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PLANTWIDE CONTROL STRUCTURE DESIGN OF METHANOL PROCESS

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A Thesis Submitted in Partial Fulfillment of the Requirements

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Department of Chemical Engineering

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กรกช นันทะน้อย : การออกแบบโครงสร้างการควบคุมแบบทั้งโรงงานของกระบวนการเมทานอล. (PLANTWIDE CONTROL STRUCTURE DESIGN OF METHANOL PROCESS) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ผศ. ดร.มนตรี วงศ์ศรี, 87 หน้า.

ในงานวิจัยนี้ เสนอการออกแบบโครงสร้างการควบคุมแบบทั้งโรงงานและผลการประเมินประสิทธิภาพของกระบวนการเมทานอลที่มีการรีไซเคิลก๊าซสามสายเพื่อผลิตเมทานอลความบริสุทธิ์สูงจากก๊าซสังเคราะห์ (synthesis gas) การออกแบบใช้วิธีของ Wongsri (2012) และโครงสร้างการควบคุมที่ได้จะนำไปเปรียบเทียบกับโครงสร้างการควบคุมที่เสนอโดย Luyben (2010) วิธีออกแบบ ของ Wongsri (2012) มี 8 ขั้นตอนซึ่งเน้นความสำคัญในการเลือกโครงสร้างการควบคุมเพื่อให้การดำเนินงานของโรงงานอยู่ในสภาวะคงที่ (fixture plant) โดยกำหนดตำแหน่งจุดสะสมของสารในกระบวนการตามเส้นทางของแต่ละสาร เพื่อที่จะสามารถกำหนดตัวแปรปรับที่เหมาะสมในการควบคุม การจัดการสิ่งรบกวนที่มีผลกับคุณภาพของผลิตภัณฑ์ การนำพลังงานที่เหลือกลับมาใช้ในกระบวนผ่านการแลกเปลี่ยนความร้อนระหว่างหน่วยของกระบวนการ การปรับปรุงกระบวนการให้ได้ประสิทธิภาพ และการทดสอบเพื่อตรวจสอบโครงสร้าง โดยกำหนดตัวแปรรบกวนเข้าสู่ระบบเพื่อทดสอบการจัดการหรือควบคุมของโครงสร้างนั้น ๆ ซึ่งตัวแปรรบกวนคือ การเปลี่ยนแปลงอัตราการไหลของก๊าซสังเคราะห์ และการเปลี่ยนแปลงส่วนประกอบภายในก๊าซสังเคราะห์ ซึ่งผลของการทดสอบการจำลองแบบไดนามิกส์พบว่า โครงสร้างการควบคุมของ Wongsri (2012) มีการควบคุมที่มีประสิทธิภาพ และให้การตอบสนองที่ดีและเสถียรกว่าโครงสร้างการควบคุมของ Luyben (2010) เนื่องจากเป็นผลของการสร้าง fixture plant และการจัดการสิ่งรบกวนที่สามารถช่วยลดการกระจายของการรบกวนที่กลับเข้าไปในกระบวนการ

ภาควิชา วิศวกรรมเคมี ลายมือชื่อนิสิต .....

สาขาวิชา วิศวกรรมเคมี ลายมือชื่อ อ.ที่ปรึกษาวิทยานิพนธ์หลัก .....

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This study presented the plantwide control structure design and the performance evaluation results of the methanol process with three gas recycled streams to produce high purity methanol from the synthesis gas. Wongsri's plantwide control structure design procedure (2012) is applied to design the plantwide control structure in order to satisfy the control objectives. The Wongsri's design procedure is explicit and systematic. It comprises of five stages with eight steps, emphasizing the establishment of a fixture plant by designing control loops, using the material quantifiers and their handlers, to regulate material component flows. The other plant level loops are designed using material and heat disturbance management for quality control. The changes of synthesis gas feed flow and synthesis gas composition are made to test the ability of the plantwide control structure proposed. The new design structures are compared with Luyben's structure (2010). Dynamic performance results show that the new control structure gives better performance than that of Luyben as a result of creating fixture plant and disturbance management supporting to reduce the disturbance propagation throughout an entire plant.

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

Page

Page

LIST OF TABLES

Page

Page

LIST OF FIGURES

Page

Page

CHAPTER I

INTRODUCTION

1.1 Importance and Reasons of Research

The plantwide process control involves to the control of the entire process which is an automatic control in the field of chemical engineering. The precise control of controlled variables is necessary in many process applications because the small changes in an initial process can significantly effect on the end result. The controlled variables and many other factors must be consistently controlled to produce the desired product satisfying control objectives. Especially, the complex process which includes the recycle streams of material and energy can have the disturbance propagations throughout the entire plant. Therefore, plantwide process control is the means that is able to achieve the operations within desired quality and safety.

The plantwide control problem is very much open-ended; therefore, there is no the best correct solution for control strategies. However, control structure designs must quickly handle the disturbances entering the process and operate easily and not too expensive. The plant's performance tests are a way of validating to select desired control structures.

This article presented the plantwide control structure design and the performance evaluation results of the designed plantwide control structures in the methanol process. Wongsri's procedure is used to design the plantwide control structure in order to satisfy the control objectives and compare with the base-case control structure obtaining from Luyben (2010). The procedure of Wongsri (2012) consist of eight steps which underline the establishment of a fixture plant by regulating material component flows using their quantifiers and handlers on their pathways; disturbance management for quality control; energy recovery through the

heat exchanger network; process modification and optimization; and design validation.

1.2 Research Objectives

Design and evaluate new plantwide control structures of methanol process proposed by Wongsri (2012).

1.3 Scopes of Research

I. Methanol process information is given by Luyben (2010).
II. Methanol process simulation is performed by using HYSYS simulation software.
III. Present new control structure design procedure of Wongsri (2012) for methanol process.
IV. Compare the new control structures design with the work proposed by Luyben (2010).

1.4 Contribution of Research

The procedure is detailed, instructive, simple, and easy to apply for novice in plantwide control structure design based on process approach.

1.5 Research Procedure

The steps of this research plants are:

I. Study concerned plantwide control theory.
II. Study and simulate the methanol process obtaining from Luyben (2010).
III. Study the plantwide control design procedure of Wongsri (2012).

IV. Design new plantwide control structures of methanol process following the Wongsri's procedure (2012).
V. Simulate methanol process in steady state mode with the new design control structures.
VI. Analyze methanol process simulation results obtaining from steady state mode.
VII. Simulate methanol process in dynamic mode with the new design control structures.
VIII. Evaluate the dynamic performance of the new plantwide control structures.
IX. Analyze and discuss the results.
X. Conclude the research.

1.6 Research Framework

The thesis consists six chapters as follows:

Chapter I: This chapter includes importance and reasons of research, research objectives, scopes of research, contributions of research, and research procedures.

Chapter II: present literature review related to plantwide control structures design procedure.

Chapter III: present the plantwide control structures design procedure.

Chapter IV: information and process description for methanol process.

Chapter V: describes the plantwide control structures design for methanol process including dynamic simulation results and discussions compared with control structures of Luyben (2010).

Chapter IV: conclusions of research and recommendations.

CHAPTER II

LITERATURE REVIEW

2.1 Review of Plantwide Control Structure Design

Price and Georgakis (1993) presented the plantwide regulatory control design procedure using two frameworks. The first design framework is Modular Framework which is the decomposition of a plant control problem into sub-problems; modules consisting of group of several linked unit operations. These modules can then be designed the control systems and combined them into a single plantwide control structure. The second design framework is Tiered Framework; the control tasks are presented in a tier including production rate control, inventory control, product specification control, equipment and operating constraints, and economic performance enhancement, where the task at first mentioned is the first to be considered. Each task provides a subset of control loops, and these control subsets are designed one at a time. The framework does not require a detailed mathematical model of the process and so can be used during the conceptual design stage before all design details of a process are fully known.

Price et al. (1994) presented the throughput manipulation in plantwide control structure. When the throughput manipulator is feed stream to the plant, the levels in each unit are controlled by manipulating the flow leaving the unit (control in the direction of flow) so that changes in production rate are passed through the plant from beginning to end by the inventory controllers. When the throughput manipulator is product stream, the levels in each unit are controlled by manipulating the flow incoming units (control in the direction opposite to flow) and if the throughput manipulator is process internal stream, the level controllers between the feed stream and the throughput manipulator are in the direction opposite to flow,

while those between the throughput manipulator and the product stream are in the direction of flow; moreover, level controllers on streams outside the primary path should also be in the direction of flow to avoid disturbance propagations throughout an entire plant.

Ng and Stephanopoulos (1996) presented the synthesis of control systems for chemical plants within an overview of the hierarchical framework. A hierarchical framework is proposed in which the plant is decomposed into a set of representations of different degrees of abstraction. Step 1 identifies overall production objectives, process constraints and sources of external disturbances. Step 2 examines the open-loop stability of the process. Step 3 performs overall system analysis. Step 4 identifies the process objectives. Step 5 prioritizes the process objectives. Step 6 synthesizes long-horizon control structure. Step 7 refines process representation. Step 8 repeats steps 4 to 7 until the dynamics of the plant becomes dominant in the representation. Step 9 refines model and process objectives and Step 10 synthesizes short-horizon control structure. This hierarchy of control strategies can be integrated to form a control system for the complex plant. The use of a hierarchy of representations reduces the complexity of the problem by allowing the designer to separately address process goals.

Luyben et al. (1997) presented the plantwide control design procedure applied to the vinyl acetate monomer process, the Eastman process, and the HDA process. The nine steps of the proposed procedure: 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. Steps 1 and 2 establish the objectives control and degrees of freedom. Step 3 ensures that heat within the process is dissipated properly. In Steps 4 and 5 satisfy the production rate, product quality, and safety. Step 6 involves total mass balance control. Step 7 checks the chemical components balance. Step 8 completes the control systems for individual unit operations. Finally, Step 9 uses the remaining degrees of freedom for optimization and improved

dynamic controllability. This heuristic procedure will generate a workable plantwide control strategy, which is not necessarily the best solution. Because the design problem is open-ended, the procedure will not produce a unique solution.

Larsson et al. (2003) presented control structure selection for reactor, separator and recycle process by systematic procedure obtained from Skogestad (2000) including seven steps; Degree of freedom analysis, Cost function and constraints, Identify the important disturbances, Optimization, Identify candidate controlled variables, Evaluation of loss, and Further analysis. The rest of prospective controlled variable is to find out a constant setpoint scheme that is satisfied economic loss. The reflux ratio L/F is an excellent controlled variable where the energy costs and the production rate are desired (minimizing energy costs and maximizing production rate) and maximizing the reactor holdup is optimal.

Konda et al. (2005) presented an integrated framework of simulation and heuristics in plantwide control of industrial process. The heuristic methodology consists of eight levels. Level 1 defines plantwide control objectives and control degree of freedom. Level 2 identifies and analyzes plantwide disturbances including setting performance and tuning criteria. Level 3 is production rate and product quality manipulator selection. Level 4 is selection of manipulators for more and less severe controlled variables. Level 5 is control of unit operations. Level 6 checks component material balances. Level 7 identifies and analyzes the effects due to recycle streams and Level 8 enhances control performance. The proposed integrated framework is applied to the HDA process. Results show that available control structure is able to be established by the proposed integrated framework of simulation and heuristics.

Seki and Naka (2007) presented control structure design for a reactor/separator process with two recycles by a hierarchical control structure including the lower level regulatory control layer and the higher level coordination control layer. The lower level regulatory layer is about the inventories and

compositions control designed on each single unit separated from plantwide process. The higher level coordination layer involves the remaining degree of freedom and process optimization designed in an entire process. The controller is designed to regulate between the subunits. To illustrate, the two recycle flows depend on the separator disturbances. The detailed dynamic model is not required, so this control structure design procedure is advantage.

Rodríguez and Gayoso (2007) presented degrees of freedom analysis for process control by the DOF expression for a complete process: DOF= $S_{ip}+\sum^{u}$ (S_{out} + H-A); where S_{ip} is the inputs to the process, S_{out} is output streams, $\sum^{u}$ is the sum of all the units in the process, H is the energy flows (one per unit), and A is the amount of inventories (liquid or gas) that are not considered. This expression is easily applied to any process and no need to write any equations. For instance, If there are the number of process streams: 39; number of inventories not accounted: 20; number of energy streams: 8, Degrees of freedom (DOF) is 39 (counting all the process streams)-20 (removing all the inventories not to be considered)+8 (adding all the energy flows (one per unit))=27.

de Andrade and Lima (2009) presented control structure design for an ethanol production plant by using the control structure design procedure of McAvoy and Ye (1994) and Price et al. (1994) in comparison. The control structure design procedure of McAvoy and Ye (1994) based on a Plantwide control approach, where single-input-single-output (SISO) control loops are used. The procedure includes control loops of simple flows and utility temperatures; closing the level loops; interaction, stability and saturation analysis; steady state disturbance analysis; tuning and testing via dynamic simulation; the quality control loops through a global material balance and; adding upper control layers, using real-time optimization tools, predictive control and others. For Price et al. (1994), the control structure design procedure based on the unit inventory management and the production rate by determining the primary path of the process and selecting a throughput manipulator to control the production rate and then inventory control loops are established in

accordance with throughput manipulator chosen to assure that the production rate changes can be passed throughout the process. The dynamic simulation results of both design procedure show good responses on handling disturbances. Nevertheless, the control structure design procedure of McAvoy and Ye (1994) is selected since it provides the best for this industrial application.

Luyben (2010) presented a design and control of a methanol reactor/column process with three gas recycle streams to produce high purity methanol from synthesis gas. The unique feature of this control scheme is a lack of control of pressure in the system, so a high-pressure override controller is used to handle component balances and pressure in the plant. The development of the plantwide control structure design is based on the heuristic procedure proposed by Luyben et al. (1999). A plantwide control structure designed can effectively handle large disturbances in the production rate and synthesis gas composition.

Luyben (2010) presented design and control of the ethyl benzene (EB) process. The economic optimization and effective plantwide control structure design are applied to minimize capital and energy costs. The reactor size and recycle flow rate of benzene are the economic optimum variables designed in this. Byproduct di-ethyl benzene (DEB) decreases in the reactor and recycle streams if reactor and benzene recycle flow rate increase. The dynamic performance results of EB process are effective by using conventional controllers. Changes of the benzene-to-ethylene ratio on changes in the DEB recycle flow rate can be efficiently regulated disturbances with the purity of EB maintained at its setpoint.

Husnil et al. (2013) presented plant-wide control for the economic operation of modified single mixed refrigerant (MSMR) process. The NGL recovery and liquefaction units were integrated in the MSMR process to provide an efficient operation. Steady-state optimality analysis is conducted to determine the variable maintaining the economic efficiency of MSMR process. The results showed that the flow rate ratio of heavy and light mixed refrigerant (HK/LK ratio) provides a self-

optimizing controlled variable and maintains the MSMR optimality. The plantwide design procedure carries on six steps. The first step is the formulation control objectives and constraints. The second step is to determine the degrees of freedom for identifying the manipulated variables. The third step is to determine the appropriate manipulated variable by sensitivity analysis that gives the relation of input-output. The fourth step is adding the necessary regulatory control loops. The fifth step is the process optimization as well as selecting the optimizing-controlled variable. The sixth step is evaluating the control structures in terms of both dynamic response and steady-state. The control structure with the HK/LK ratio loop provided better performance than the system with the HK flow control loop.

Luppi et al. (2013) presented decentralized plantwide control strategy for large-scale processes of pulp mill benchmark. Plantwide control strategy consists of five steps, namely define the stabilizing control loops (stabilizing the plant by establishing control loop of level or pressure in tanks and vessels), obtain a reduced process model (estimating steady-state gains and simplified dynamic linear models), select the CVs set together with the optimal CVs–MVs pairing, determine the algorithm and tuning parameters for each control loop, and evaluate the dynamic performance of the designed strategy. The proposed methodology considers tools as the normalized relative gain array (NRGA) and the Hungarian Algorithm (HA). The approach is based on steady-state information, and tries to reduce the use of heuristic considerations. The dynamic simulation results show stable and acceptable dynamic performance under several disturbances and setpoint changes.

CHAPTER III

PLANTWIDE CONTROL STRUCTURE DESIGN PROCEDURE

Plantwide process control is the tool used to control an entire plant that includes many interconnected unit operations, not just the individual unit operations. The control structure of a single unit may not operate a plant when that unit is connected to other unit operations with the integrated chemical processes consisting the recycle streams and energy integration. The need for a plantwide control perspective arises from three important features of integrated processes: the effects of material recycle, the effects of energy integration, and the effects of chemical component inventories.

The procedure decomposes the plantwide control problem into each level and forces us to focus on the unique features and issues that involve a control strategy for an entire plant. The nine basic steps of a general heuristic plantwide control design procedure (Luyben et al, 1997) satisfy the two fundamental chemical engineering principles, namely the overall conservation of energy and mass; moreover, the procedure accounts for chemical component inventories and entropy.

3.1 Plantwide Control Design Procedure of Luyben

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

Step 1: Establish Control Objectives. Assess the steady-state design and dynamic control objectives for the process. These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine Control Degrees of Freedom. Count the number of control valves available. This is the number of degrees of freedom to control, i.e., the number of variables that can be controlled to setpoint. The valves will be used to achieve basic control of the process: set production rate, maintain gas and liquid inventories, control product qualities, and avoid safety and environmental constraints.

Step 3: Establish Energy Management System. Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system; to provide a control system that removes exothermic heats of reaction from the process and provide a control system that prevents the propagation of thermal disturbances. Process to process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom to 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 rates, we must increase overall reaction rates. This can be accomplished by raising temperature (higher specific reaction rate), increasing reactant concentrations, increasing reactor holdup (in liquid-phase reactors), or increasing reactor pressure (in gas-phase reactors). First choice for setting production rate should be to alter one of these variables in the reactor. The variable we select must be dominant for the reactor and significant effects on reactor performance. For example, temperature is often a dominant reactor variable. Once we identify the dominant variables, we must also identify the manipulators (control valves) that are most suitable to control them. The manipulators are used in feedback control loops to hold the dominant variables at setpoint.

