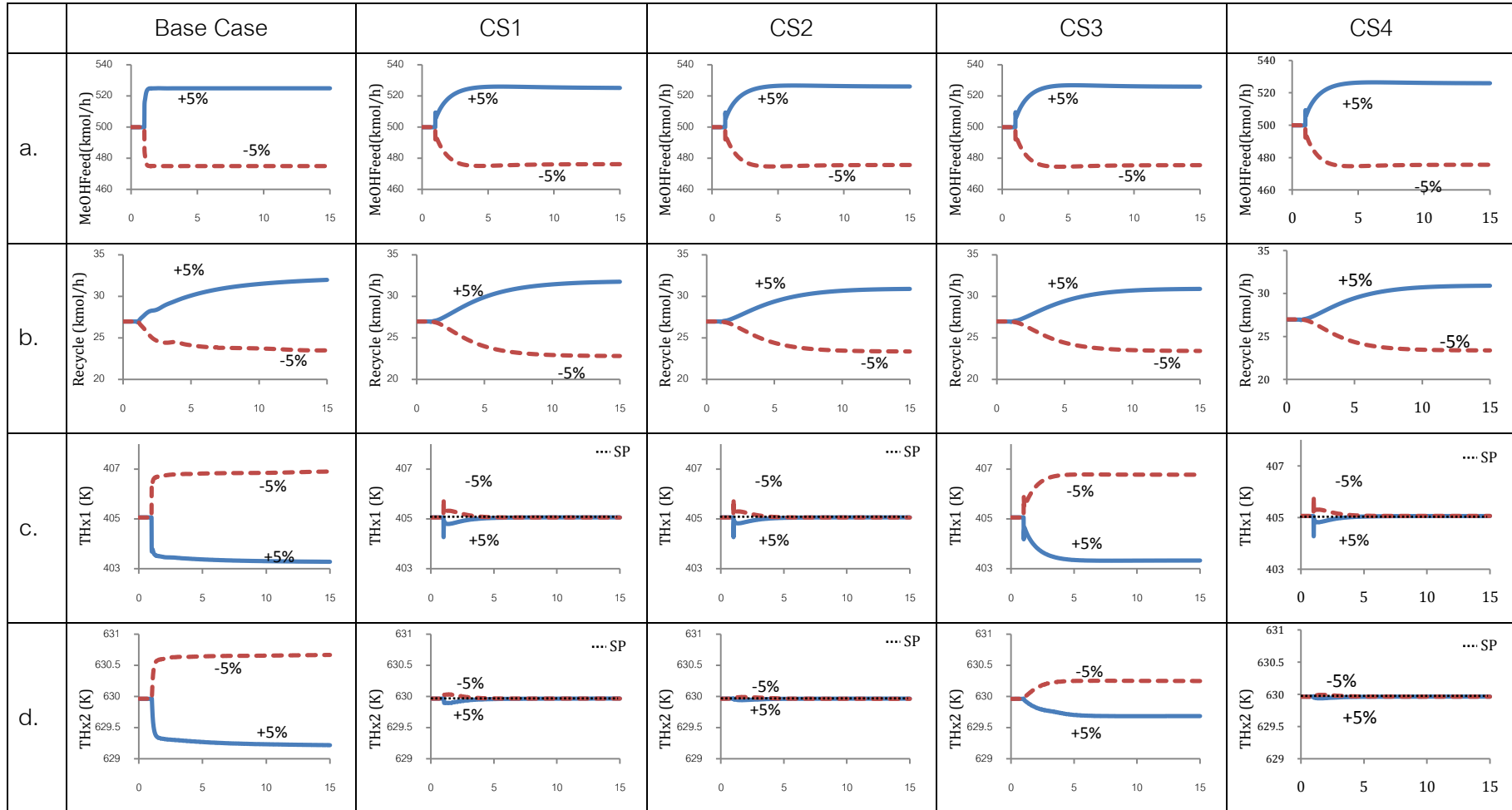


Table 5.6 (continue) Dynamic responses with total fresh methanol feed change.

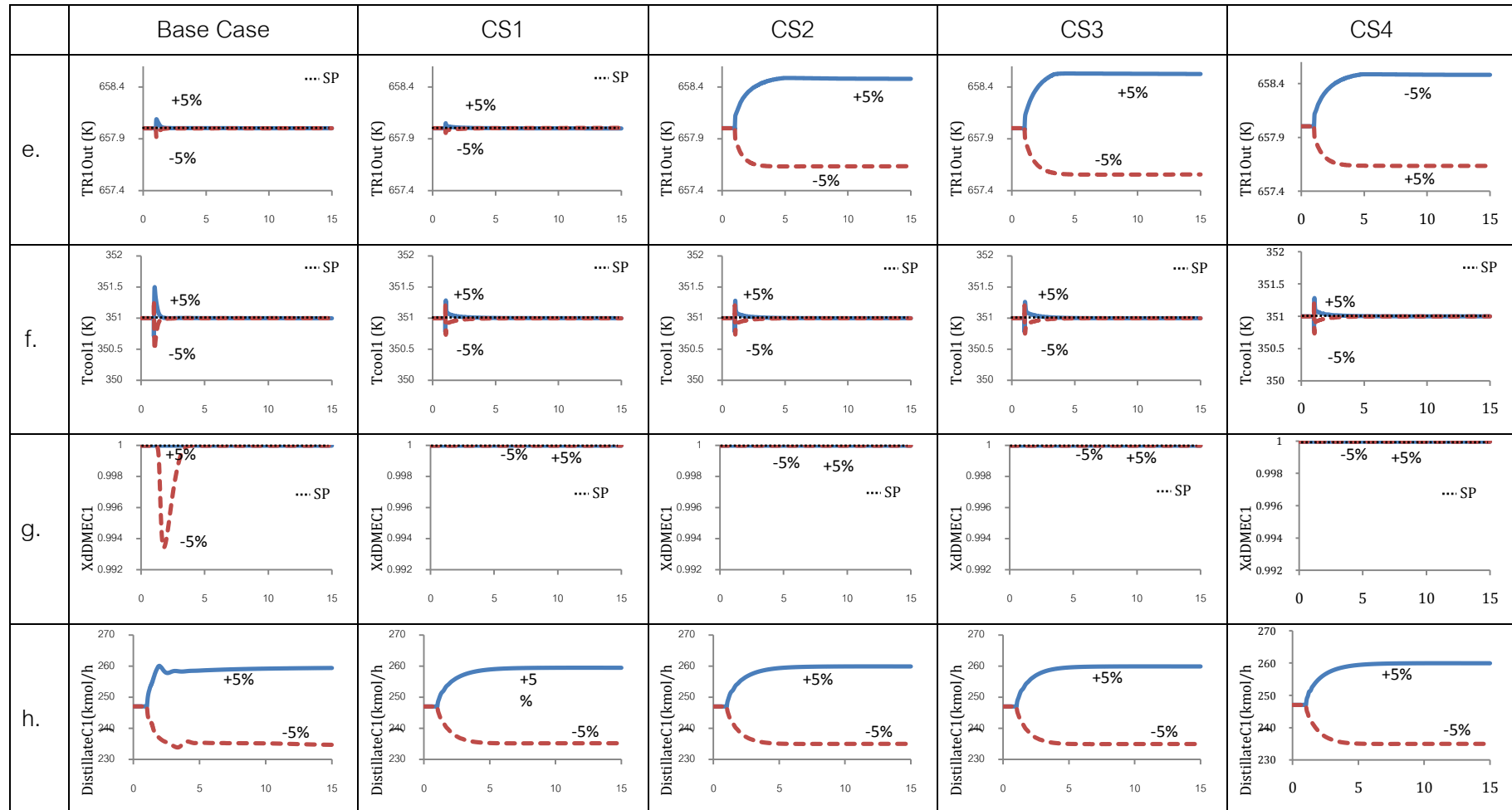


Table 5.6 (continue) Dynamic responses with total fresh methanol feed change.