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 such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times and large steady-state gains.

Step 6: Control Inventories (Pressures and Levels) and Fix a Flow in Every Recycle Loop. Flow controlling a stream somewhere in all recycle loops is an important simple part of any plantwide control strategy. Once we have fixed a flow in each recycle loop, we then determine what valve should be used to control each inventory variable. Inventories include all liquid levels and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit. Because we have fixed a flow in each recycle loop, our choice of available valves has been reduced for inventory control in some units.

Step 7: Check Component Balances. Identify how chemical components enter, leave, and are generated or consumed in the process. The buildup of chemical components in recycling streams must be prevented by keeping track of chemical component inventories (reactants, products, and inerts) inside the system and identify the specific mechanism or control loop to guarantee that there will be no uncontrollable buildup of any chemical component within the process by controlling their reaction, or adjusting their outflow from the process.

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.

Step 9: Optimize Economic or Improve Dynamic Controllability. Establish the best way to use the remaining control degrees of freedom. After satisfying all of the basic regulatory requirements, we usually have additional degrees of freedom involving control valves that have not been used and setpoints in some controllers that can be adjusted. These can be used either to optimize steady-state economic process performance (e.g., minimize energy, maximize selectivity) or to improve dynamic response.

3.2 Plantwide Control Design Procedure of Wongsri

Wongsri (2012) presented the new plantwide control design procedure carried out in five stages with eight steps, the major steps deal with plant level design; establishing a fixture plant. The component balances are accounted by identifying the material quantifiers that indicate the amounts of the components and using their handlers to control them. The disturbances entering into the process must be directed by using the proposed material and energy disturbance management for avoiding the disturbance propagation throughout the plant. Each step is as follows:

Stage 1. Plant Information and Analysis.

Step 1: Gather of relevant plant information and control objectives, including constraints for control. It is necessary to obtain all information relevant to process control, such as product quality, production rate, smooth operation, process and equipment constraints, plant safety, and environmental regulations.

Step 2: Plant analysis. Several tasks to assist design decision in Step 3 are:

2.1 Control degree of freedom (CDOF). Each single independent stream, physical or virtual, material or energy, must have a handle or one control degree of freedom.

2.2 Heat pathways. The first pathway is heat generated by exothermic reactions and flows out to the environment. A second pathway carries heat from utilities into the process and to the environment. The third pathway is internal to the process. The fourth pathway is accounted for the enthalpies entered and left the plant.

2.3 Material pathways. The pathway is the flow path of a component from an entry point or an originated point to an exit point or an end point.

2.4 Material quantifier. A material quantifier is the place indicating the significant amounts of a chemical component (or a group of the components) in the plant which can be handled quite readily by regulating at their handlers. In the case that the quantifier is a flow, it is, but not necessarily, the place that has the highest gain of component flow is the total flow.

2.5 Reaction section. It is necessary to obtain required information for control design of reactor section. In general, what kind of controlled variables used to regulate the reaction yield and where to measure such controlled variables? What is the best control strategy and all? If feeds and recycle streams are fixed, the only places that the material (total or component) flow rates altered are a reactor and also a separator.

2.6 Separation section. The appropriate directions of disturbances are analyzed and specified. A plus disturbance, D+ is the plus deviation of the mass load from the nominal load and the minus disturbance, D- is the minus deviation of the mass load. The paths of D^+ and D^- in the separation section are analyzed and then designed in order to shift plus or minus mass loads to the desired targets to achieve the plant operation objective, e.g. maintaining product quality and avoiding disturbance propagation and recycling. The paths of D+ and D- in the separation section must be shifted to the proper exits. In the case that there is no proper exit for D^+ or shifting it through available exits will disturb the product quality, recycling it would be allowed.

Next, a good location of temperature control is the tray with the largest changes in the temperature from the initial steady state by changing of composition, total flow, temperature, and component flow during keeping the reboiler heat duty and reflux flow or reflux ratio or reflux fraction or boil up ratio constants.

2.7 Production rate control. Throughput changes must be achieved by altering reactor condition. However, reactor temperature, reactant concentration, reactor holdup would be somehow limited.

The production or throughput rate change by increasing/decreasing feed rate, should be accompanied by adjusting recycle flow accordingly.

Mode of operation: On-supply, On-demand, and on-internal. The mode of operation is dictated by a business objective and the mode of operation, such as on-supply (fixed feed rate), on-demand (fixed product rate), and on-internal (fixed internal flow rate) based on throughput manipulator (TPM) decision Price and Georgakis (1994). For on-internal control scheme, the throughput manipulator (where the production rate is set) is located inside the plant downstream of this location

(normally at the bottleneck), the plant has to process whatever comes in, and upstream of this location the plant has to produce the desired quantity. The selection of on-supply, on-demand or on-internal should depend on the completeness of total control of components.

In some processes, the separation section is placed before the reactor section, there are two locations to fix the material flows into the process: at the entrances of the reactor section or of the separation section. In the case that the influent reactor is fixed, the quantifiers (inventories) prior to this point must be controlled as 'on-demand production'.

Stage 2. Fixture Plant and Disturbance Management.

This stage is a major design stage; plant control structure is created at plant level in two steps: Step 3 and Step 4. The plant control loop design procedure presented in this paper is explicit and systematic while the Luyben design procedure has some shortcomings, Konda (2005). There are two objectives: the plant nominal material balance is maintained; the heat and material disturbances must be rejected to the nearest exits or directed to less significant streams.

Step 3: Establish fixture plant. The principal idea of establishing a fixture plant is first to have a material-balanced in the plant by controlling each component at its quantifier, i.e., fixture point.

3.1 Keep the materials entered and/or reentered fixed. A fresh feed and/or a combined stream of make-up feed and recycle stream must be kept constant to maintain the plant inventory by flow/composition controls. A recycle flow should not be fixed. This leaves the recycle flow free to be adjusted; one degree of freedom is restored to the plantwide control design process. If the composition of the recycle stream differs from the fresh feed stream significantly, each recycle stream may be flow-controlled. However, in the case that the composition of the recycle reactant can be measured, the composition of the combined stream is controlled to keep the combined reactant flow in check.

In the case of changing throughput, the combined stream of make-up feed and recycle or the recycle stream is adjusted accordingly to maintain the material

balance principle. Normally, the liquid recycle is adjusted automatically by its level somewhere in the process. However, it might be not the case for the gaseous recycle flow, the additional ratio loop of the recycle and the feed is recommended.

3.2 Adjust the flow of exit material streams (products, byproducts, and inert) according to their accumulations. If the flows of the products are controlled (mode of operation is on-demand) the quantifiers of the products, e.g. levels of reflux drums indicating the plus/minus will be used to control the feeds.

3.3 Handle the material that's not leaving the process. The reactor is the logical place to regulate a component fed or formed in the process and not leaving the process. If there is only one reactor and there is more than one component that not leaving the process, their kinetics must be similar, e.g. increasing the reactor temperature reduces or increases the amount of both components. Handlers of these components must be identified. If their kinetics are not compatible, we must provide exits for the incompatible components.

3.4 Control the amount of the rest of the component at their quantifiers. This step assures the rest of component inventory is regulated from a plantwide perspective. Setting the control at the specified quantifiers is like providing coordination over different sections of the plant to ensure that the rate of accumulation of each component in the overall process is zero.

3.5 Maintain the production rate.

3.5.1 Consume the limiting reactant. Determine the most appropriate manipulated variable to control the limiting reactant for the economic reason, i.e., the reactor temperature, the reactor pressure, or the reactor holdup.

3.5.2 Maintain the production rate. The product rate can be maintained through 3.5.1. If this is done and the production rate does not reach the objective or the production demand, the limiting reactant feed rate must be increased. However, the design constraints may limit this strategy concerning increasing the reactant feed rate.

Step 4: Disturbance management for quality control. The nominal conditions of process streams are maintained by specifying the disturbance shifting directions. The principles of disturbance management are following:

4.1 Heat disturbance management. The heat disturbance is divided into two categories. Heat disturbance of category 1 (HDC1) is the heat disturbance that does not instantly affect on the qualities of process streams, such as heat disturbance in a process stream toward a heater, a cooler, or a process-to-process heat exchanger. Heat disturbance of category 2 (HDC2) is the heat disturbance that will affect the process stream qualities where an additional phase is created or introduced, and the equilibrium is altered; or where chemical reactions are undergoing, such as separators and reactors.

4.1.1 Direct the HDC1 to the environment via the next and nearest exit points, usually heaters or coolers, to keep the thermal conditions of the process stream fixed.

4.1.2 Direct the HDC2 to less significant output streams of separators. This rule is generally apt to a separator using heat as a separating agent.

4.2 Material disturbance management. The configurations of the control loop are decided based on the desired material pathways. As in the case of heat disturbance management, we should direct the material disturbances to the environment via the next and nearest exit points to avoid disturbance recycling and propagation.

Many industrial distillation columns use some type of single-end temperature control because of its simplicity and low maintenance cost. This step presents a procedure to determine the control structure of a distillation column with desired material disturbances (D+ and D-) following step 2.6 by using a dynamic process simulator for various single-end control structures, namely constant reflux flow (R), constant reflux ratio (RR), constant reflux-to-feed ratio (R/F), constant reflux fraction (R/(R+D)), constant boil-up ratio (V/B). Several kinds of material disturbances in feed, such as temperature, flow rate, composition, and component flow rate are generated to test the disturbance shifting ability of these control structures. In addition, the principals of the material disturbance management are as follows:

4.2.1 Direct the material disturbances of byproducts, inerts, and unconverted raw materials to the environment via the next and nearest exit points.

4.2.2 For the main products, the minus disturbances should follow Rule 4.2.1. However, the main product plus disturbances should be allowed to propagate to their exits.

4.2.3 MDM rule for the recycle streams: their plus disturbances of unreacted raw materials are permitted, however, their minus disturbances must not be allowed to economize the make-ups.

The selection of the distillation control structures is carried out in two steps: preliminary screening using steady-state simulation and the selected candidates are further tested by rigorous dynamic simulation.

Stage 3. Unit Level Design.

Control loop design at this stage is solely based on individual unit operations.

Step 5: Design the rest of the control loops. Normally, the rest of the control loops is inventory loops which are self-regulating and less crucial. They can be designed using unit-based approach.

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

5.2 Adding simple enhanced controls, e.g. cascade, feed forward control.

Stage 4. Energy Management and Optimization.

The supplementary design activities involve heat exchanger network design and control, and plant operation and design optimization.

Step 6: Energy management via heat exchanger networks. In the case that the exothermic heat of reaction is large enough to heat some process cold streams, i.e., potential heat exchanger networks or alternative heat integrated processes (HIPs) exist, a heat exchanger network must be designed and a HEN must be resilient, i.e. delivering the exchange streams to their target temperature. The resilient heat exchanger network with specified load disturbances can be designed using Wongsri's method. The design of a control system that prevents the propagation of the heat disturbance of Wongsri and Hermawan is recommended.

Step 7: Optimize economics or improve control performance. The design and control issue remains an open research area regarding the plantwide control design, so the opportunity to alter the process design is possible.

Stage 5. Design Validation.

The validation of the design control structures using rigorous nonlinear simulation is inevitable; whatever may be the design procedure.

Step 8: Validate the designed control structures by rigorous dynamic simulation. The measures would be costs, raw material and energy consumptions, control performances of the total plant or some selected loops, etc. Expected disturbances must be listed to perform the disturbance test on the plant with designing control structures.

Plantwide control design procedure of Luyben et al., (1997) subdivided the big task of designing the overall plantwide control system into smaller tasks. However, in each step (especially set production rate and material inventory steps) with specific guideline is not apparent from this discussion.

Wongsri's design procedure is explicit, systematic, and easy to apply as well as more specific and generic guidelines, which will be very useful to beginners to understand the potential alternatives at each stage and choose the better one based on the process knowledge and requirements. It comprises of five stages with eight steps emphasizing the establishment of a fixture plant by designing control loops, using the material quantifiers and their handlers, to regulate material component flows. The other plant level loops are designed by using material and heat disturbance management for quality control. This design procedure is clearly more detailed and useful guidelines on how to go about the plantwide control problem. Wongsri's design procedure is reasonably developed and has several new features compared with that of Luyben as shown in Table 1.

Table 1 Plantwide control design procedure of Wongsri and Luyben in comparison

Plantwide Control Design Procedure	
Wongsri (2012)	**Luyben et al., (1997)**
Stage 1. Plant Information and Analysis Step 1: Gather of relevant plant information and control objectives, including constraints for control Step 2: Plant analysis 2.1 Control degree of freedom (CDOF) - Each single independent stream must have a handle or one control degree of freedom 2.2 Heat pathways 2.3 Material pathways 2.4 Material quantifier 2.5 Reaction section 2.6 Separation section - The appropriate directions of disturbances are analyzed and specified - Sensitivity test for selecting temperature control tray location 2.7 Production rate control - Mode of operation: On-supply, On-demand, and on-internal	**Step 1: Establish Control Objectives** **Step 2: Determine Control Degrees of Freedom** - Count the number of control valves available **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

Table 1 Plantwide control design procedure of Wongsri and Luyben in comparison (Continued)

Plantwide Control Design Procedure	
Wongsri (2012)	**Luyben et al., (1997)**
Stage 2. Fixture Plant and Disturbance Management Step 3: Establish fixture plant 3.1 Keep the materials entered and/or reentered fixed 3.2 Adjust the flow of exit material streams (products, byproducts, and inert) according to their accumulations 3.3 Handle the material that's not leaving the process 3.4 Control the amount of the rest of the component at their quantifiers 3.5 Maintain the production rate - 3.5.1 Consume the limiting reactant - 3.5.2 Maintain the production rate Step 4: Disturbance management for quality control 4.1 Heat disturbance management - The heat disturbance that does not instantly affect on the qualities of process streams	**Step 7: Check Component Balances** - Identify how chemical components enter, leave, and are generated or consumed in the process **Step 3: Establish Energy Management System** - Transferring the variability to the plant utility system

Table 1 Plantwide control design procedure of Wongsri and Luyben in comparison (Continued)

Plantwide Control Design Procedure	
Wongsri (2012)	**Luyben et al., (1997)**
- The heat disturbance that will affect the process stream qualities 4.2 Material disturbance management - The configurations of the control loop are decided based on the desired material pathways	**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
Stage 3. Unit Level Design Step 5: Design the rest of the control loops 5.1 Design the control loops for the remaining control variables, i.e. the rest of the inventory 5.2 Adding simple enhanced controls, e.g. cascade, feed forward controls	**Step 6: Control Inventories (Pressures and Levels) and Fix a Flow in Every Recycle Loop** **Step 8: Control Individual Unit Operations**
Stage 4. Energy Management and Optimization Step 6: Energy management via heat exchanger networks Step 7: Optimize economics or improve control performance	**Step 9: Optimize Economic or Improve Dynamic Controllability**
Stage 5. Design Validation Step 8: Validate the designed control structures by rigorous dynamic simulation	

CHAPTER IV

METHANOL PROCESS

4.1 Introduction to Methanol Process

Methanol is the essential chemical commodities, most of which is produced from natural or synthesis gas. Methanol is the simplest alcohol, with the lowest carbon content and the highest hydrogen content of any liquid fuel. It is utilized in many forms such as transportation fuel, a hydrogen carrier for fuel cell technologies, and an efficient fuel for electric power generation. Hence, the methanol process is one of the examples considered here. The process description and conditions obtained from Luyben (2010).

The mixture feed of carbon dioxide, carbon monoxide, water, and hydrogen in the synthesis gas is fed into the process, including a reaction unit, separation section, and three recycle streams for recovery of reactants. The synthesis gas is then converted to the methanol in the solid catalyst in the plug flow reactor and then the methanol is purified to high quality by removing water and impurities in the separators and distillation column, respectively. The impurities and reactants are circulated back to the reactor.

4.2 Reaction Kinetics

The reactions are exothermic; therefore, the chemical equilibrium constants decrease with increasing temperature, which results in lower conversion, more excess components, and increases of system pressure are built. The reactor temperatures must be low for improving conversion; however, the reactor temperatures are not so low that the specific reaction rates are too small. The kinetics are given by vanden Bussche and Froment by using the water-shift reaction:

$CO_2+3H_2 \leftrightarrow CH_3OH+H_2O$ (1)

$CO+H_2O \leftrightarrow CO_2+H_2$ (2)

The reactions are exothermic and use a solid catalyst. The original data use pressures in bar and reaction rates in kmol min^{-1} kg^{-1} catalyst. These must be transformed to use Pascals. The kinetics are described by LHHW-type equations:

$$R = (kinetic\ term)\frac{(driving-force\ term)}{(adsorption\ term)} \quad (3)$$

The first reaction is given in eq 4.

$$R_1 = (k_4 P_{CO2} P_{H2})\frac{\left[1-\frac{1}{K}\left(\frac{P_{CH3OH}P_{H2O}}{P_{CO2}P_{H_2}^3}\right)\right]}{\left[1+k_8\left(\frac{P_{H2O}}{P_{H_2}}\right)+k_1\sqrt{P_{H_2}}+k_2 P_{H2O}\right]^3} \quad (4)$$

The second reaction is given in eq 5.

$$R_2 = (k_5 P_{CO2})\frac{\left[1-\frac{1}{K}\left(\frac{P_{CO}P_{H2O}}{P_{CO2}P_{H_2}}\right)\right]}{\left[1+k_8\left(\frac{P_{H2O}}{P_{H_2}}\right)+k_1\sqrt{P_{H_2}}+k_2 P_{H2O}\right]} \quad (5)$$

Table 2 gives the kinetic and adsorption parameters entered into the Heterogeneous Catalytic model in Hysys.

Table 2 Kinetic LHHW Parameters

$R_1(CO_2+3H_2 \leftrightarrow CH_3OH+H_2O)$	$R_2(CO+H_2O \leftrightarrow CO_2+H_2)$
kinetic factor k = 1.07e-3	**kinetic factor** k = 1.22e9
E = 36696 kJ/kmol	E = 94765 kJ/kmol
driving-force expressions	**driving-force expressions**
term 1	term 1
conc. exponents for reactants: CO_2 = 1; H_2 = 1	conc. exponents for reactants: CO_2 = 1; H_2 = 0
conc. exponents for products: CH_3OH = 0; H_2O = 0	conc. exponents for products: CO = 0; H_2O = 0
coefficients: A = -23.02581; B = C = D = 0	coefficients: A = -11.512952; B = C = D = 0
term 2	term 2
conc. exponents for reactants: CO_2 = 0; H_2 = -2	conc. exponents for reactants: CO_2 = 0; H_2 = -1
conc. exponents for products: CH_3OH = 1; H_2O = 1	conc. exponents for products: CO = 1; H_2O = 1
coefficients: A = 24.388981; B = -7059.7258;	coefficients: A = -16.184871; B = 4773.2589;
C = D = 0	C = D = 0
adsorption expression	**adsorption expression**
adsorption term exponent: 3	adsorption term exponent: 1
concentration exponents:	concentration exponents:
term 1: H_2 = 0; H_2O = 0	term 1: H_2 = 0; H_2O = 0
term 2: H_2 = -1; H_2O = 1	term 2: H_2 = -1; H_2O = 1
adsorption constants:	adsorption constants:
term 1: A = 0, B = 0, C = 0, D = 0	term 1: A = 0, B = 0, C = 0, D = 0
term 2: A = 8.1471087, B = 0, C = 0, D = 0	term 2: A = 8.1471087, B = 0, C = 0, D = 0

4.3 Methanol Process Description

The process studied is the economically optimum design of a methanol reactor/distillation column system with three gas recycle streams to produce high-purity methanol from synthesis gas.

Luyben (2010) optimized the process plant parameters, namely reactor pressure, reactor size, vent/recycle split, flash tank pressure, and distillation column design according to capital cost, energy cost, income, and the return on investment (ROI).

Effect of Pressure. Higher pressure in the reactor, resulting in more production of methanol, which results in smaller the recycle and reduce compressor

power K3 of recycle. Both capital and energy costs increase in net effect, but income increases as methanol product increases. Based on the return on investment (ROI), the reactor pressure is set at 110 bar.

Effect of Reactor Size. Increase the reactor size, by increasing the number of tubes in the reactor, increases the conversion. Therefore, the recycle flow decreases and so the cost of K3 compressor. The total capital cost of reactor size and K3 increases since the capital cost of increases in reactor size is greater than the one of the decreases in recycling compressor K3. The optimum design value is 8000 tubes in the reactor.

Effect of Vent/Recycle Split. When vent/recycle split is decreased, vent rate decreases, and recycle flow increases, so the energy and capital cost of the recycle compressor K3 increases. The methanol product is more produced due to smaller losses of reactants in vent. The vent/recycle split of 0.022 gives the maximum income.

Effect of Flash Tank Pressure. The energy cost of the compressor K4, recycling the gas from flash separator S2 back to the reactor, rapidly increases as the flash pressure is decreased from 2 to 1 bar. In contrast, the energy cost of the compressor K5, recycling the gas from the reflux drum of column C1 back to the reactor, decreases as the flash pressure is decreased. A pressure of 2 bar gives the maximum income and at the same time gives the minimum capital investment.

Effect of Distillation Column Design. The minimum reboiler duty is determined the optimum feed stage of 27 and the minimum total annual cost (TAC) is considered at total stages of 42.

Figure 1 shows the flow sheet of the methanol process and Table 3 gives the operating conditions and design specification of process units. The process description and conditions obtained from Luyben (2010).

The synthesis gas at 51.2 bars including the reactants mostly containing the hydrogen, carbon dioxide, and carbon monoxide and the small inert gases of methane and nitrogen is compressed by two compressors to 110 bars to mix with three recycle gas streams, and the total gas stream is then heated to 150 °C in a reactor preheater HX3 for proper thermal condition on converting to methanol in the

plug flow reactor PFR. The reactor outlet stream is cooled to 38 ℃ in HX4 for partially condensing and then the stream is separated in a separator S1 operating at 106.5 bar and 38 ℃ for removing the uncondensed gases and recycling. A small vapor stream containing the inert components must be purged out of the system at a flow rate about 900 kmol/h by vent valve. The liquid from the separator S1 is fed to the flash tank S2 operating at 2 bars, which is used to remove the light components remaining for recycling before feeding into the column C1. The liquid from the flash tank S2 is fed on stage 27 of a 42-stage distillation column C1 operating at 1 bar. The specifications set the compositions of the bottoms of 0.01 mole % methanol, the distillate of 0.1 mole % water, and the reflux-drum temperature at 50 ℃, which establishes the amount of vapor for recycling. The column C1 required the reflux ratio of 1.03 and the reboiler energy is 80.12 MW for base temperature is 110 ℃.

Table 3 Operating conditions and design specification of process units

Units	**Reactor**	**Separator S1**	**Flash tank S2**	**Column C1**
Type	PFR	Adiabatic	Adiabatic	Simple tray
Operating Temp	265 °C	38 °C	38 °C	50-110 °C
Operating Pressure	110 bar	106.5 bar	2 bar	1-1.4 bar
Feed	Combined stream	Reactor effluent	S1 bottoms	S2 bottoms
Size	8000 tubes, 12.2 m length, 0.03675 m diam., and 0.5 void volume.	6.5 m diam.	2.8 m diam.	42 trays 6.5 m diam.
Feed stage	-	-	-	27
Reflux ratio	-	-	-	1.03

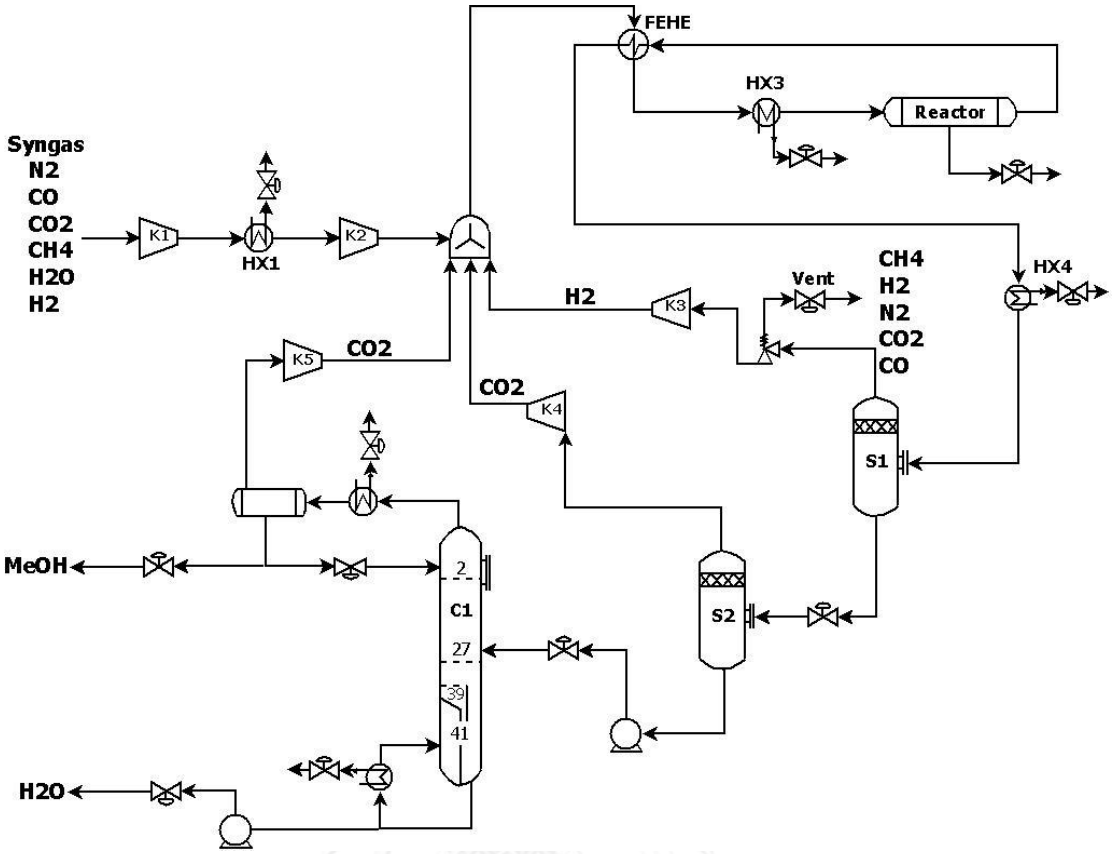


Figure 1 Methanol process flow sheet

CHAPTER V

CONTROL STRUCTURE DESIGN

5.1 Control Structure Design Procedures Applied to the Methanol Process

The proposed new design procedure of Wongsri demonstrated in chapter 2 is applied to the methanol process obtained from Luyben (2010). Discussion in each step of the design procedure carried out in five stages with eight steps in detail as follows:

Stage 1. Plant Information and Analysis.

Step 1: Gather of relevant plant information and control objectives, including constraints for control. The information mentioned above, is used in the control structure design and simulation. The performances of control structure must satisfy the seven control objectives, namely the compositions of the bottoms (0.01 mole % methanol), the distillate (0.1 mole % water), the recycle gas (0.32 mole % methane), the pressure of separator S1 is not over of 120 bar, the pressure of flash separator S2 (2 bar), the column temperature at tray 39 (101°C), and the reactor inlet temperature (150°C) in a stable manner under operation constraints.

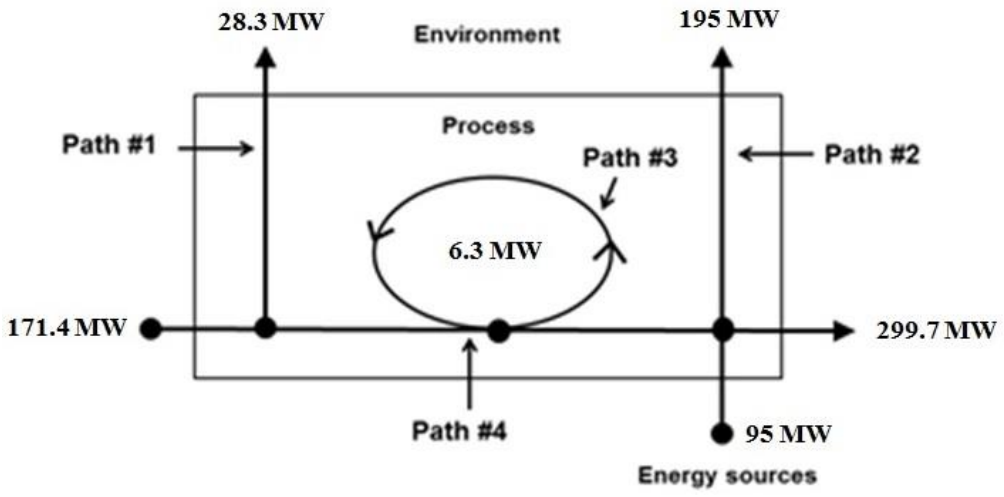
Step 2: Plant analysis

2.1 Control degree of freedom (CDOF). Each single independent stream should be provided the handling given in Table 4. There are a total of 17 independent streams, hence 17 CDOFs, namely vent flow 1, compressor work 5, reactor cooling flow 1, heater and cooler 3, column 5 (condenser heat removal, bottoms flow, distillate flow, reboiler heat input, and reflux rate), and separator liquid flow 2.

Table 4 The control degree of freedom for the methanol process

Unit	Manipulated variable	Quantity	CDOF
Vent stream	Vent Flow rate	1	1
Compressor	Work	5	5
Plug flow reactor	Coolant flow rate	1	1
Heater and Cooler	Heat input and Coolant flow rate	3	3
Distillation column	Condenser heat removal, Bottoms flow rate, Distillate flow rate, Reboiler heat input, Reflux rate	1	5
Adiabatic separator	Liquid flow rate	2	2
Total			17

2.2 Heat pathway. The heat pathways are used to design control loops regulating the thermal condition of the process streams as well as rejecting the thermal disturbances. The heat pathways are presented in Figure 2. The first pathway is heat generated by the exothermic reactions (28.3 MW). A second pathway is heat from utilities into the process (95 MW) and to the environment (195 MW). The third pathway is internal to the process (6.3 MW). The fourth pathway is the enthalpies entered (171.4 MW) and left the plant (299.7 MW) via process stream.



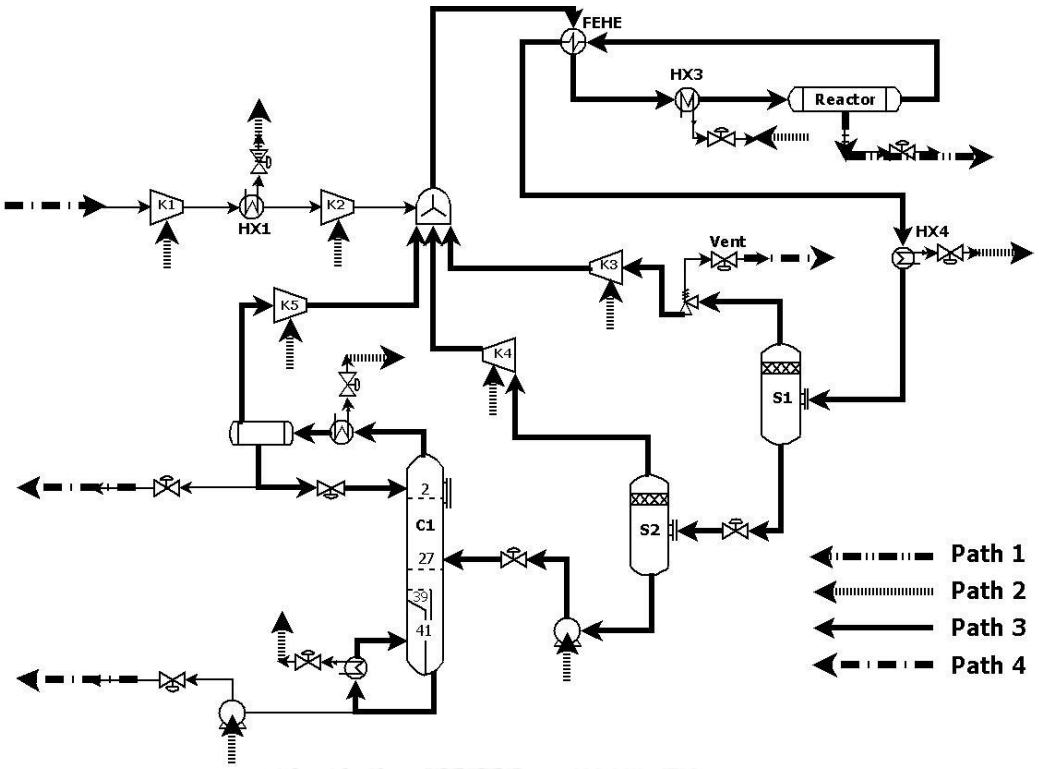


Figure 2 Heat pathways

2.3 Material pathway. The material pathways are useful to identify the material quantifier as discussed in Section 2.4. The material pathways are predicted in Table 5.

2.4 Material quantifier. The material quantifiers are useful to design control loops for component balance as discussed in Step 3. The quantifier is the place indicating the significant amounts of a chemical component in the plant as shown in Table 5 and the quantifiers are described with its handler as shown in Table 6.

The place indicating the significant amounts of methanol is level of C1 reflux drum. Similarly, the quantifier of H_2O is C1 bottoms level. The exit point of inert gases (CH_4 and N_2) is vent valve, so their quantifiers are CH_4 composition from top S1. The reactants (H_2, CO, and CO_2) are fed to the process together with CH_4, H_2O, and N_2. H_2 is excess and unreacted H2 is recycled. Fixing the combined flow of recycle streams and feed of several components will result in the combined stream with varying composition. Notice that CO and CO_2 are supposed to be consumed to extinction at the reactor. To regulate their amount is adjusting the reactor temperature by measuring their composition at the reactor outlet. The alternative is

increasing the vent flow. The quantifier for CO and CO_2 is their composition in the reactor effluent in the former case and S1 pressure in the latter case.

Notice that the quantifier of inert gases (CH_4 and N_2) and reactants (H_2, CO, and CO_2) are identified at the same place, which is the vapor stream from separator S1 because the vent flow rate is the only way to regulate the flow of exit material stream unless distillate and bottoms stream. A vent valve position is controlled from two signals; CH_4 composition and high pressure controller. CH_4 composition controller is normally set for keeping CH_4 composition. The rest of such components can accumulate and cause to high pressure in the system. When the pressure in the separator S1 rises more than the specified value, the controlled signal of CH_4 is replaced by the one of pressure from pressure override controller.