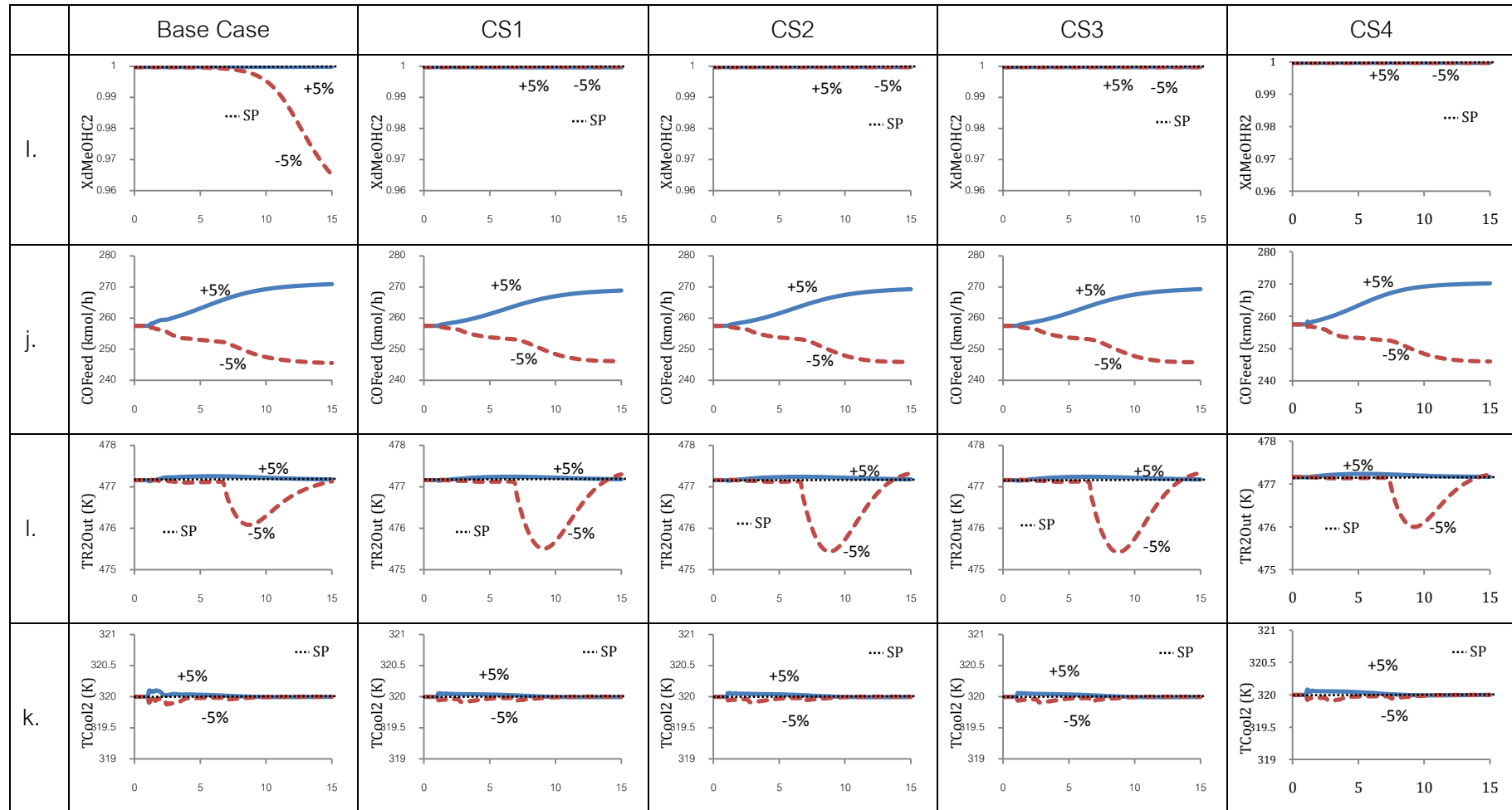
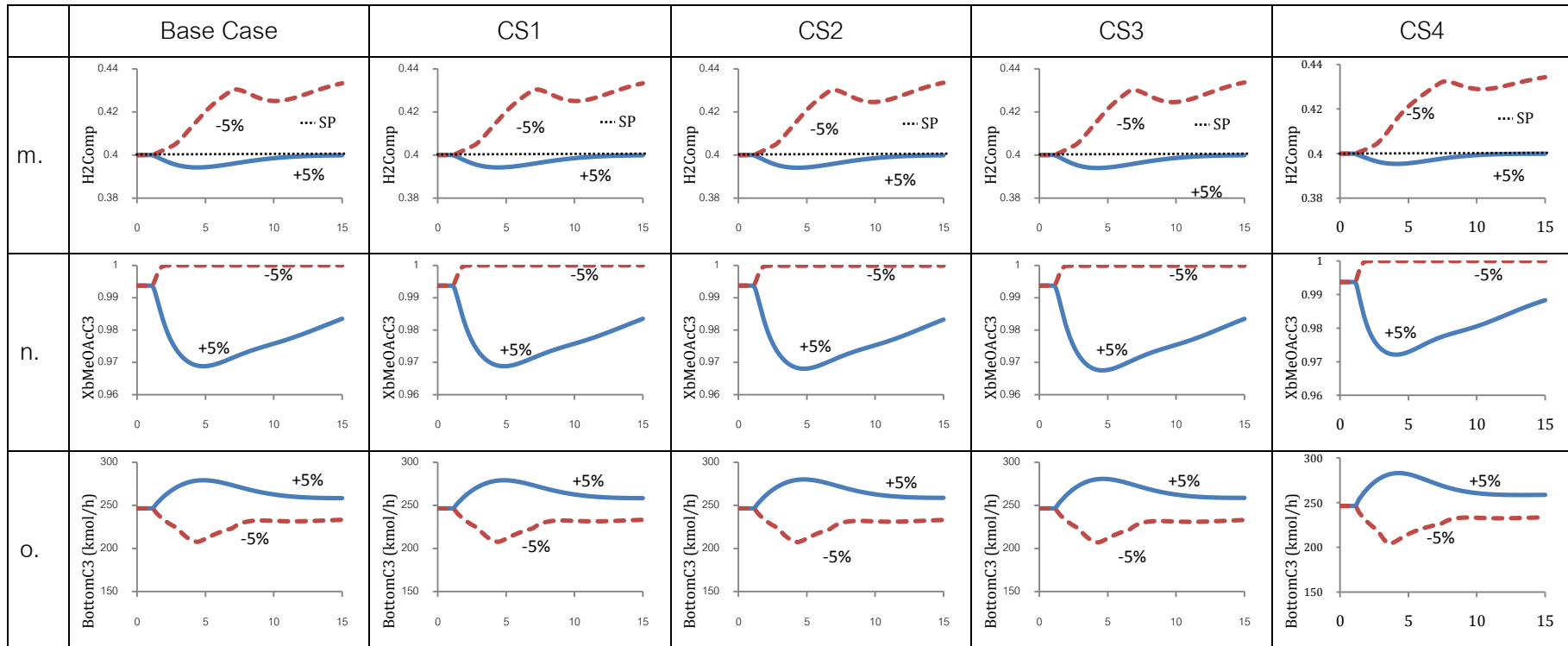


Table 5.6 (continue) Dynamic responses with total fresh methanol feed change.



2. Feed temperature change

Feed temperature change is taken place by step change the feed temperature by 3 K. The temperature feed change effects the deviation of the recycle flow around 0.04 kmol/h in base case and case CS1 but smaller change in case CS2, CS3 and CS4 because of temperature peak control of reactor R1. The temperature of exchanger HX1 outlet is deviate from the steady value in case CS1 and base case because there is no control in temperature outlet as same as exchanger HX2 but is no significantly deviation. It is know that controlling the temperature out of heat exchanger of case CS1, CS2 and CS4 can control the heat disturbances giving the temperature out of a set point.

Temperature of R1 outlet is disturbed and converges to new value in case CS2, CS3 and CS4 because it is controlled by temperature peak control but no control the outlet temperature. Responses of temperature outlet of cooler Cool1 are not different in all case, base case, CS1, CS2 and CS3. The disturbance can be handled less than 1 hour. The difference in control loop of column C1 causes the oscillation in distillate flow rate in first period. The results show that the flow rate of the distillate of column C1 in case CS4 is smooth compared with case CS1, CS2 and CS3 because of using the PID controller.

The oscillation of dimethyl ether out of the column C1 affect fresh CO feed flow rate also waved at the first period. In case CS4, the PID controller of fresh CO feed cause the flow rate responses highly wave in the first period. The reverse respond of dimethyl ether flow out of column C1 in case CS3 compared with the others affect the reverse respond of the variables in the second section, carbonylation section.

Amount of methyl acetate product flow is different in each case because of quantity of CO feed and the dimethyl ether entering the second section relating to the methanol fresh feed but small deviation, less than 0.1 kmol/h.

Table 5.7 Dynamic responses with feed temperature change.