Table 5 Material pathways, Material quantifiers and Handles of each component

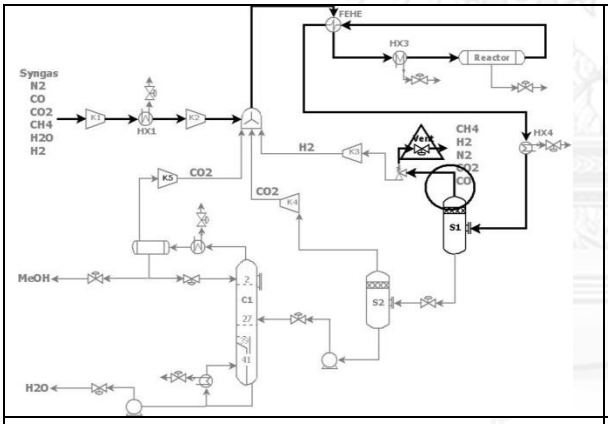
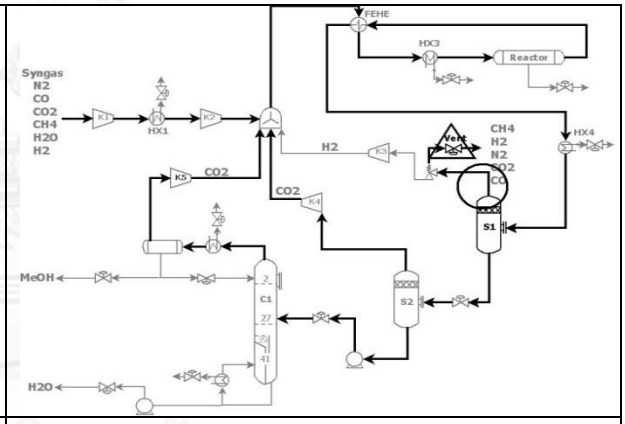
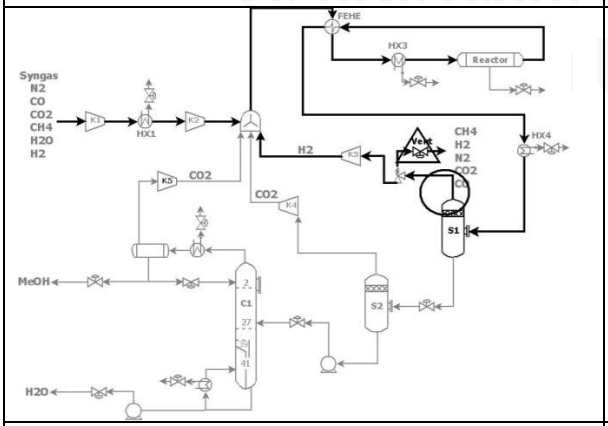
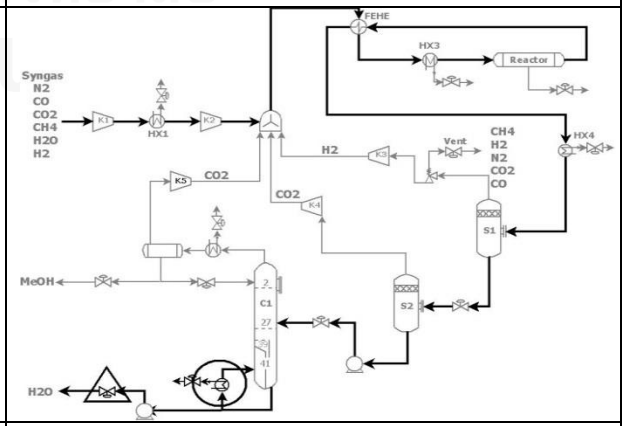
	
CO, CH_4, and N_2 pathway	CO_2 pathway
	
H_2 pathway	H_2O pathway

Table 5 Material pathways, Material quantifiers and Handles of each component (Continued)

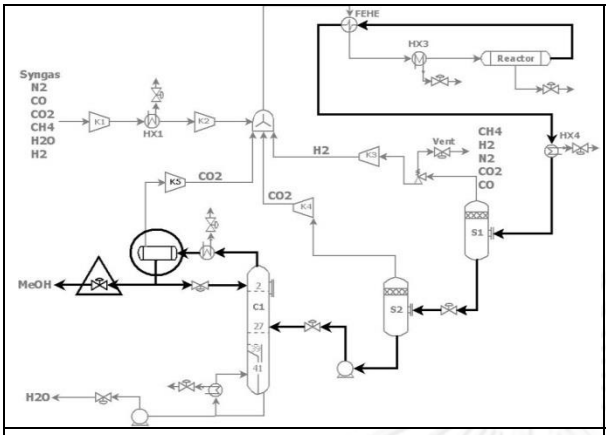
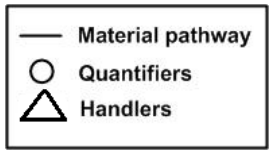
	
CH_3OH pathway	Legend

Table 6 Quantifiers and handlers of components

Component	Quantifier	Handler
CH_4	CH_4 composition from separator S1	Vent flow rate
CO, N_2, H_2, and CO_2	Pressure in separator S1	Vent flow rate
MeOH	C1 Reflux drum level	C1 Distillate flow rate
H_2O	C1 Reboiler level	C1 Bottoms flow rate

2.5 Reaction section. The kinetic information obtained from Luyben (2010) as mentioned above. The dominant controlled variable used to regulate the reaction yield is determined in this section. The kinetics are given by vanden Bussche and Froment by using the water-shift reaction:

$CO_2+3H_2 \leftrightarrow CH_3OH+H_2O$

$CO+H_2O \leftrightarrow CO_2+H_2$

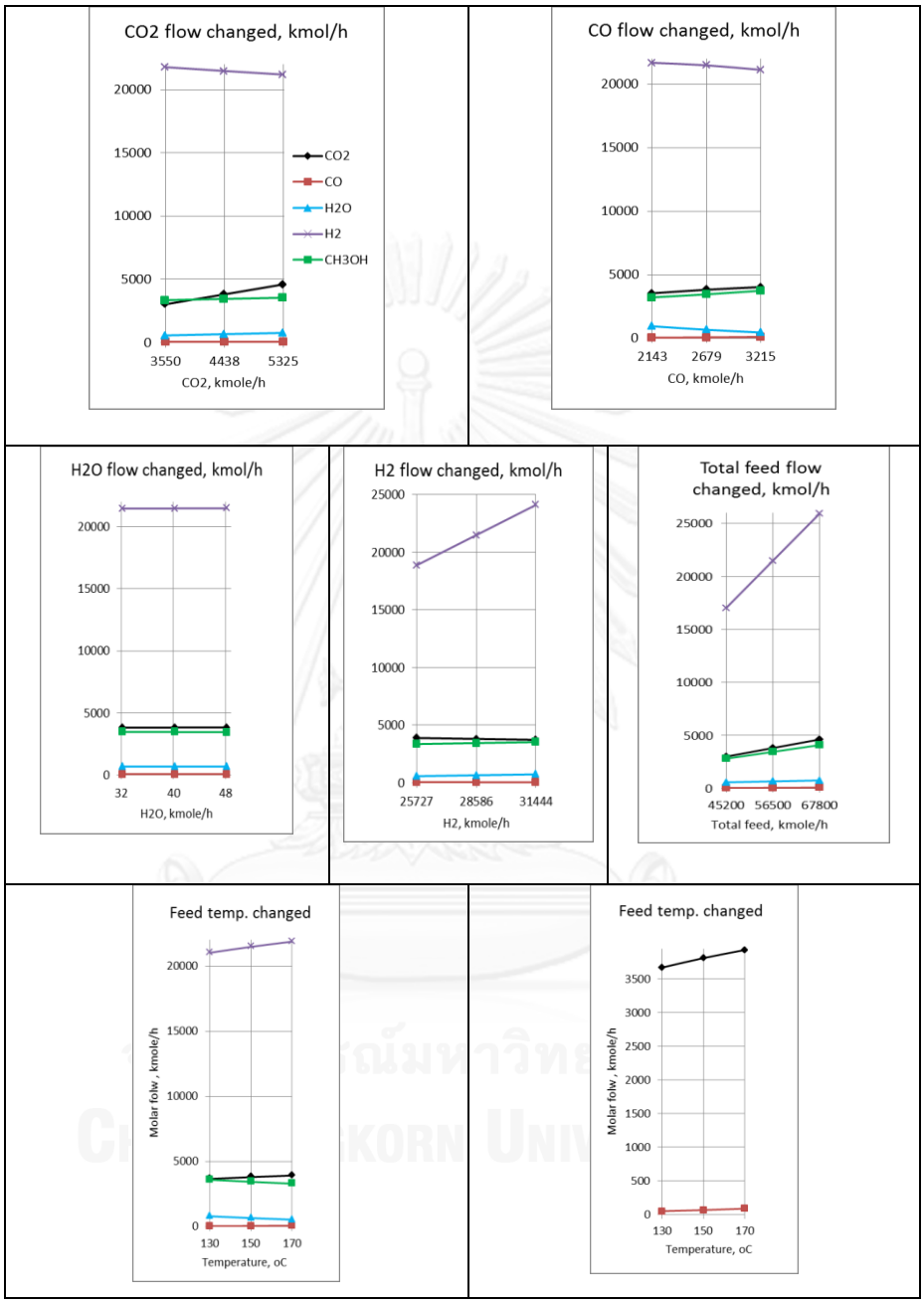
Figure 3 gives the results for the effects of changes in each component feed flow rate, total feed flow rates, and reactor inlet temperatures stream on the

changes in each component leaving the reactor. The vertical axis is component flow rate, leaving the reactor and the horizontal axis are each component feed flow rate, total feed flow rate, and temperature changed in the reactor inlet stream.

The simulation results show that water has negligible effects on methanol production rate. The methanol products increase for carbon dioxide, carbon monoxide, hydrogen, and total feed flow increase, so which one of them could be the dominant controlled variable such as the limiting reactant, carbon monoxide. However, the design constraints limit this strategy concerning increasing the reactant feed rate. That is, the synthesis gas feed containing all reactants as a single stream.

The methanol product increases as reactor inlet temperature decreases since the reactions are exothermic. In other words, to decrease the reactor temperature improves the conversion. Therefore, the dominant controlled variable should be the reactor temperature adjusted by manipulating the cooling rate. Moreover, the limiting reactants CO and CO2 change the same way as reactor temperature changes.

Figure 3 The components leaving the reactor outlet stream with input disturbances



2.6 Separation section analysis. The proper directions of material disturbances are analyzed and specified in this section. To begin with, the separator S1 separates the cooled reactor effluent into liquid and gas stream at 106.5 bar. The gas stream is rich in CH_4, N_2, H_2, and CO_2 while the liquid stream contains H_2O and CH_3OH. The minus disturbance of carbon dioxide and hydrogen (DCO_2^-, DH_2^-) should

be shifted to the top of S1 and their plus should be kept in the process. The plus and minus disturbance of the inert (CH_4 and N_2) should be directed to the top of S1. However, the plus disturbances of raw material and inert cannot be shifted to the bottoms liquid flow because the separator condition and their availability in the bottoms.

The minus disturbance of methanol product DMe^- should be shifted to the top of S1 to maintain its purity in the product stream. But this is not possible because the amount of methanol in S1 top stream is very small. DMe^+ should be directed to the bottoms S1 and this is possible. Since H_2O is heavier than methanol, its disturbance goes to the bottoms.

The desired and actual disturbance paths of the components for S2 are the same the ones as S1.

For the C1 column, since the top product is methanol, DMe^+ goes to the top. To maintain the product purity, DMe^- of 270.59 kmole/h should go to the bottoms, but the bottoms availability is 0.0759 kmole/h; hence, this is not possible. Figure 4 and Table 7 shows the actual disturbance paths.

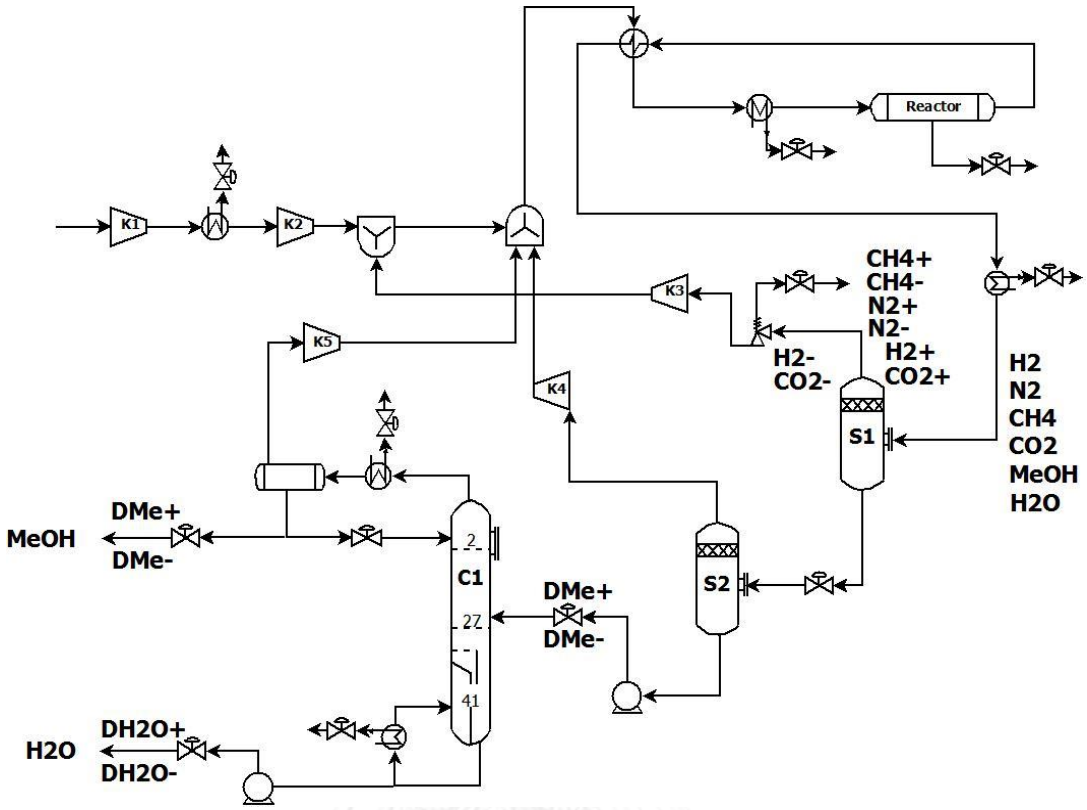


Figure 4 The directions of material disturbances predetermined

Table 7 Plus and minus disturbances shifting direction

Separation Unit	Top	Bottoms
S1	DCO_2^+, DCO_2^-, DH_2^+, DH_2^-, DCH_4^+, DCH_4^-, DN_2^+, DN_2^-	-
S2	-	DMe^+, DMe^-
C1	DMe^+, DMe^-	DH_2O^+, DH_2O^-

Selecting Temperature/Composition Control Tray Location. To select the temperature control tray location of C1, the tray sensitivities to important disturbances are performed. The important disturbances are feed changes in total flow, composition, component flow, and temperature. To select a tray where there are significant changes in temperature from tray to tray while keeping reboiler duty and reflux flow or reflux ratio fixed. This test is done in a series of steady-state

simulations. The most sensitive tray of column C1 is 39 as shown in Figure 5 and Figure 6.

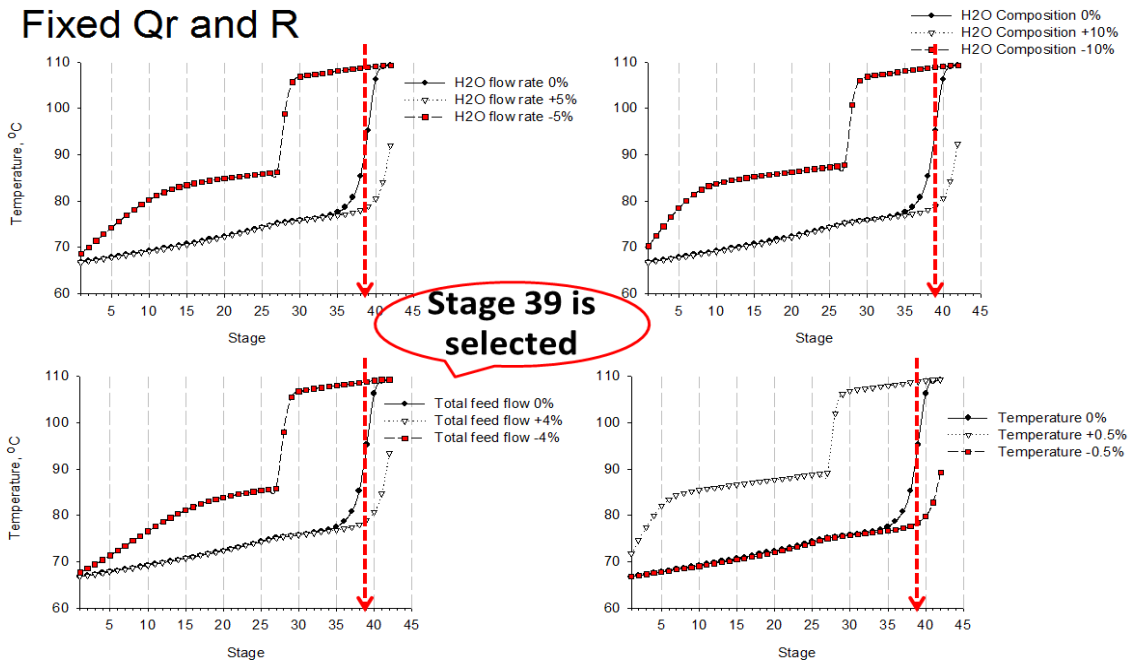


Figure 5 Selecting temperature control tray location by keeping the reboiler heat duty (Qr) and reflux flow (R)

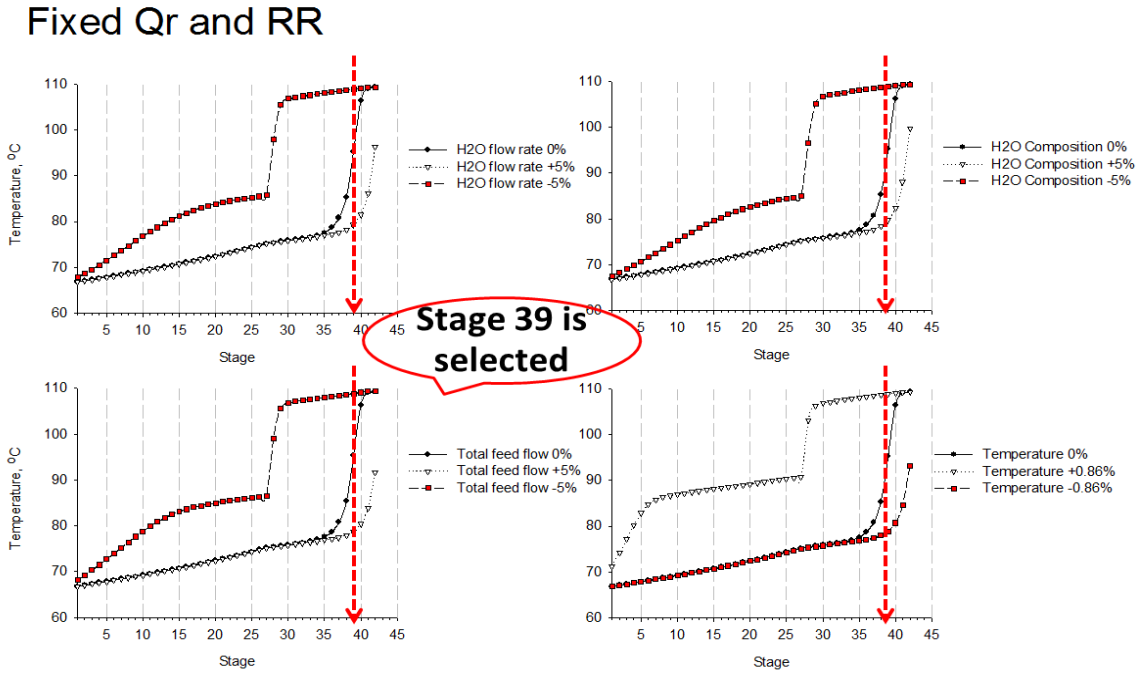


Figure 6 Selecting temperature control tray location by keeping the reboiler heat duty (Qr) and reflux ratio (RR)

2.7 Production rate control. The production rate control is set at the synthesis gas feed control loop as on-supply mode and set at the product flow control loop as on-demand mode.