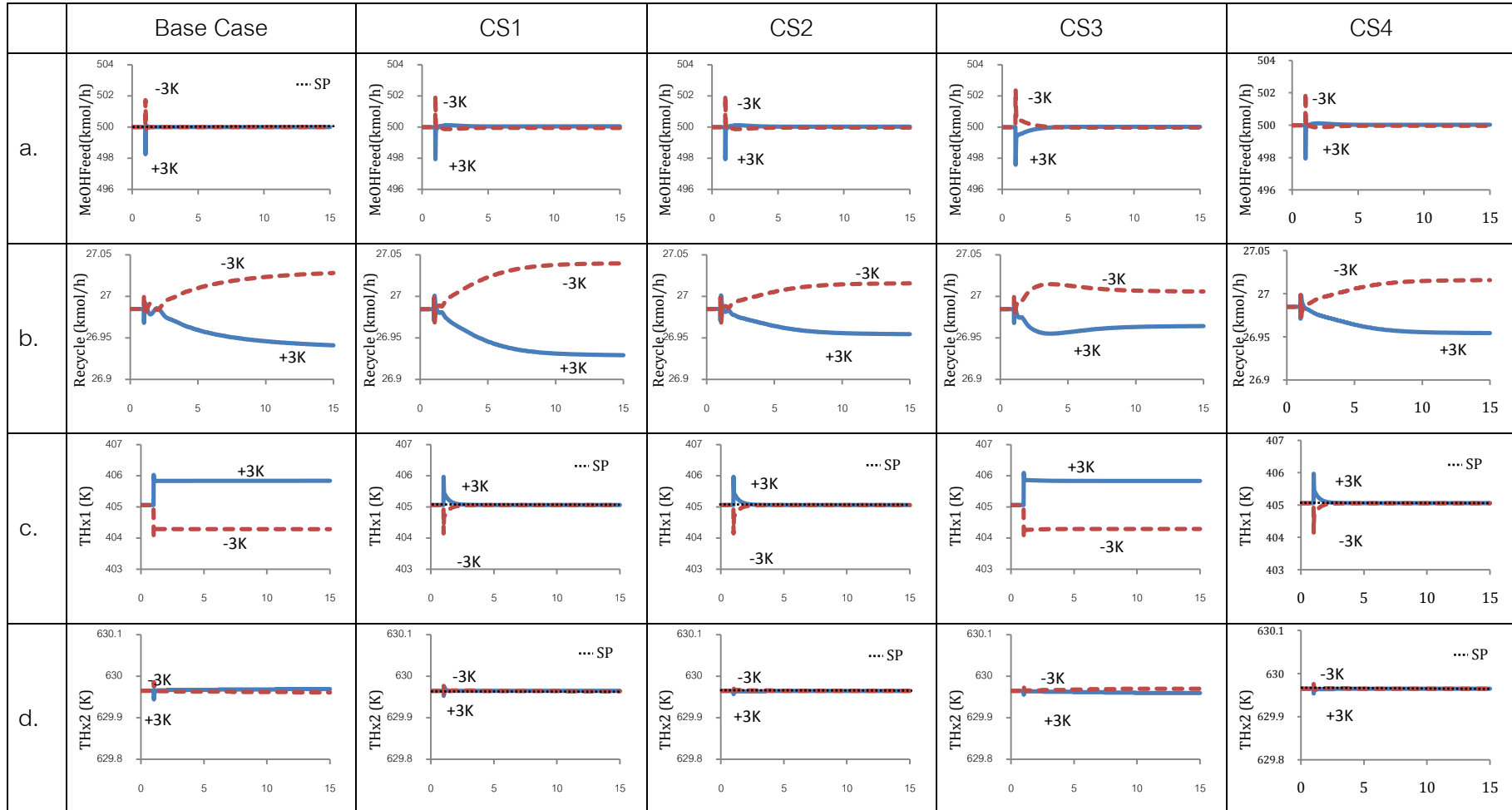


Table 5.7 (continue) Dynamic responses with feed temperature change.

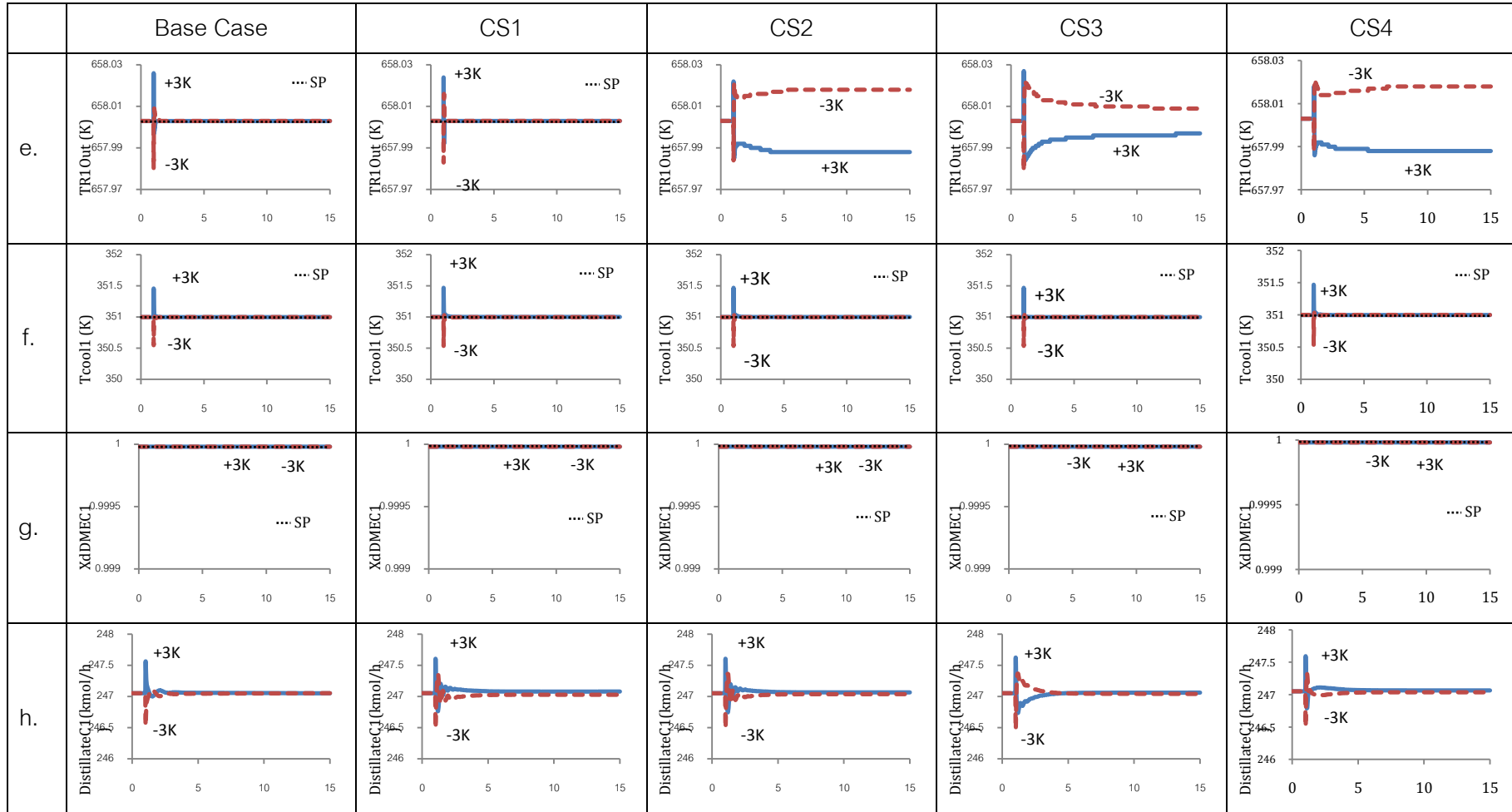


Table 5.7 (continue) Dynamic responses with feed temperature change.

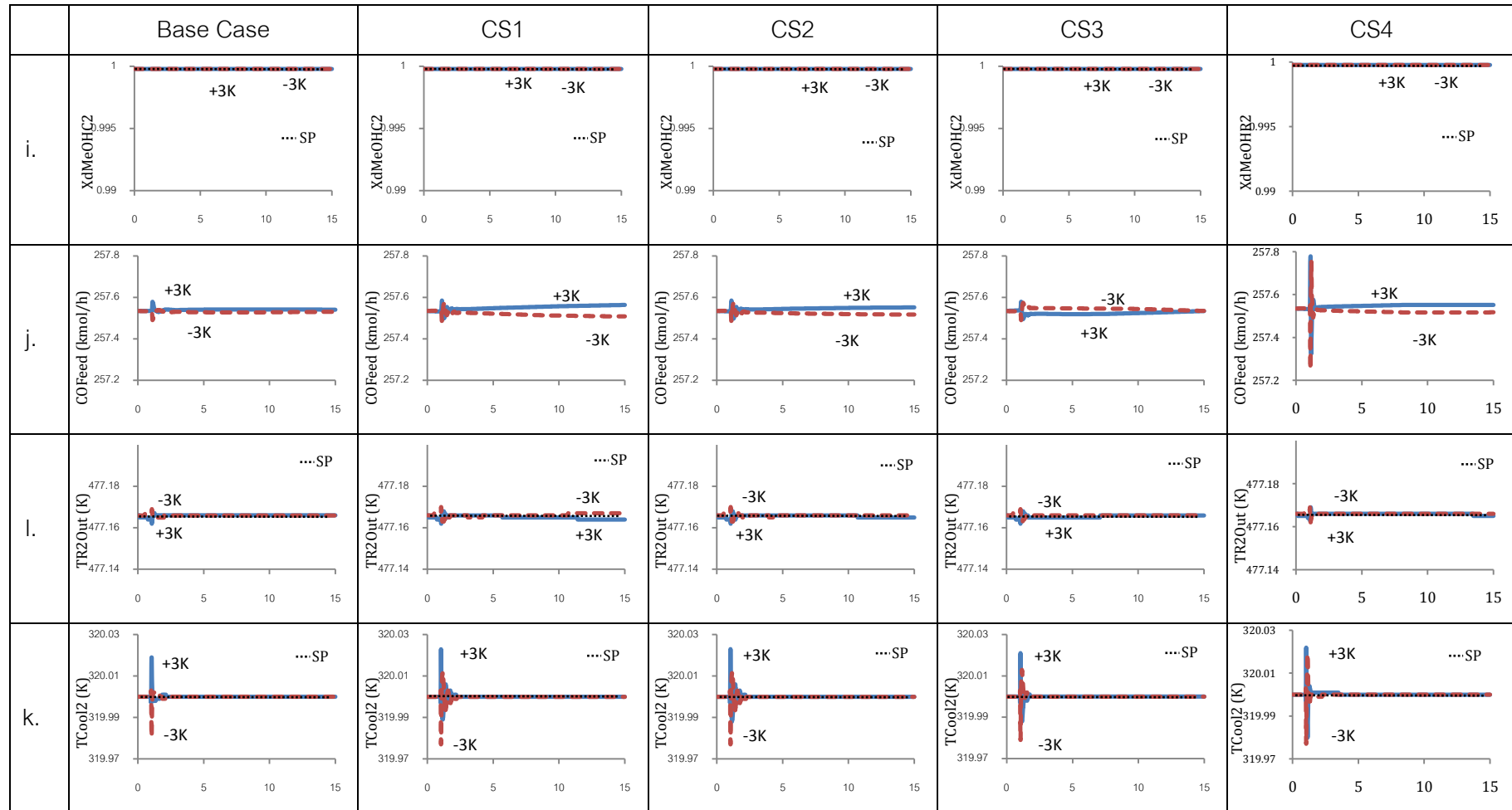
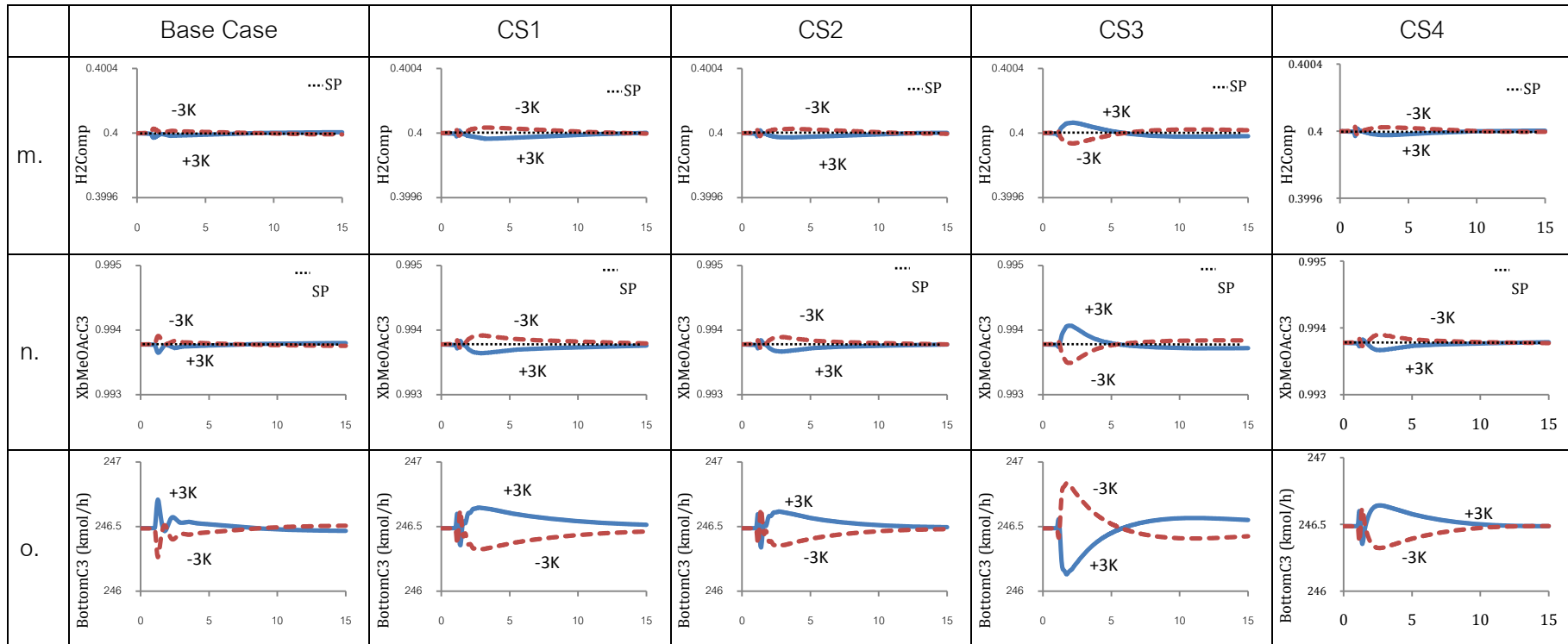


Table 5.7 (continue) Dynamic responses with feed temperature change.



3. Composition change

Compositions of H_2O and H_2 in methanol and carbon monoxide feed are increased by 0.01, from 0.01 to 0.02 and 0.02 to 0.03 respectively. The responses of the variable are collected for considering the effect of composition change.

3.1 Increase H_2O in methanol feed

The results show that the fresh feed of methanol in case CS2, CS3 and CS4 are converged to higher values than steady-state value because the conversion of dehydration reaction increase effecting the recycle decreases. The recycle decreasing causes the total feed control adjusts the total flow to reach the set point. Because of the temperature peak control, the conversion is increased by allow the temperature of the reactor to reach the limited value. If the temperature inlet is low, the temperature deviation is higher. The higher temperature deviation affect the amount of reactant reacted.

The temperature control of exchanger HX1 and HX2 affect the responses of outlet temperature of case CS1, CS2 and CS4 converge to the steady-state value but there are off sets in base case and case CS3. The temperature outlet of cooler Cool2 is disturbed but not significantly changes in all case.

Dimethyl ether flow rate out of column C1 is decreased with amount of H_2O increasing. The results show that the flow rate of dimethyl ether in case CS4 is smoothest. There is highly oscillation of dimethyl ether flow rate outlet from column C1 in base case. Decreasing of dimethyl ether affect the CO feed decreasing in the same as decreasing of amount of methyl acetate product. There are no significantly changes in temperature control loops with H_2O composition increasing. The deviation of composition of methyl acetate in case CS4 is smallest.

3.2 Increasing H₂ in carbon monoxide feed

Increasing in H₂ in fresh carbon monoxide feed stream does not affect the dehydration section because H₂ is only fed to the carbonylation section. H₂ increasing requires the amount of feed flow rate to give the concentration of carbon monoxide in total feed constant. The higher of flow rate causes the temperature deviation in reactor R2 outlet about 0.2 K and about 0.06 K at cooler Cool2. There is the oscillation in the first period of case CS4. The oscillation in case CS4 affecting the temperature of reactor R1 and cooler Cool2 outlet is taken place by the PID fresh CO controller.

The higher composition of hydrogen can be controlled by purge stream in 8 hours and deviation of 0.07 but it is smaller in case CS4, deviation of 0.05. In the carbonylation section, there are no different characteristic changes in comparison of base case, case CS1, case CS2 and case CS3.

Table 5.8 Dynamic responses with composition of H₂O and H₂ change.

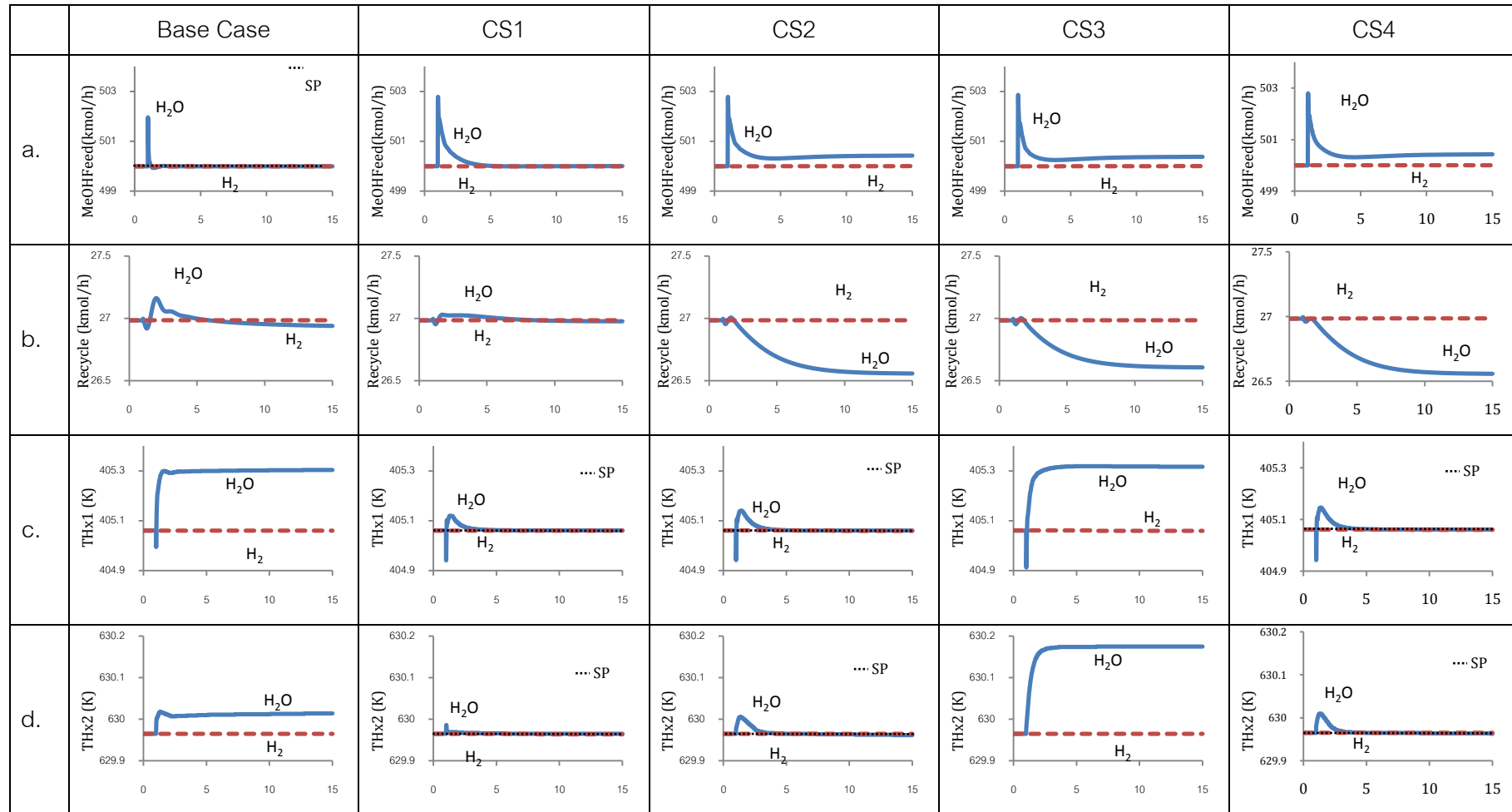


Table 5.8 (continue) Dynamic responses with composition of H₂O and H₂ change.