Mode of operation. The modes of operation considered are on-supply and on-demand. For on-demand control, its choices of manipulated variables in inventory control in the main path, relying on the basic layout of the inventory control presented by Price and Georgakis (1994), are incoming flows, which is opposite to on-supply control. The dynamic performance results are presented in Section 5.2.

Stage 2. Fixture Plant and Disturbance Management.

Step 3: Establish fixture plant. Creating material balances in an entire plant by controlling each component at its quantifier.

3.1 Keep the materials entered and reentered fixed. Since the composition of feed stream differs considerably from the composition of the recycle streams, the gas feed stream containing all reactants is fixed flow. The two recycle streams are flow controlled by manipulating works to compressor K4 and K5, which recycle the gas back to the reactor. For control loop at K3, the controller of recycle flow from separator S1 to synthesis gas feed ratio is considered and its setpoint will come from output signal of vent controller so that the recycle flow can be adjusted along the changes of production or throughput rate and vent flow accordingly. The compressor K4 may also be used to be manipulator in pressure controller because such a recycle stream is the gas phase.

3.2 Adjust the flow of exit material streams. Product methanol leaving the process is adjusted by manipulating the distillate flow rate, according to the level of C1 reflux drum, its quantifier. Similarly, H2O flow rate is adjusted by C1 bottoms level, its quantifier. The quantifier of CH_4 is its amount at S1 vent. Therefore, CH4 is regulated by vent valve.

3.3 Handling the material that is not leaving the process. There is no component not leaving the process.

3.4 Control the amount of the rest of the component at their quantifiers. The rest of the components are N_2, CO, CO_2, and H_2 which are circulated through the process and they are not leaving the process under normal circumstance (except some of them leaving the process accompanying CH4 through the vent valve). However, regulating their amounts by adjusting the reactor temperature is complicated, if not implausible. If any of them is accumulated in the process, the system pressure will increase. Hence, their amount is measured at S1 and adjusted via pressure override controller.

3.5 Maintain the production rate. The production rate is maintained by measuring the reactor outlet temperature and manipulating the reactor temperature by adjusting the heat removal rate or cooling rate. The control structure obtained in this step is shown in Figure 7.

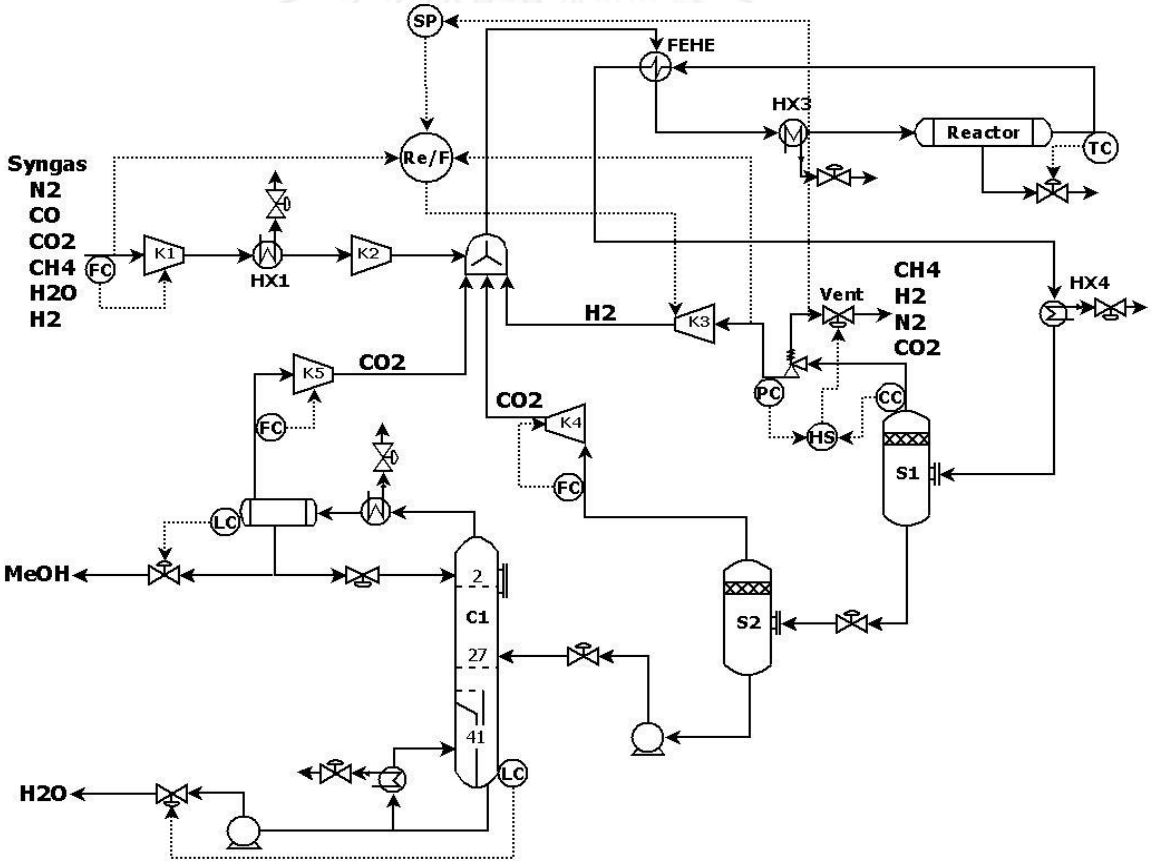


Figure 7 The control structure obtained in step 3

Step 4: Disturbance management for quality control.

4.1 Heat disturbance management. According to the analysis made in Step 2.2, the temperatures of the stream going into the compressor K2, the stream entering the reactor and the stream leaving the reactor must be maintained by shifting the heat disturbances to the environment.

4.1.1 The temperature of the stream going into the compressor K2 is controlled by manipulating heat removal in the cooler HX1. The temperature of the stream entering the reactor is controlled by manipulating the reactor preheater duty HX3. The temperature of the stream entering S1 is controlled by manipulating the heat removal in the cooler HX4.

4.1.2 The column temperature at tray 39 is controlled by manipulating the heat input in reboiler.

4.2 Material disturbance management. Several disturbance tests are made to identify control structure to achieve the desired material disturbance shifting directions. Four single temperature control structures of column C1 as shown in Figure 8, namely R, R/D, R/F, and R/(R+D) are tested to select which one of them that is suitable to the desired disturbance propagation schemes as discussed in section 2.6.

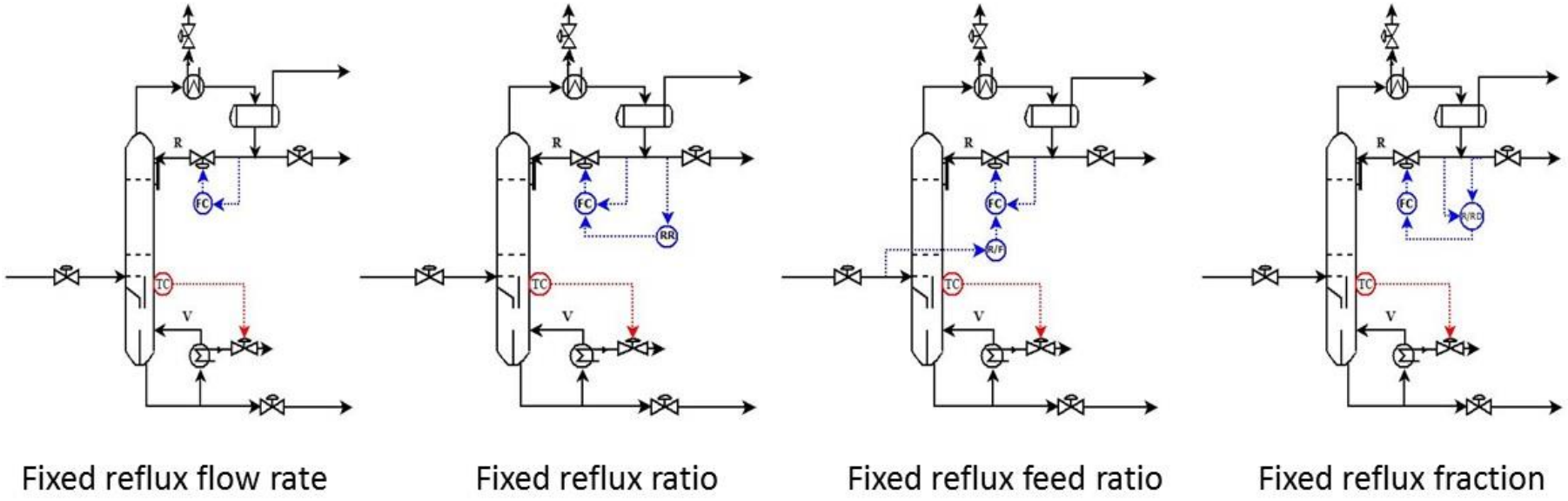


Figure 8 Four single temperature control structures of column C1

To examine this problem, the effects of changes in feed component flows on each prospect distillation control structure are made in a series of steady-state simulations. The disturbances must be directed to the desired pathways. Table 8 gives the results from analyzing the material disturbances of water and methanol in a distillation column. The values in parentheses are differential molar flow rate.

The water flow rate in the bottoms of all control structures increases for increases in water feed flow rate and decrease for decreases in the water feed flow rate since the water is a heavy key which must be shifted to the bottoms. The methanol flow rate in distillate of all control structures increases for increases in the methanol feed flow rate and decrease for decreases in the methanol feed flow rate as well. From the results, all of control structures are possible to be chosen to handle component feed flow rate disturbances because differential molar flow rates in each prospect distillation control structure are not quite different. Hence, the column dynamic simulation runs are made to find out desired control structures.

Table 8 Plus and minus disturbances shifting test results for water and methanol in distillation column

Distillation column	Product stream	R	RR	R/F	R/(R+D)
C1	Distillate	DMe^+ (+271.51) DMe^- (-271.52)	DMe^+ (+271.48) DMe^- (-271.49)	DMe^+ (+271.48) DMe^- (-271.50)	DMe^+ (+271.48) DMe^- (-271.49)
	Bottoms	DH_2O^+ (+58.45) DH_2O^- (-58.47)	DH_2O^+ (+58.44) DH_2O^- (-58.48)	DH_2O^+ (+58.96) DH_2O^- (-58.96)	DH_2O^+ (+58.45) DH_2O^- (-58.48)

Dynamic simulation tests of four disturbances of feed rate, feed temperature, feed composition and feed component flow on each control structure are shown in Figure 9-Figure 13. The distillate rate, product quality, and reboiler duty are the key performance indices.

Figure 9 Column dynamic results for ±5% changes of methanol column feed flow

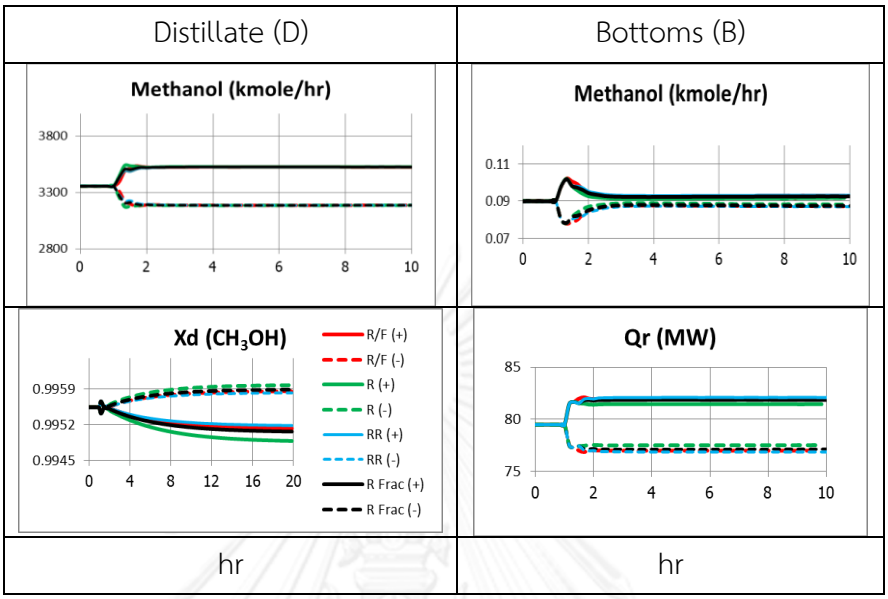


Figure 9 gives results for ±5% changes of the component flow rate of methanol. Notice that the methanol flow rate in the distillate (D) increases and decreases for increases and decreases in the methanol feed flow rate, respectively. Meanwhile, the methanol flow rate in bottoms (B) is very low and quite unchanged. In other words, the plus and minus disturbances of methanol are shifted to the top of column C1.

To change with methanol feed flow, only if plus disturbance of all structures gives the desired methanol disturbance shifting whereas minus disturbance gives no structures due to limit in the column design and the availability of methanol in bottoms. However, the RR and R/F structures give the best performance in maintaining methanol composition in distillate close to the specified values.

Figure 10 Column dynamic results for ±10% changes of water column feed flow

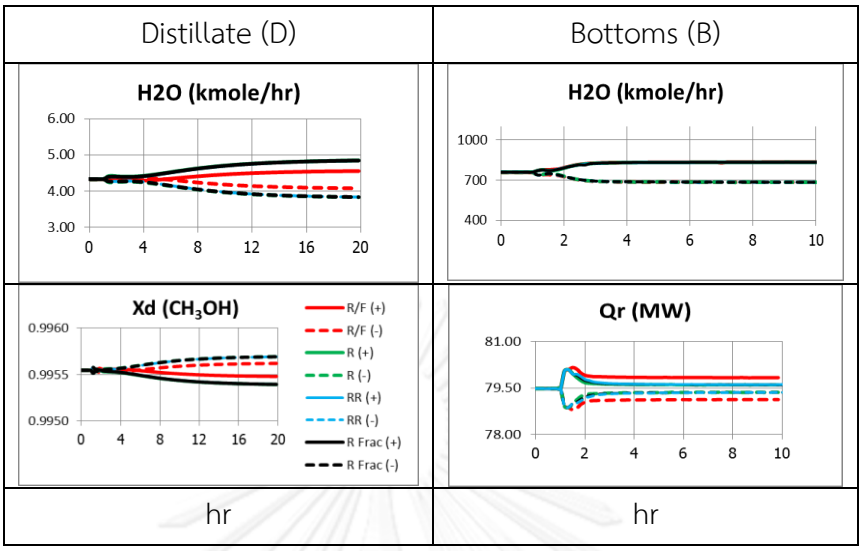


Figure 10 gives results for ±10% changes of the component flow rate of water. Notice that the water flow rate in bottoms (B) increases and decreases for increases and decreases in the water feed flow rate, respectively. Meanwhile, the water flow rate in distillate (D) is low and less changed. That is, the plus and minus disturbances of water are shifted to the bottoms of column C1.

For change in water feed flow, all structures yield the desired water disturbance shifting. The R/F structure is the best candidate in maintaining methanol composition in distillate. However, to achieve the best candidate, the R/F structure utilizes more reboiler duty.

Figure 11 Column dynamic results for ±5% changes of total flow in column feed

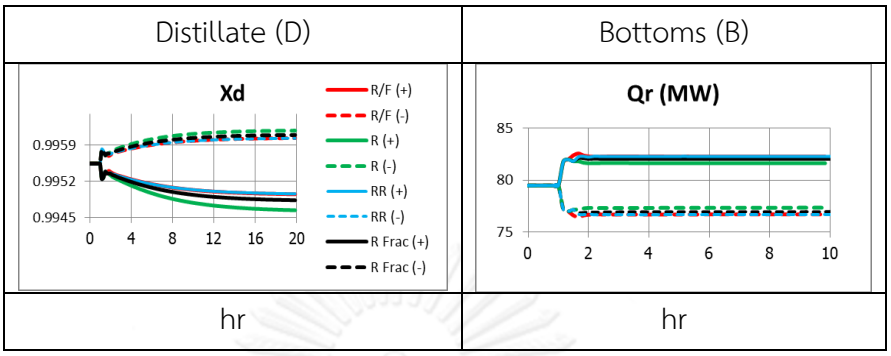


Figure 11 gives results for ±5% changes of the total flow in column feed. The desired performance is maintaining methanol composition in distillate and less utilizing reboiler duty, the RR and R/F structures are the best in term of maintaining product composition while are the worst in term of utilizing energy.

Figure 12 Column dynamic results for ±2 mole % methanol changes in column feed

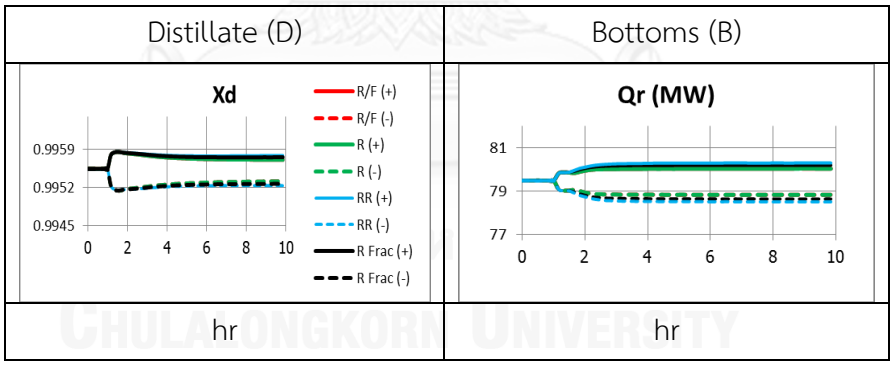


Figure 12 gives results for ±2 mole % methanol changes. All structures yield about the same methanol composition in distillate, while the R structure obviously uses less reboiler duty.

Figure 13 Column dynamic results for ±4 oC changes in column feed

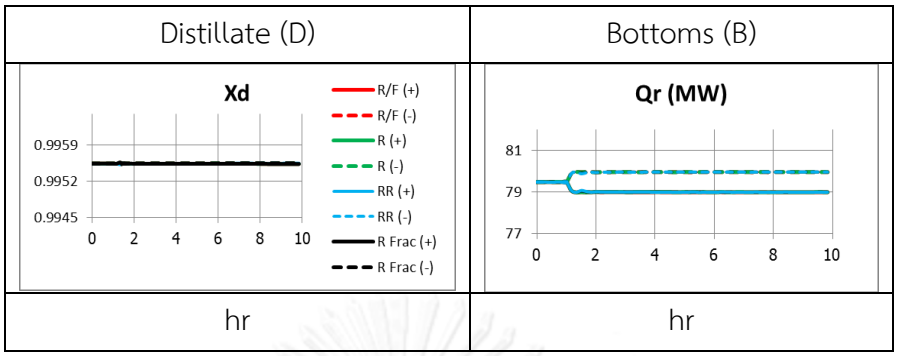


Figure 13 gives results for ±4°C changes in column feed. All structures compensate the disturbance well enough using about the same reboiler duty, so the product composition is well maintained.

From all of the performance results mentioned above, the control structures that are possible to be chosen to handle material disturbances in the column are RR and R/F control structures because of giving the best performance results for all cases. The control structures obtained in this step are shown in Figure 14 and Figure 15.

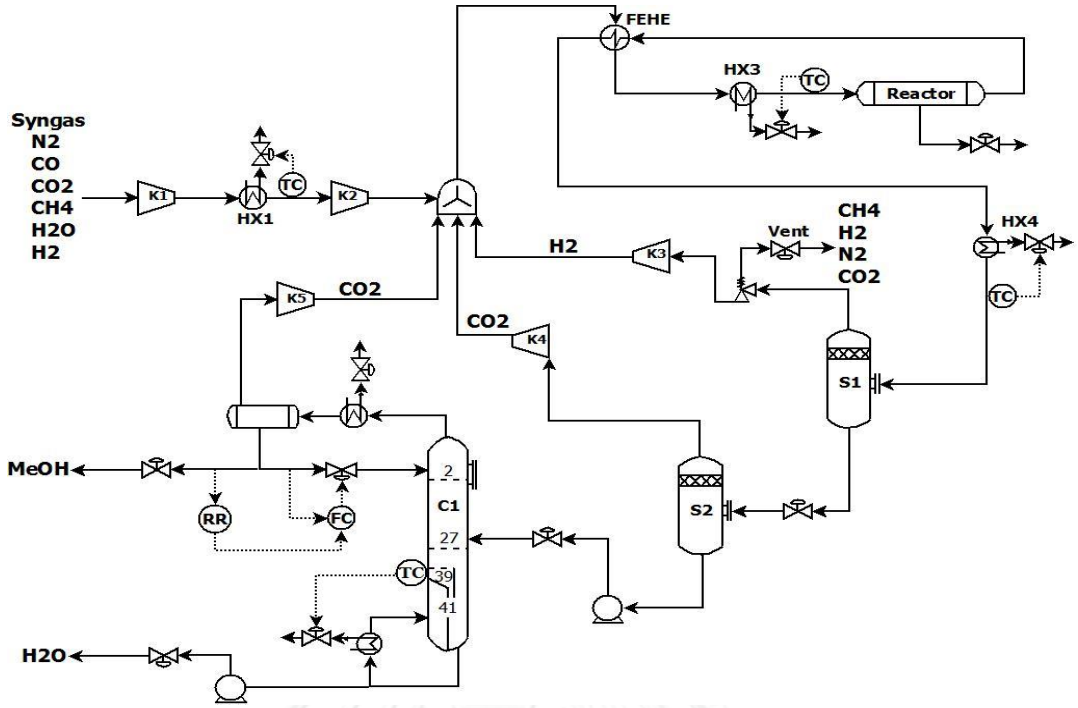


Figure 14 The control structure obtained in step 4 with RR column control structure

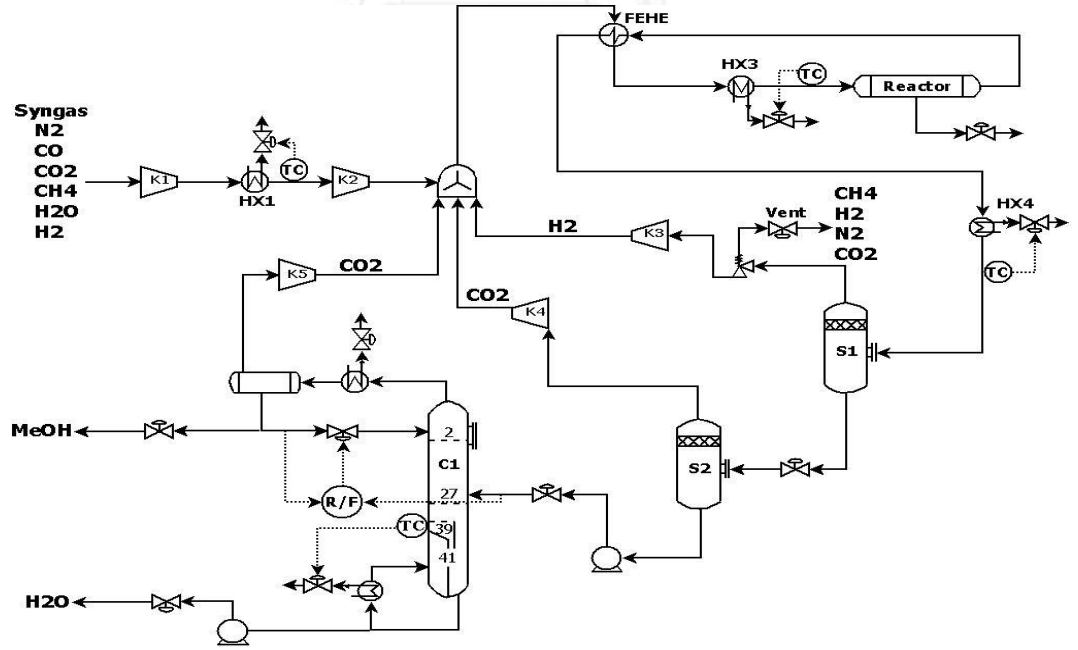


Figure 15 The control structure obtained in step 4 with R/F column control structure

Stage 3. Unit Level Design.

Step 5: Design the rest of the control loops.

5.1 The units to be considered in this step are compressor K2, separators S1 and S2, and column C1. The pressure of a stream going into the compressor K2 and the pressure of condenser in the C1 column are controlled by manipulating the compressor work K2 and cooling rate, respectively. The liquid levels in the separators S1 and S2 are controlled by manipulating the liquid flow rates leaving its bottoms. The control structure obtained in this step is shown in Figure 16.

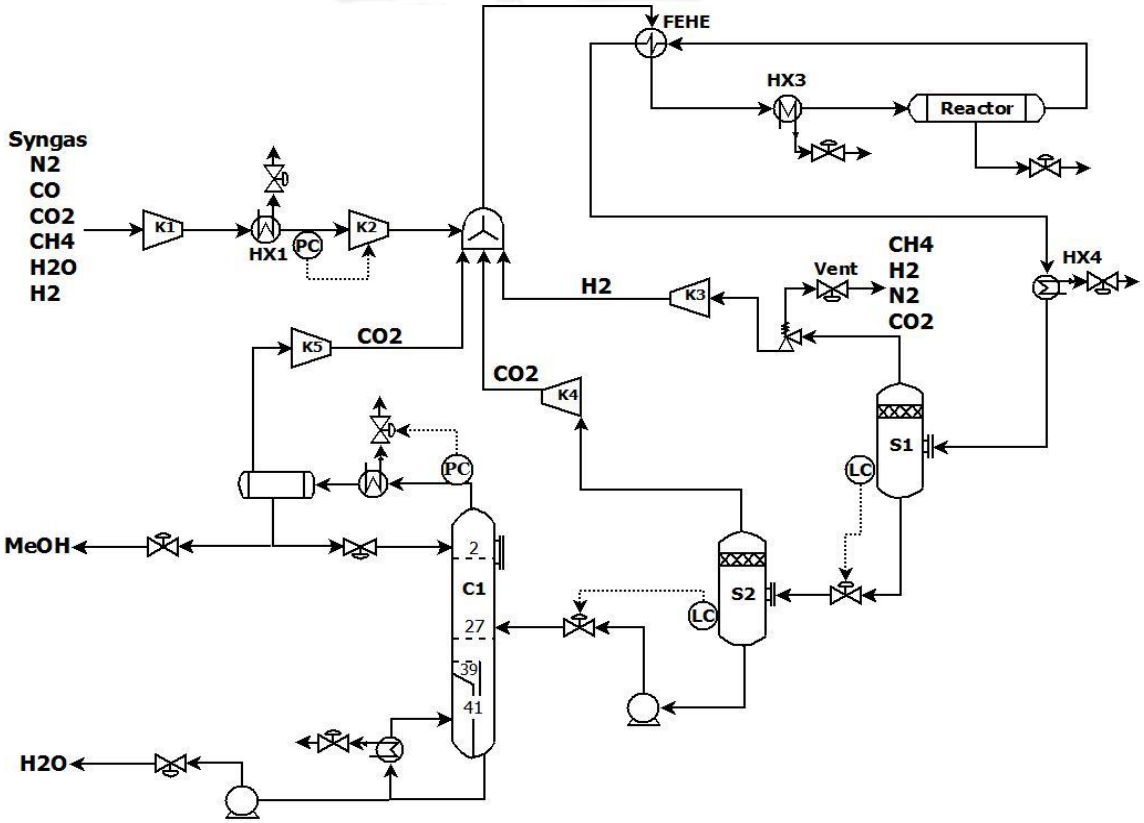


Figure 16 The control structure obtained in step 5.1

Stage 4. Energy Management and Optimization.

The supplementary design is considered in this step.

Step 7: Optimize economics or improve control performance. The design of a methanol process is altered by removing the reactor preheater HX3 and adding the heat transfer area of 2906 m^2 in feed-effluent heat exchanger (FEHE). The reactor inlet temperature is regulated by measuring and bypassing (10% flow rate) on the cold stream, i.e., reactor inlet stream. The control structure obtained in this step is shown in Figure 17.

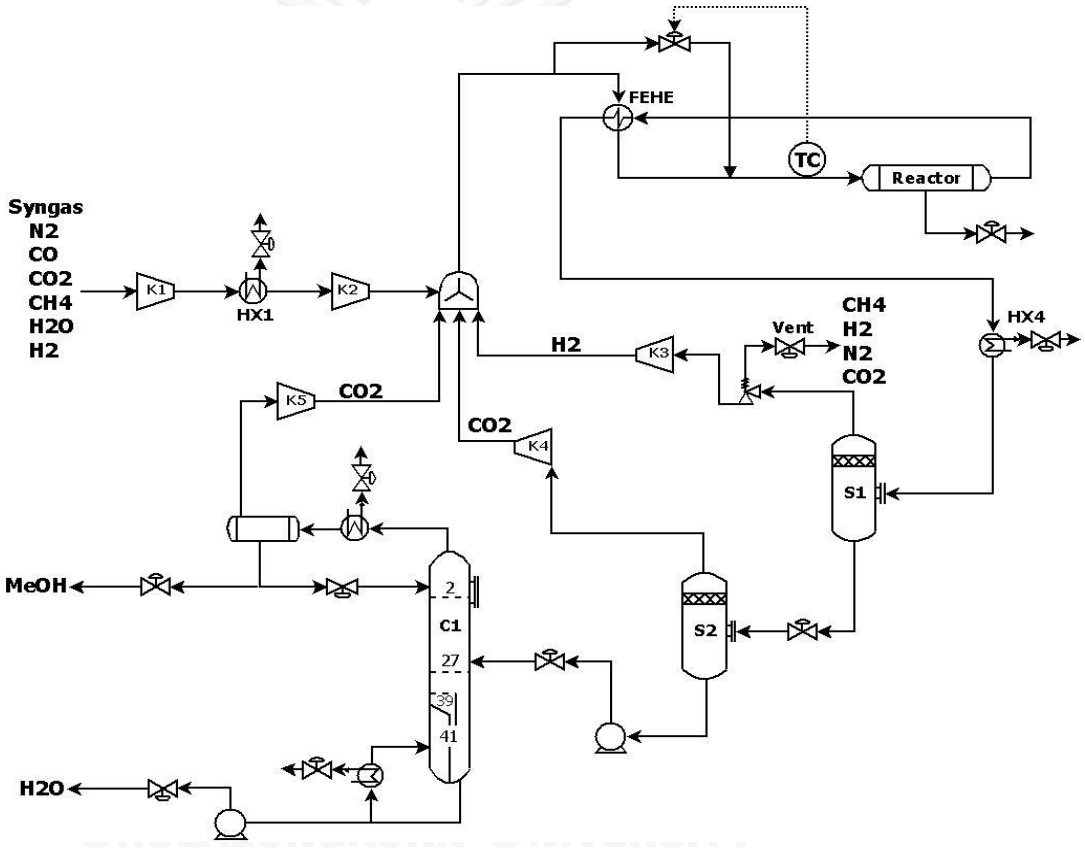


Figure 17 The control structure obtained in Step 7

Stage 5. Design Validation.

Step 8: Validate the designed control structures by rigorous dynamic simulation via HYSYS process simulation software. The changes of synthesis gas feed flow rate (production rate) and the disturbance of synthesis gas composition (inert gas methane) are made to test the performance of the plantwide control structures designed (CS1 and CS2). The control structure designed by Luyben (2010)

(CS0) is also tested in comparison. The three control structures shown in Figure 18, Figure 19, and Figure 20.

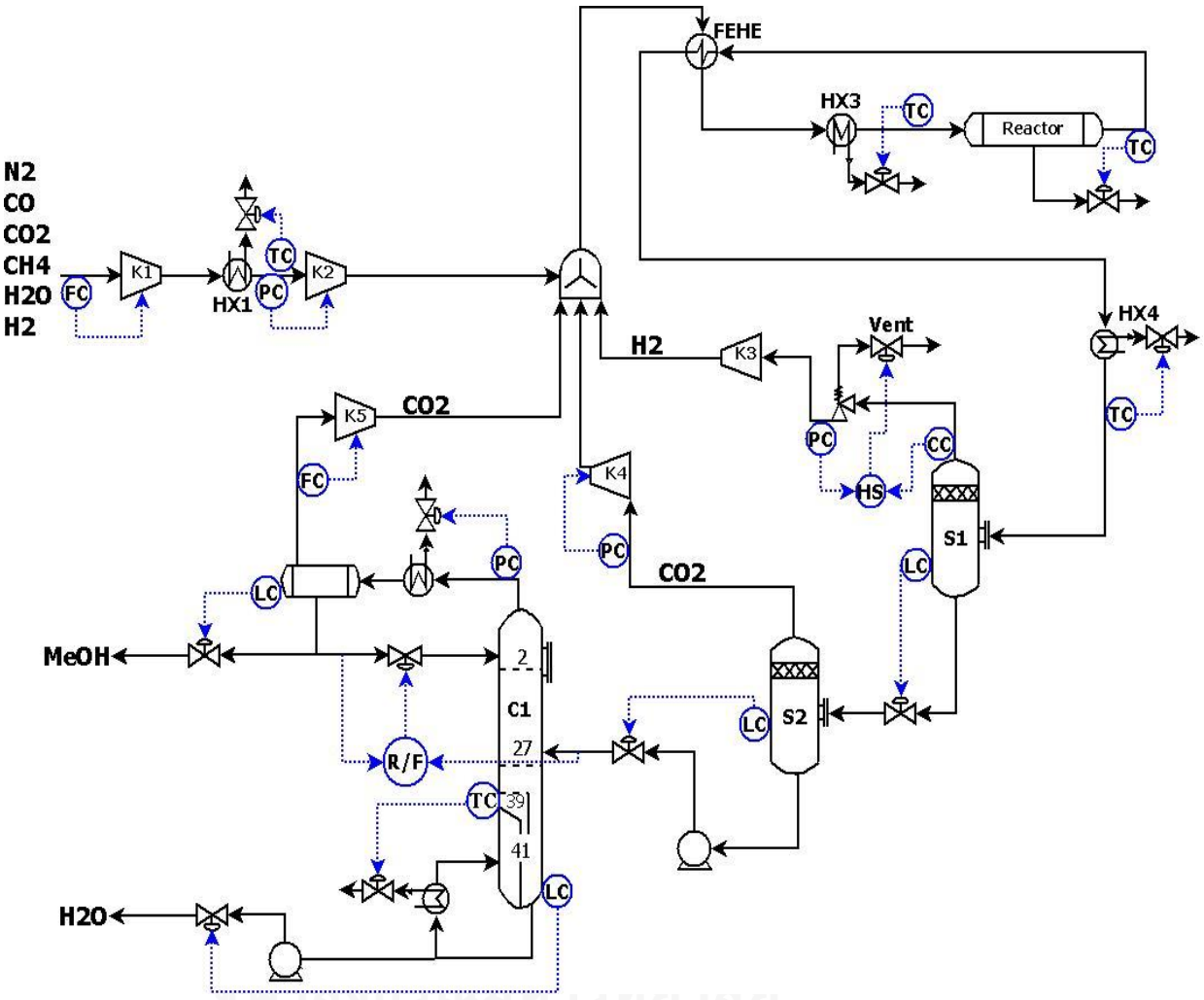


Figure 18 Luyben's control structure (CS0)