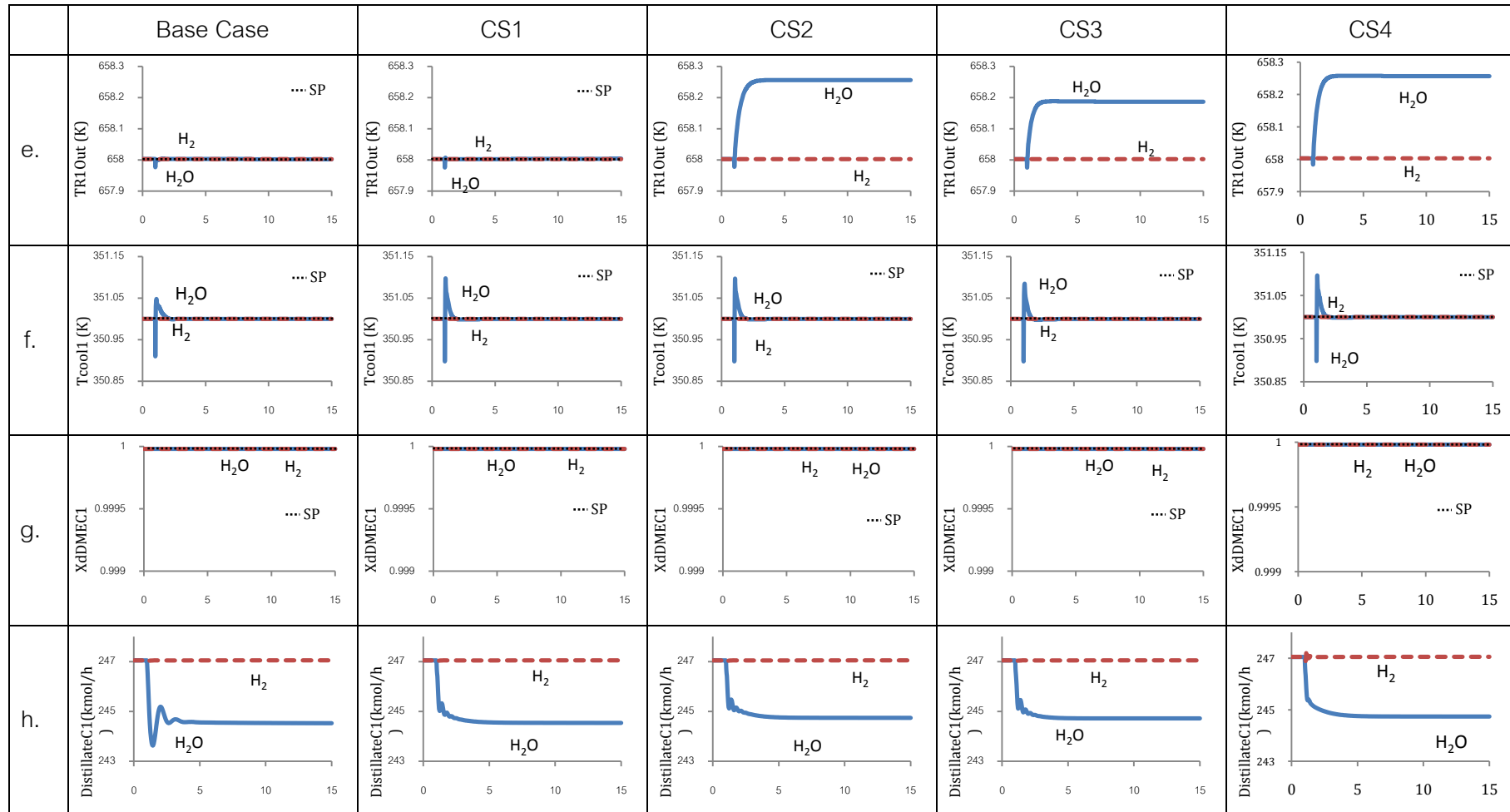


Table 5.8 (continue) Dynamic responses with composition of H₂O and H₂ change.

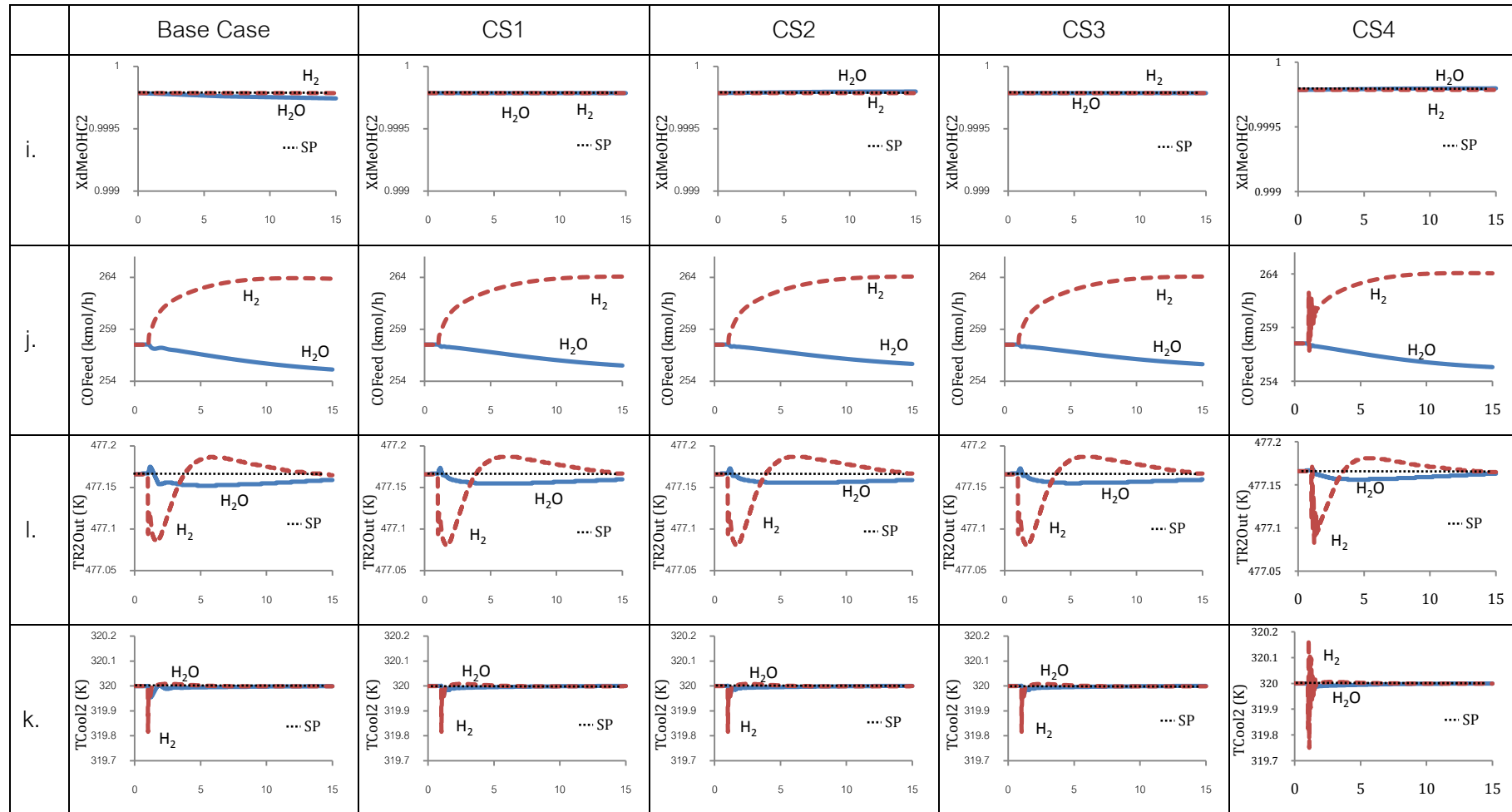
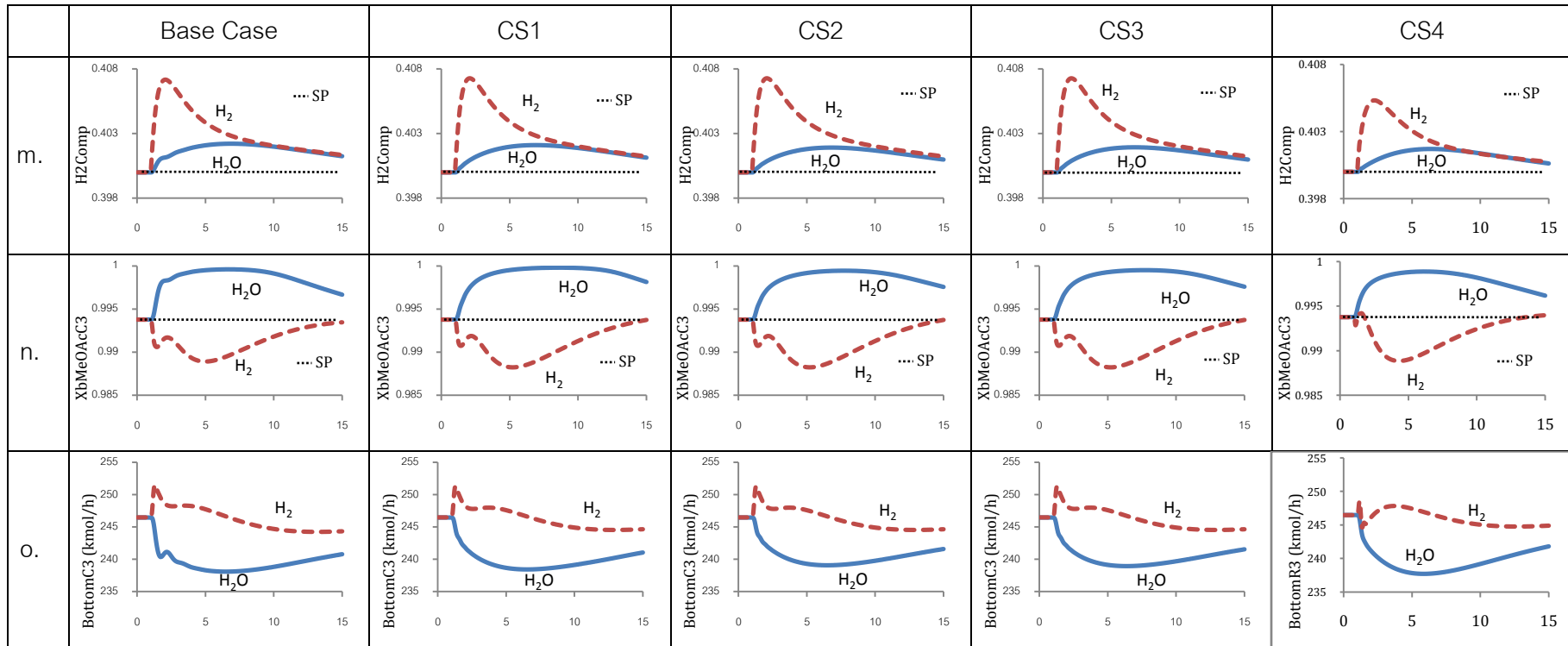


Table 5.8 (continue) Dynamic responses with composition of H₂O and H₂ change.



5.2 IAE analysis

The IAE (integral absolute errors) are analyzed from the safety loop control, temperature and pressure control, and the composition of products loops. The temperature and pressure control are considered because the safety loop is important. The safety control in the process operation causes the operation smoothly and securely. The IAE value is calculated after the disturbances are tested and the values are measured. The qualities of product are also important because of requirement of the commercial product quality.

By the way, the IAE are considered to select the best control structure (compare in 5 cases). The minimum IAE value means the best control structure handling the temperature and pressure disturbances smoothly and securely operation and can keep the product quality in commercial requirement.

Table 5.9 IAE of safety control loop with total feed change.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.375765	0.130571	0.332351	0.838686
CS1	0.050458	0.090927	0.332343	0.473728
CS2	0.107656	0.024862	0.339773	0.472290
CS3	0.376032	0.024726	0.341294	0.742053
CS4	0.093177	0.024600	0.279204	0.396981

Table 5.10 IAE of safety control loop with feed temperature change.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.109075	0.002192	0.000539	0.111806
CS1	0.002523	0.002772	0.001732	0.007026
CS2	0.004362	0.000460	0.001096	0.005919
CS3	0.110429	0.000616	0.002051	0.113096
CS4	0.004290	0.000325	0.000886	0.005501

Table 5.11 IAE of safety control loop with H₂ and H₂O composition change.

Control structure	Temperature	Pressure	Composition	Sum IAE
Base case	0.022888	0.022635	0.103944	0.149467
CS1	0.003335	0.023681	0.114476	0.141492
CS2	0.020839	0.002903	0.108417	0.132160
CS3	0.047158	0.002656	0.109466	0.159280
CS4	0.020335	0.002311	0.087065	0.109711

From the IAE value shown in table 5.9-11, the minimum IAE value is the value of case CS4. The second challenger CS2 in which rang two of IAE number is greater than base case, case CS1 and CS3. The smaller IAE values of case CS1 and CS2 indicate that the control of temperature out of heat exchanger give high performance in temperature control loops. Moreover, the temperature peak control affect the temperature of the reactor directly that more safety than the case with only outlet temperature control.

The difference of the IAE value in pressure loop is the effect of the temperature control loops affected the pressure in the column and the vessel. In the composition control loop, the IAE of case CS4 is smallest because of using of the PID controllers in temperature and concentration controls. The smallest IAE of case CS4 shows the good controlling of the product purities and the good operation.

5.3 Utilities cost

Utilities costs are calculated from the duties used in cooling and heating and the works used in pumps and compressors. The cost of cooling water used in the process is \$0.354/GJ. The steam used in the process is assumed to be high pressure steam in which cost is \$17.7/GJ. The electric cost is \$16.8/GJ which is multiplied with 0.0036 to convert the unit to \$/kWh.

In the table 5.12, the results shows the utilities cost of the case CS1 is smallest followed by case CS2 and CS3. The feed temperature disturbances, the utilities cost of

case CS4 is smaller followed by case CS3. The utilities cost of case CS1 and CS2 is the same, \$21,002.38. But in the composition change, base case requires the utilities cost smallest.

Table 5.12 Utilities cost with total feed change.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	\$	GJ	\$	kWh	\$	
Base case	-2101.18	743.8161	1085.383	19211.28	21007.79	1270.551	21225.64
CS1	-2097.61	742.5533	1083.348	19175.26	20965.15	1267.972	21185.79
CS2	-2097.87	742.6477	1083.487	19177.72	20974.96	1268.565	21188.94
CS3	-2098.46	742.8565	1083.958	19186.05	20979.97	1268.869	21197.78
CS4	-2100.29	743.502	1083.819	19183.59	21064.23	1273.965	21201.06

Table 5.13 Utilities cost with feed temperature change.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	\$	GJ	\$	kWh	\$	
Base case	-2051.68	726.2956	1085.383	19211.28	21007.79	1270.551	21208.12
CS1	-2083.45	737.5427	1073.058	18993.13	21026.91	1271.707	21002.38
CS2	-2083.45	737.5426	1073.058	18993.13	21026.88	1271.706	21002.38
CS3	-2083.44	737.5395	1073.050	18992.98	21026.88	1271.706	21002.22
CS4	-2083.45	737.5425	1073.057	18993.11	10512.12	635.7727	20366.43

Table 5.14 Utilities cost with H₂O and H₂ composition change.

Case	Cooling Water		Steam		Work		Utilities cost
	GJ	\$	GJ	\$	kWh	\$	
Base case	-2078.09	735.6437	1071.392	18963.64	21138.25	1278.441	20977.72
CS1	-2078.99	735.9624	1071.997	18974.34	21148.92	1279.087	20989.39
CS2	-2079.12	736.0072	1071.936	18973.26	21157.01	1279.576	20988.85
CS3	-2078.79	735.8922	1071.652	18968.24	21155.27	1279.471	20983.60
CS4	-2078.62	735.8309	1071.546	18966.36	21139.13	1278.495	20980.68

The utilities cost required for the operation with the disturbances of base case are highest in total feed and feed temperature disturbances but smallest in composition disturbances. However, the selection of the best case is focused on all three type of disturbances with requiring lowest cost. The smallest required cost is case CS4 followed by case CS1 and CS2 closely required.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The wongsri procedure, 8-step plantwide control structures design can be used to design the effective control structure of any plant. There are easy steps and the operator can follow easily. For the designed control structures of the methyl acetate process, the disturbances can be handled.

The control structure of all case can handle the disturbances (total feed, feed temperature and composition change). The temperature peak control of the reactor give the deviation of the conversion less than controlling the outlet temperature.

IAE comparison, the results show the best control structure (compare in 5 cases) is CS4 which could handle the process safety and smoothly operation. Furthermore, the utility cost required is small in comparison with base case, case CS1, case CS2 and case CS3.

6.2 Recommendation

The performances of the controller can be improved for more effectively control by adjusting the control parameters, gain and integral time of the controllers. Furthermore, adding the enhanced controllers can also improve the performances of control.