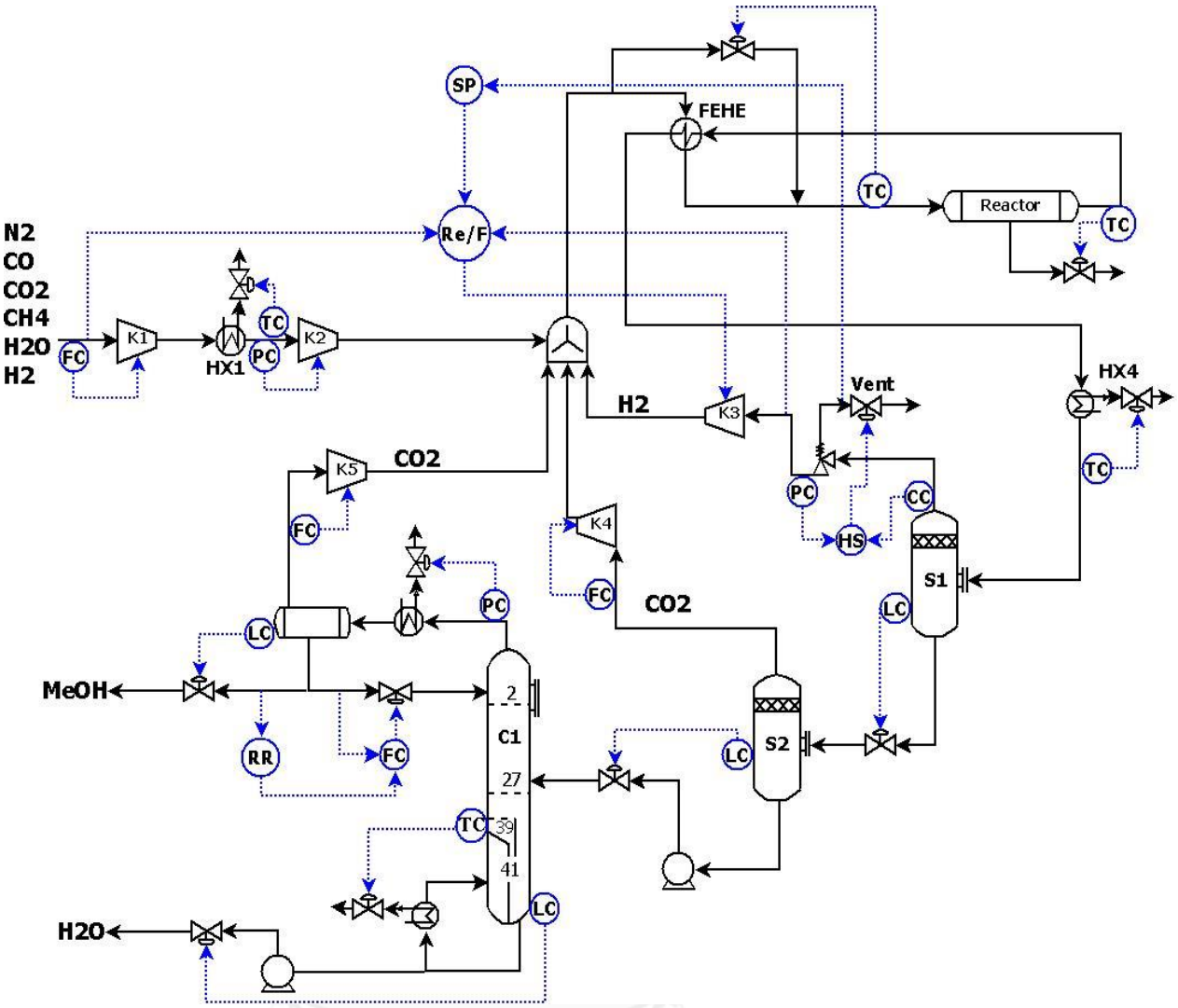


Figure 19 New control structure 1 (CS1)

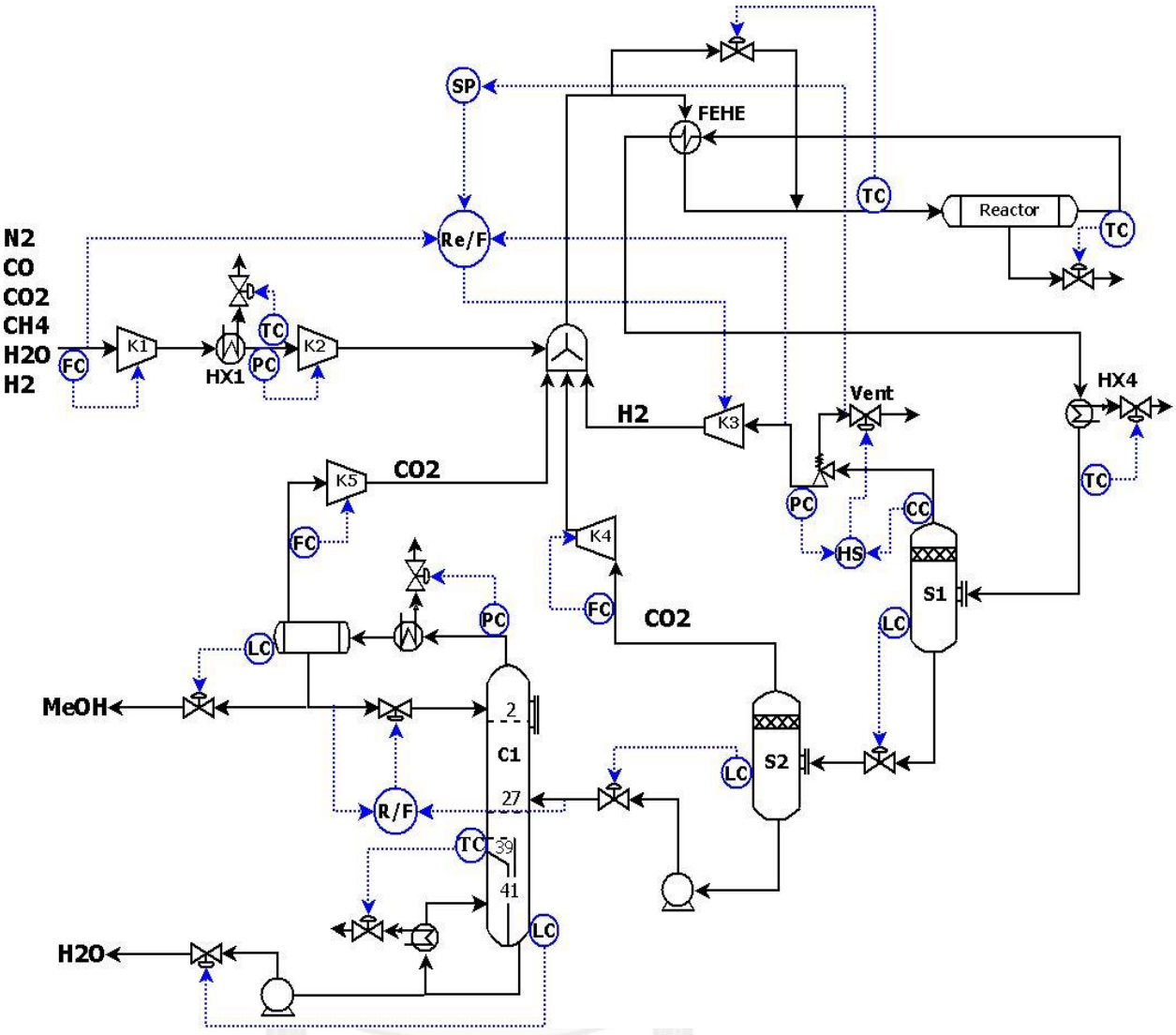


Figure 20 New control structure 2 (CS2)

5.1 Dynamic Performance Results and Discussions

Figure 21 ±10% changes in the set point of the synthesis gas flow controller for CS0 and CS1

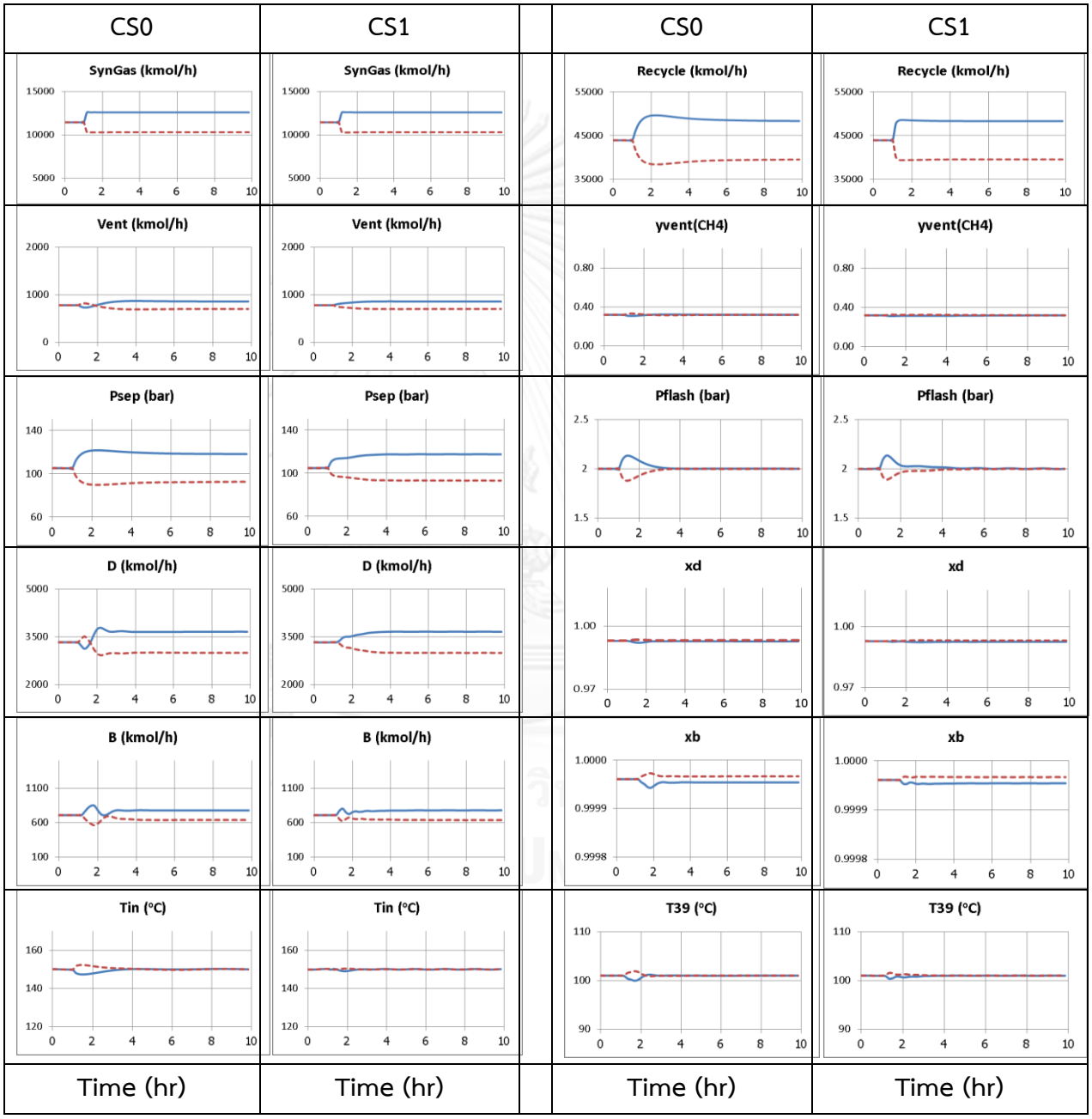
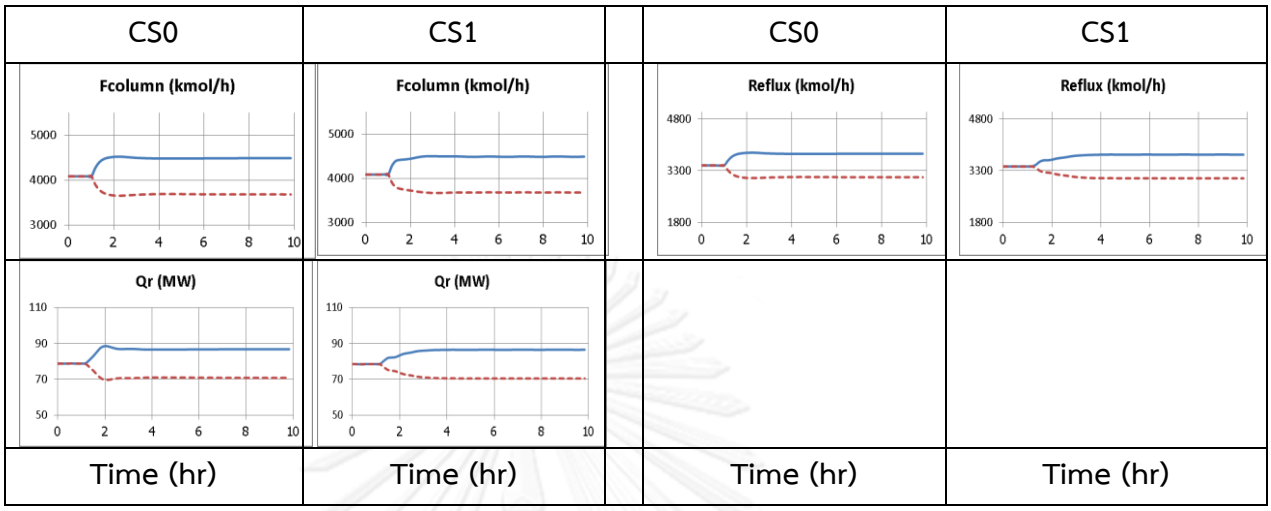


Figure 22 ±10% changes in the set point of the synthesis gas flow controller for CS0 and CS1 (Continued)



Production Rate Change. Figure 21 and 22 give results for ±10% changes in the set point of the synthesis gas flow controller at 1 hr. The solid lines are 10% increases; the dashed lines are 10% decreases.

Recycle flow rate of CS0 and CS1 changes about the same way as total feed increases and decreases; however, the response of CS1 is smoother than that of CS0 because of recycle to feed ratio control. Because of this, there is well initial response in the vent flow rate of CS1. The methane composition (yvent) of both control structures is well kept at its setpoint. The pressure in the separator S1 (Psep) indicating the pressure in the system is not controlled, so the pressure increases and decreases to a new level as total feed changes. The pressure in flash separator S2 (Pflash) is well controlled. Because of more reactants, distillate (D), bottoms (B), and column feed flow rates increase. The reactor inlet temperature (Tin) and the stage 39 temperature (T39) are well controlled by manipulating the heat input to reactor preheater and reboiler (Qr), respectively. Reflux flow rate changes as total feed changes so as to keep the reflux to column feed R/F of CS0 and the reflux ratio RR of CS1 constant. The methanol composition in distillate (xd) and the water composition in bottoms (xb) are quite close their setpoint. Notice that the dynamic results of the most cases for CS1 provide better performance in initial response since aftereffect of establishing recycle to feed ratio leads to have stability in recycle and

vent streams. In addition, altering plant process by removing the reactor preheater HX3 and adding heat transfer areas in FEHE for maintaining reactor inlet temperature gives lower cost as shown in Table C. 5 of appendix C.

Methane Impurity Change. Figure 23 gives results for changes of the methane impurity in synthesis gas feed at 1hr. The solid lines are the methane composition increases from 2.17 to 3.17 mole % and decreases in the hydrogen composition from 67.46 to 66.46 mole %. The dashed lines are the methane composition decreases from 2.17 to 1.17 mole % and increases in the hydrogen composition from 67.46 to 68.46 mole %.

In case of increasing methane composition in the synthesis gas feed, there is a substantial increase in the vent flow rate to maintain the level of CH4. Consequently, the recycle flow of CS0 decreases significantly. This means that the reactor inlet flow is disturbed accordingly. For CS1 the reactor inlet flow is disturbed less than that of CS0 by the recycle flow to feed ratio control. In conjunction, the pressure in Psep of CS1 drops more than that of CS0. The vent flow rate of CS1 rises up to almost the same new steady-state level and CH4 composition of CS1 is slightly higher than that of CS0. Therefore, the CS1 reactants loss is slightly lesser than that of CS0. The pressure in Pflash of CS1 is settled quicker.

Consequently, the distillate feed flow is better maintained for CS1. This brings about holding product purities closer to their specifications for CS1.

In case of decreasing methane composition in the synthesis gas, the vent flow rate decreases in order to maintain the methane composition. The recycle flow rate of CS1 increases less than that of CS0 due to the recycle flow to feed ratio control. Hence, the new steady state vent flow rate of CS1 is slightly higher than that of CS0. As the pressure in Psep reaches 120 bar, the override controller takes over the vent valve and removes gas from the system for both structures. More methanol D and water B are produced because there are lesser losses of reactants. As a result of establishing a fixture plant and executing disturbance management using the new design procedure, the responses in Tin, T39, Qr, xd, xb, column feed flow rate, and column reflux flow rate of CS1 are held closer to their specifications. Notice that the

production rate D of CS0 is slightly higher than that of CS1 (about 0.57 %) due to higher recycle flow (about 13.59 %).