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APPENDICES

APPENDIX A

EQUIPMENT DATA AND STREAM INFORMATION

Table A.1 Equipment data

Units operation	Properties	Size
Reactor R1	Length (m)	10
	Diameter (m)	0.0245
	Number of tubes	300
	U (kW/m ³ ·K)	0.28
Reactor R2	Length (m)	10
	Diameter (m)	0.05
	Number of tubes	1000
	U (kW/m ³ ·K)	0.28
Reflux drum column C1	Length (m)	2.3
	Diameter (m)	1.6
Reflux drum column C2	Length (m)	1.68
	Diameter (m)	1.12
Reflux drum column C3	Length (m)	1.6
	Diameter (m)	1.07
Separator S1	Length (m)	6.79
	Diameter (m)	4.53
Sump column C1	Length (m)	4.46
	Diameter (m)	2.97
Sump column C2	Length (m)	1.56
	Diameter (m)	1.04
Sump column C3	Length (m)	2.79
	Diameter (m)	1.86

Table A.1 (continue) Equipment data

Units operation	Properties	Size
Vaporizer V1	Length (m)	2.4
	Diameter (m)	1.6
Vaporizer V2	Length (m)	2.07
	Diameter (m)	1.38

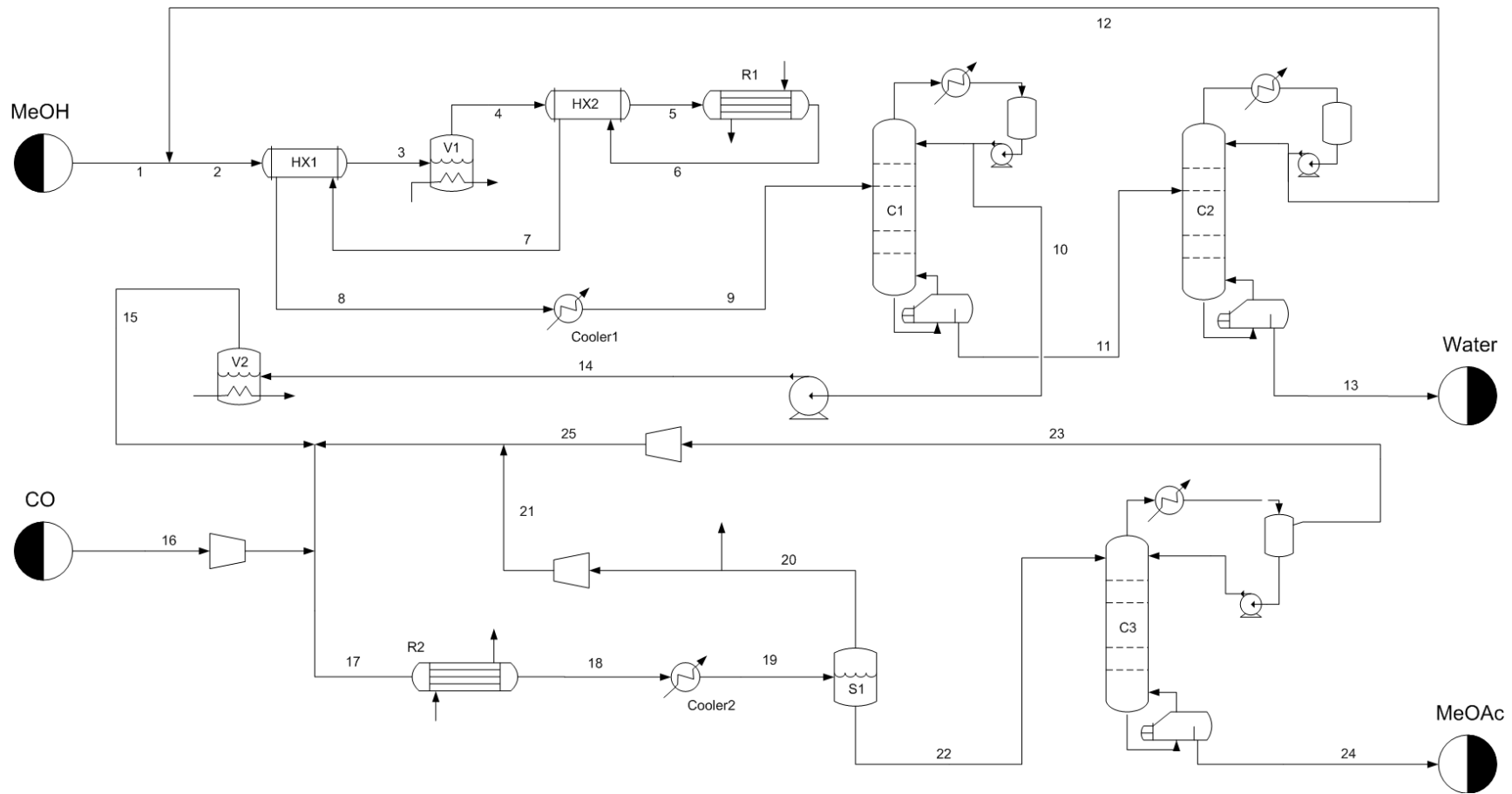


Figure A.1 Process flow sheet

Table A.2 Stream information

Stream	1	2	3	4	5	6	7	8	9	10
Flow (kmol/hr)	500.00	526.99	526.99	526.99	526.99	526.99	526.99	526.99	526.99	247.05
Temperature (C)	45.00	46.26	131.91	147.66	356.82	384.85	196.00	146.95	351.00	44.92
Pressure (bar)	15.91	13.93	13.54	13.04	12.63	12.22	11.82	11.42	10.65	10.13
Mole fraction										
CO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
DME	0.0000	0.0000	0.0000	0.0000	0.0000	0.4688	0.4688	0.4688	0.4688	1.0000
H ₂	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0100	0.0095	0.0095	0.0095	0.0095	0.4783	0.4783	0.4783	0.4783	0.0000
MeOAc	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MeOH	0.9900	0.9905	0.9905	0.9905	0.9905	0.0529	0.0529	0.0529	0.0529	0.0000

Table A.2 (continue) Stream information

Stream	11	12	13	14	15	16	17	18	19	20
Flow (kmol/hr)	279.93	26.98	252.95	247.05	247.05	257.54	1152.22	907.00	907.00	637.60
Temperature (C)	165.64	68.83	103.46	47.34	99.27	35.00	117.17	204.02	46.85	46.85
Pressure (bar)	10.27	13.93	1.17	33.44	32.42	5.78	31.44	31.08	30.40	30.40
Mole fraction										
CO	0.0000	0.0000	0.0000	0.0000	0.0000	0.9800	0.5253	0.3970	0.3970	0.5561
DME	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.2414	0.0363	0.0363	0.0230
H ₂	0.0000	0.0000	0.0000	0.0000	0.0000	0.0200	0.2218	0.2818	0.2818	0.4000
H ₂ O	0.9004	0.0002	0.9964	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MeOAc	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0114	0.2849	0.2849	0.0209
MeOH	0.0996	0.9998	0.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table A.2 (continue) Stream information

Stream	21	22	23	24	25
Flow (kmol/hr)	624.73	269.40	22.91	246.49	22.91
Temperature (C)	50.84	46.94	286.85	112.03	127.15
Pressure (bar)	31.44	30.39	5.07	5.23	31.44
Mole fraction					
CO	0.5561	0.0205	0.2416	0.0000	0.2416
DME	0.0230	0.0679	0.7319	0.0062	0.7319
H ₂	0.4000	0.0019	0.0227	0.0000	0.0227
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000
MeOAc	0.0209	0.9096	0.0038	0.9938	0.0038
MeOH	0.0000	0.0000	0.0000	0.0000	0.0000

APPENDIX B

TUNNING PARAMETERS

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_c	τ_i
Methanol feed	FC	Flow rate	Feed flow rate	PI	Reverse	500 kmol/h	0-1000	0.5	0.5
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	1.2 m	0-2.4	2	-
Reactor (R1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	658 K	558-758	3.67	5.28
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	351 K	251-451	6.04	5.28
Column (C1)	TC	Temperature tray 11-15	Reboiler duty	PI	Reverse	299.3 K	273-399	0.134	51.48
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.181	0-0.36	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.15 m	0-2.3	2	-
	LC	Reflux drum level	Pump work	P	Direct	2.23 m	0-4.46	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	10.3 bar	0-20	4.2	5.28
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	372 K	273-472	1.76	52.8
	FC	Reflux ratio	Reflux flow rate	PI	Reverse	3.55	0-7.00	0.3	52.8
	LC	Reboiler level	Bottom flow rate	P	Direct	0.78 m	0-1.56	2	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.84 m	0-1.68	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	1.013 bar	0-2	1.14	5.28

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct	1.035 m	0-2.07	2	-
CO feed	CC	Composition R2 out	Set point of FC	PI	Reverse	0.397	0-0.8	0.84	132
	FC	Flow rate	Compressor work	PI	Reverse	257.5 kmol/h	0-515	0.5	0.5
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	477.2 K	273-681	0.453	26.4
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	320 K	273-367	1.665	5.28
Separator (S1)	LC	Level	Liquid flow out	P	Direct	3.395 m	0-6.79	2	-
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	0.4	0-1.0	25.42	262.68
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	287 K	273-300	0.082	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.46	0-0.91	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.395 m	0-2.79	2	-
	LC	Reflux drum level	Condenser duty	P	Direct	0.8 m	0-1.6	2	-
	PC	Condenser pressure	Compressor work	PI	Reverse	5.07 bar	0-10.13	17.37	7.92

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	527 kmol/h	0-1054	0.5	10
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	405 K	305-505	27.35	10.56
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	630 K	530-730	7.92	10.56
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	1.2 m	0-2.4	2	-
Reactor (R1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	658 K	558-758	3.67	5.28
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	351 K	251-451	6.04	5.28
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	367 K	273-461	0.411	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.181	0-0.36	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.15 m	0-2.3	2	-
	LC	Reflux drum level	Pump work	P	Direct	2.23 m	0-4.46	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	10.3 bar	0-20	4.2	5.28
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	372 K	273-472	1.76	52.8
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	352 K	273-430	1.12	26.4
	LC	Reboiler level	Bottom flow rate	P	Direct	0.78 m	0-1.56	2	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.84 m	0-1.68	2	-

Table B.2 (continue) Type of controllers and tuning parameters of CS1

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Column (C2)	PC	Condenser pressure	Condenser duty	PI	Reverse	1.013 bar	0-2	1.14	5.28
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct	1.035 m	0-2.07	2	-
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	0.5253	0-1	0.84	132
	FC	Flow rate	Compressor work	PI	Reverse	257.5 kmol/h	0-515	0.5	0.5
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	477.2 K	273-681	0.453	26.4
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	320 K	273-367	1.665	5.28
Separator (S1)	LC	Level	Liquid flow out	P	Direct	3.395 m	0-6.79	2	-
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	0.4	0-1.0	25.42	262.68
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	287 K	273-300	0.082	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.46	0-0.91	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.395 m	0-2.79	2	-
	LC	Reflux drum level	Condenser duty	P	Direct	0.8 m	0-1.6	2	-
	PC	Condenser pressure	Compressor work	PI	Reverse	5.07 bar	0-10.13	17.37	7.92

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	527 kmol/h	0-1054	0.5	10
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	405 K	305-505	27.35	10.56
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	630 K	530-730	7.92	10.56
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	1.2 m	0-2.4	2	-
Reactor (R1)	TC	Temperature peak	Duty flow rate	PI	Reverse	680 K	580-780	0.08	5.28
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	351 K	251-451	6.04	5.28
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	367 K	273-461	0.411	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.181	0-0.36	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.15 m	0-2.3	2	-
	LC	Reflux drum level	Pump work	P	Direct	2.23 m	0-4.46	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	10.3 bar	0-20	4.2	5.28
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	372 K	273-472	1.76	52.8
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	352 K	273-430	1.12	26.4
	LC	Reboiler level	Bottom flow rate	P	Direct	0.78 m	0-1.56	2	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.84 m	0-1.68	2	-

Table B.3 (continue) Type of controllers and tuning parameters of CS2

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Column (C2)	PC	Condenser pressure	Condenser duty	PI	Reverse	1.013 bar	0-2	1.14	5.28
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct	1.035 m	0-2.07	2	-
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	0.5253	0-1	0.84	132
	FC	Flow rate	Compressor work	PI	Reverse	257.5 kmol/h	0-515	0.5	0.5
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	477.2 K	273-681	0.453	26.4
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	320 K	273-367	1.665	5.28
Separator (S1)	LC	Level	Liquid flow out	P	Direct	3.395 m	0-6.79	2	-
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	0.4	0-1.0	25.42	262.68
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	287 K	273-300	0.082	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.46	0-0.91	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.395 m	0-2.79	2	-
	LC	Reflux drum level	Condenser duty	P	Direct	0.8 m	0-1.6	2	-
	PC	Condenser pressure	Compressor work	PI	Reverse	5.07 bar	0-10.13	17.37	7.92

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

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	527 kmol/h	0-1054	0.5	10
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	1.2 m	0-2.4	2	-
Reactor (R1)	TC	Temperature peak	Duty flow rate	PI	Reverse	680 K	580-780	0.08	5.28
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	351 K	251-451	6.04	5.28
Column (C1)	TC	Temperature tray 13	Reboiler duty	PI	Reverse	367 K	273-461	0.411	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.181	0-0.36	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.15 m	0-2.3	2	-
	LC	Reflux drum level	Pump work	P	Direct	2.23 m	0-4.46	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	10.3 bar	0-20	4.2	5.28
Column (C2)	TC	Temperature tray 23	Reboiler duty	PI	Reverse	372 K	273-472	1.76	52.8
	TC	Temperature tray 13	Reflux flow rate	PI	Reverse	352 K	273-430	1.12	26.4
	LC	Reboiler level	Bottom flow rate	P	Direct	0.78 m	0-1.56	2	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.84 m	0-1.68	2	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	1.013 bar	0-2	1.14	5.28
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct	1.035 m	0-2.07	2	-
CO feed	CC	Feed R2 composition	Set point of FC	PI	Reverse	0.5253	0-1	0.84	132

Table B.4 (continue) Type of controllers and tuning parameters of CS3

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters	
								K_C	τ_i
	FC	Flow rate	Compressor work	PI	Reverse	257.5 kmol/h	0-515	0.5	0.5
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	477.2 K	273-681	0.453	26.4
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	320 K	273-367	1.665	5.28
Separator (S1)	LC	Level	Liquid flow out	P	Direct	3.395 m	0-6.79	2	-
Purge stream	CC	Hydrogen composition	Purge flow rate	PI	Direct	0.4	0-1.0	25.42	262.68
Column (C3)	TC	Temperature tray 1	Reboiler duty	PI	Reverse	287 K	273-300	0.082	26.4
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.46	0-0.91	0.5	0.5
	LC	Reboiler level	Bottom flow rate	P	Direct	1.395 m	0-2.79	2	-
	LC	Reflux drum level	Condenser duty	P	Direct	0.8 m	0-1.6	2	-
	PC	Condenser pressure	Compressor work	PI	Reverse	5.07 bar	0-10.13	17.37	7.92

Table B.5 Type of controllers and tuning parameters of CS4

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	τ_i	τ_D
Methanol feed	FC	Total feed flow rate	Feed flow rate	PI	Reverse	527 kmol/h	0-1054	0.5	10	-
Exchanger (HX1)	TC	Temperature outlet	By-pass flow rate	PI	Direct	405 K	305-505	27.35	10.56	-
Exchanger (HX2)	TC	Temperature outlet	By-pass flow rate	PI	Direct	630 K	530-730	7.92	10.56	-
Vaporizer (V1)	LC	Level	Duty flow rate	P	Direct	1.2 m	0-2.4	2	-	-
Reactor (R1)	TC	Temperature peak	Duty flow rate	PID	Reverse	680 K	580-780	0.116	5.28	0.38
Cooler (Cool1)	TC	Temperature outlet	Duty flow rate	PI	Reverse	351 K	251-451	6.04	5.28	-
Column (C1)	TC	Temperature tray 13	Reboiler duty	PID	Reverse	367 K	273-461	0.598	26.4	1.9
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.181	0-0.36	0.5	0.5	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.15 m	0-2.3	2	-	-
	LC	Reflux drum level	Pump work	P	Direct	2.23 m	0-4.46	2	-	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	10.3 bar	0-20	4.2	5.28	-
Column (C2)	TC	Temperature tray 23	Reboiler duty	PID	Reverse	372 K	273-472	2.55	52.8	3.8
	TC	Temperature tray 13	Reflux flow rate	PID	Reverse	352 K	273-430	1.63	26.4	1.9
	LC	Reboiler level	Bottom flow rate	P	Direct	0.78 m	0-1.56	2	-	-
	LC	Reflux drum level	Distillate flow rate	P	Direct	0.84 m	0-1.68	2	-	-
	PC	Condenser pressure	Condenser duty	PI	Reverse	1.013 bar	0-2	1.14	5.28	-

Table B.5 (continue) Type of controllers and tuning parameters of CS4

Equipment	Controller	Controlled variable	Manipulated variable	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_C	τ_i	τ_D
Vaporizer (V2)	LC	Level	Duty flow rate	P	Direct	1.035 m	0-2.07	2	-	-
CO feed	CC	Feed R2 composition	Set point of FC	PID	Reverse	0.5253	0-1	1.22	132	9.52
	FC	Flow rate	Compressor work	PI	Reverse	257.5 kmol/h	0-515	0.5	0.5	-
Reactor (R2)	TC	Temperature outlet	Duty flow rate	PID	Reverse	477.2 K	273-681	0.659	26.4	1.9
Cooler (Cool2)	TC	Temperature outlet	Duty flow rate	PI	Reverse	320 K	273-367	1.665	5.28	-
Separator (S1)	LC	Level	Liquid flow out	P	Direct	3.395 m	0-6.79	2	-	-
Purge stream	CC	Hydrogen composition	Purge flow rate	PID	Direct	0.4	0-1.0	36.98	262.7	18.95
Column (C3)	TC	Temperature tray 1	Reboiler duty	PID	Reverse	287 K	273-300	0.12	26.4	1.9
	FC	Reflux/feed ratio	Reflux flow rate	PI	Reverse	0.46	0-0.91	0.5	0.5	-
	LC	Reboiler level	Bottom flow rate	P	Direct	1.395 m	0-2.79	2	-	-
	LC	Reflux drum level	Condenser duty	P	Direct	0.8 m	0-1.6	2	-	-
	PC	Condenser pressure	Compressor work	PI	Reverse	5.07 bar	0-10.13	17.37	7.92	-

VITAE

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