Because the control structure of CS1 and CS2 is only different in column C1 and the amount of methane in column C1 is very small, the dynamic performance results of CS2 are similar to the ones of CS1 for all input disturbances as shown in Figure 24 and 25. In other words, the new control structures (CS1 and CS2) are possible to satisfy the dynamic performances.

Figure 23 Methane impurity changes in synthesis gas feed for CS0 and CS1

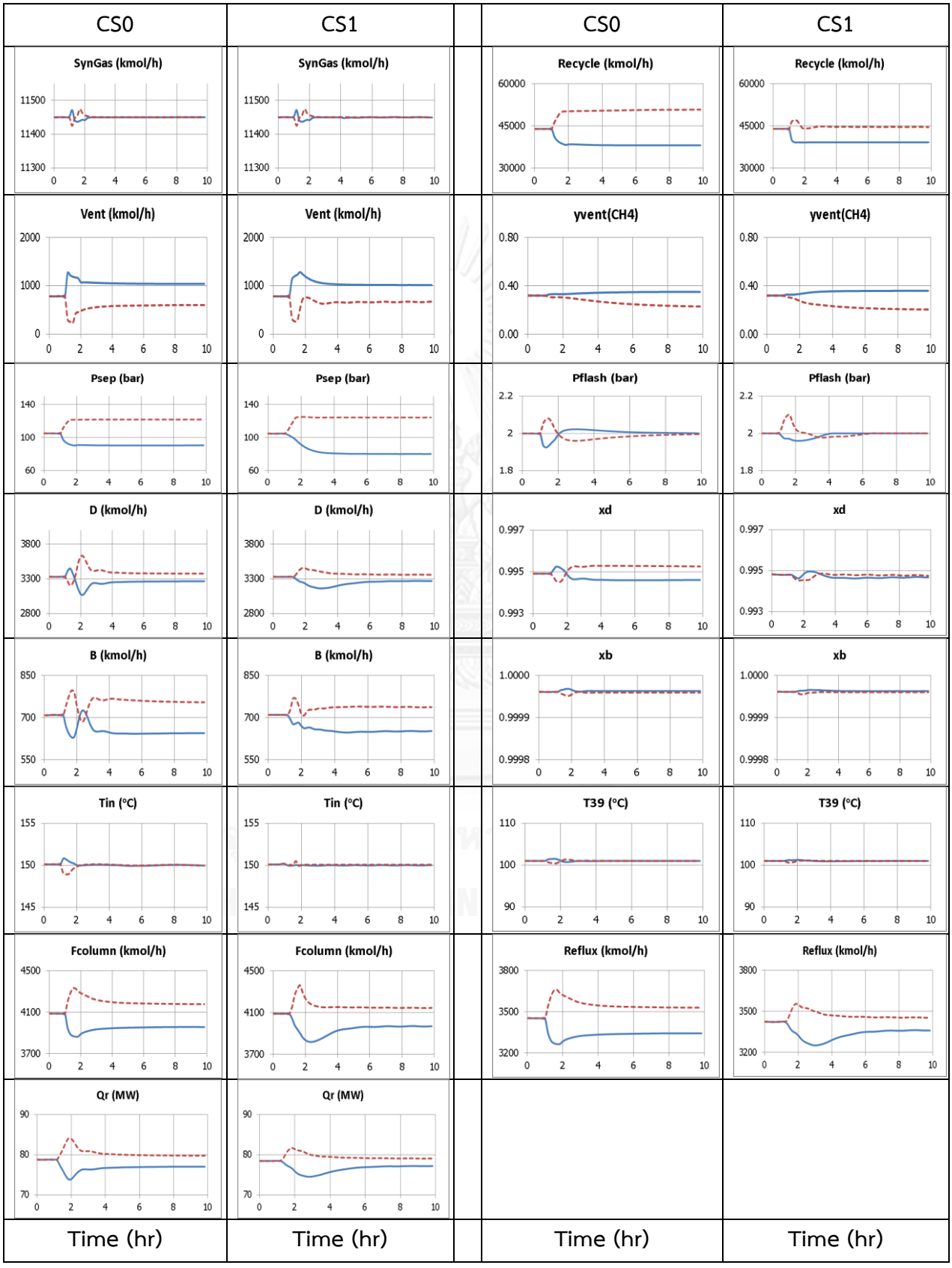


Figure 24 ±10% changes in the set point of the synthesis gas flow controller for CS0 and CS2

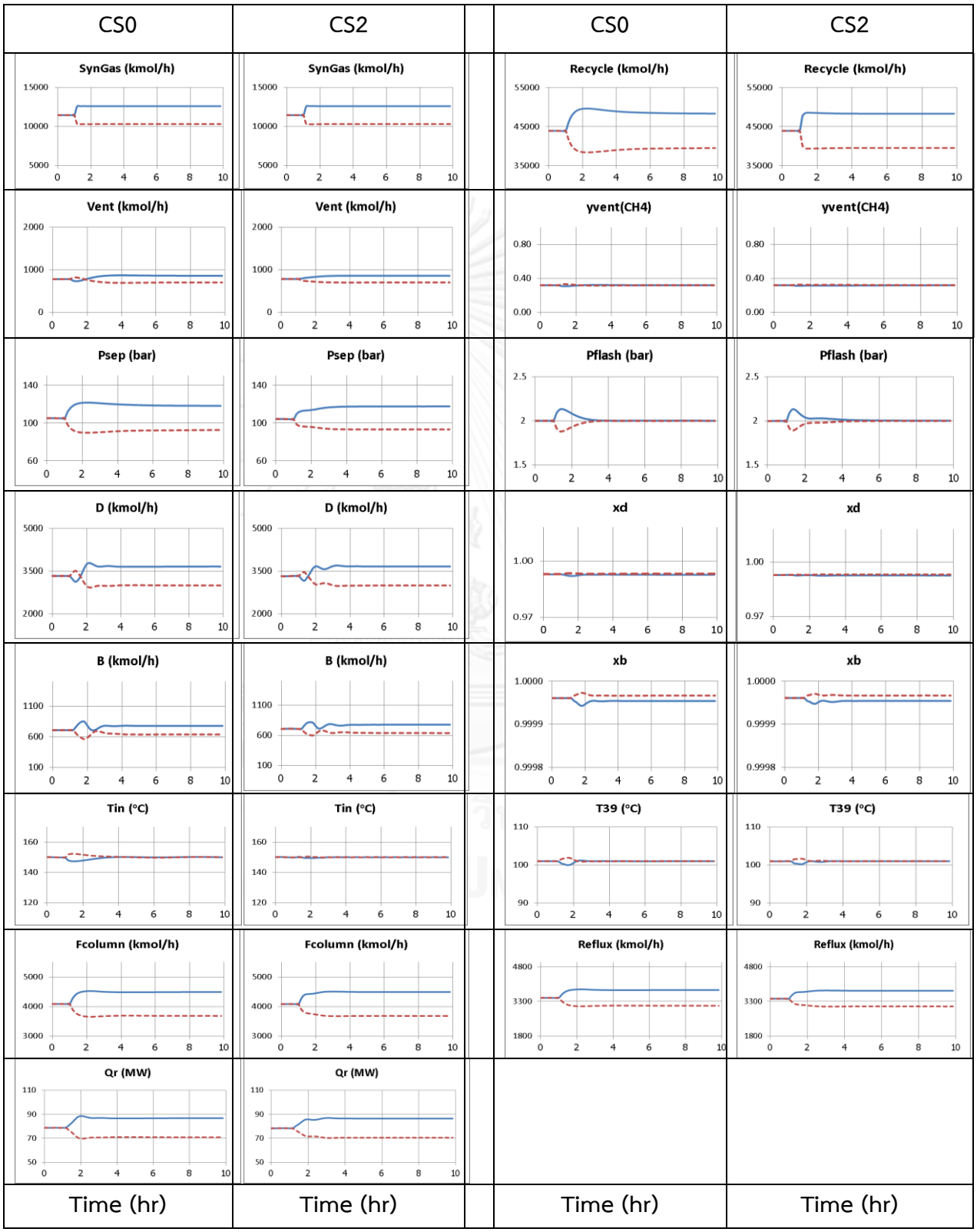
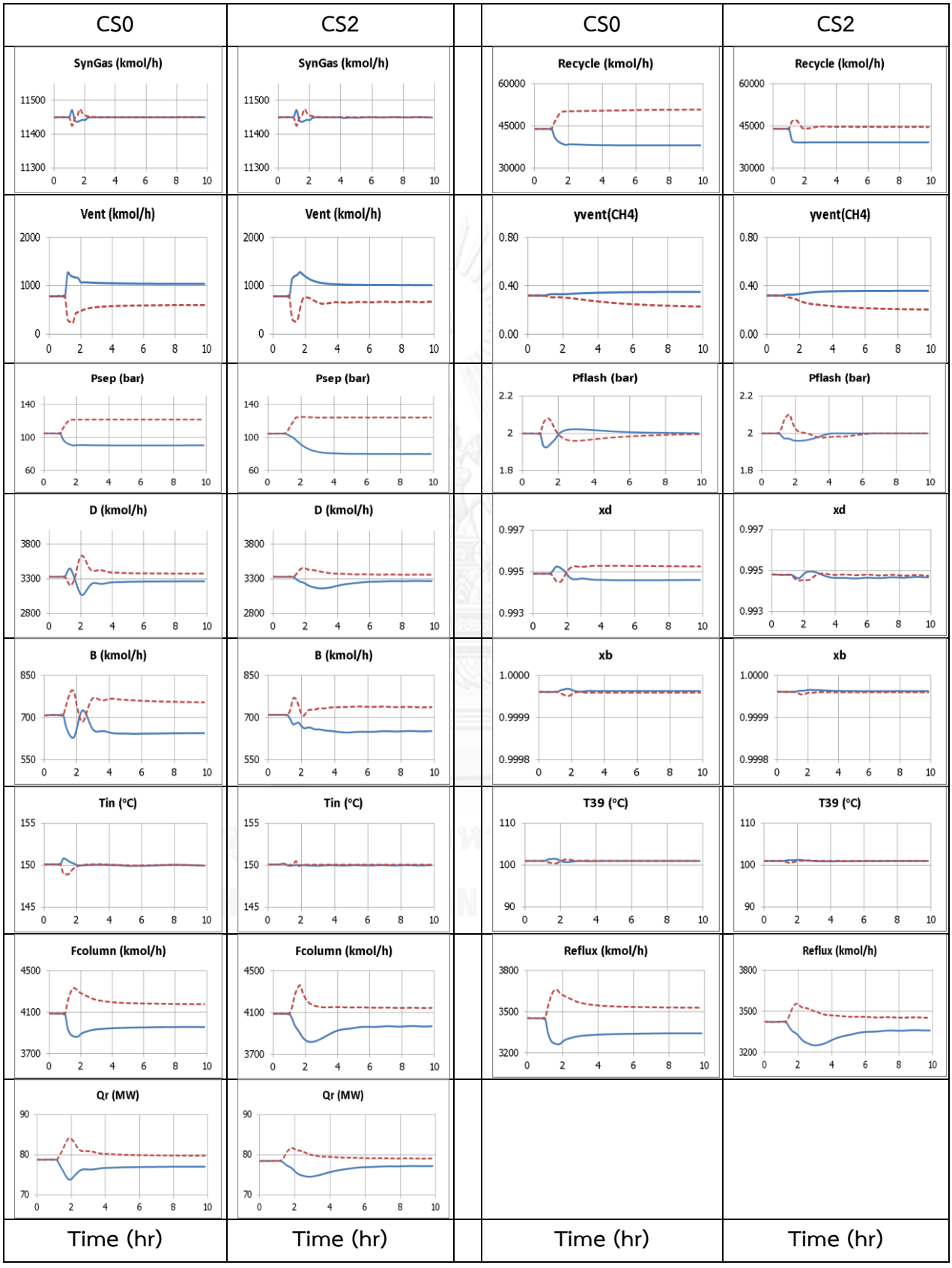


Figure 25 Methane impurity changes in synthesis gas feed for CS0 and CS2



On-demand Structure. The design of the plantwide control structure for on-demand mode using Wongsri's procedure while keeping the inventory flow control in logical order. The performance of both on-supply and on-demand structures in face of changes in synthesis gas feed and methanol product rate of about 5%. Figure 26 shows the performance on several plant conditions.

In case of on-demand, changes in the product rate result in the disturbances propagated in the direction opposite to flow, so levels in each unit are regulated by manipulating incoming streams. For example, responses in the feed flow (synthesis gas) gradually change since the time lag brings about the required change in manipulating flows slowly for handling the liquid level of S1. For this reason, Vent, yvent (CH4), and xd values of on-demand compared with ones of on-supply have gradual responses better.

The on-demand yield better performance in initial stage in terms of product composition xd, product rate D, raw material loss via a vent, while utilizing more energy Qr initially. Furthermore, the on-demand provides slightly lower energy cost as shown in Table C. 4 of Appendix C.

Figure 26 Changes in the set point of the synthesis gas flow controller for On-supply and changes in the set point of the product flow controller for On-demand

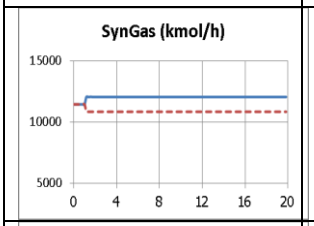
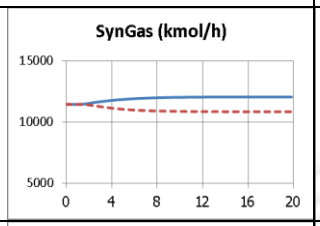
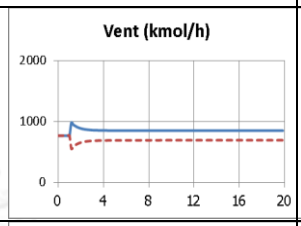
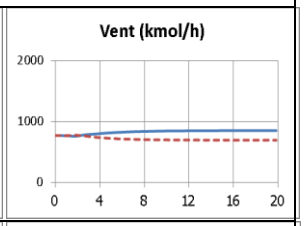
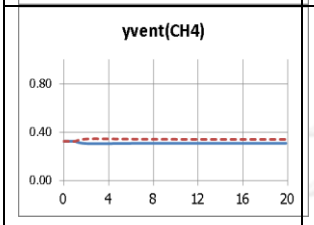
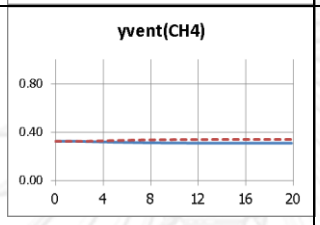
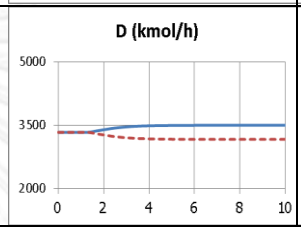
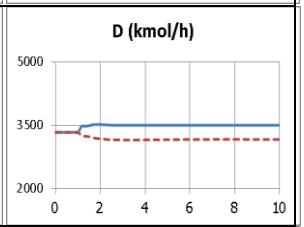
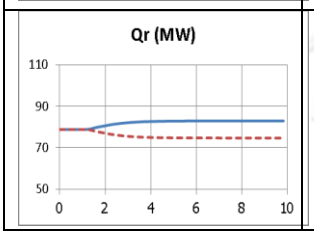
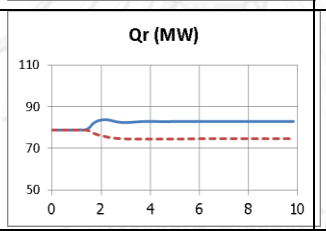
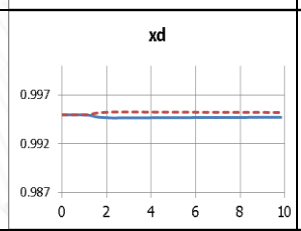
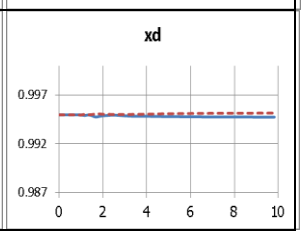
On-supply	On-demand	On-supply	On-demand
			
			
			
Time (hr)	Time (hr)	Time (hr)	Time (hr)

Table 9 Controlled variable (CV) and Manipulated variable (MV) for methanol process control in CS0, CS1, and CS2

Unit	CS0		CS1 and CS2	
	CV	**MV**	**CV**	**MV**
Reactor	Syngas feed flow rate	Compressor work K1	Syngas feed flow rate	Compressor work K1
	Temperature of stream going into the compressor K2	Cooler heat removal HX1	Temperature of stream going into the compressor K2	Cooler heat removal HX1
	Pressure of stream going into the compressor K2	Compressor work K2	Pressure of stream going into the compressor K2	Compressor work K2
	Reactor inlet temperature	**Reactor preheater duty HX3**	**Reactor inlet temperature**	**Flow rate of bypass stream at FEHE**
	Reactor outlet temperature	Reactor heat removal	Reactor outlet temperature	Reactor heat removal
Separator S1	Temperature of stream leaving the reactor	Condenser heat removal HX4	Temperature of stream leaving the reactor	Condenser heat removal HX4
	CH_4 composition from separator S1	Vent flow rate	CH_4 composition from separator S1	Vent flow rate
	Pressure in separator S1	Vent flow rate	Pressure in separator S1	Vent flow rate
	Liquid level in the separator S1	Liquid flow rate leaving bottoms of S1	Liquid level in the separator S1	Liquid flow rate leaving bottoms of S1
			Flow of recycle gas from separator S1 to Synthesis gas feed flow ratio	**Compressor work K3**
Flash separator S2	Liquid level in the separator S2	Liquid flow rate leaving bottoms of S2	Liquid level in the separator S2	Liquid flow rate leaving bottoms of S2
	Pressure in separator S2	**Compressor work K4**	**Flow rate of recycle gas from separator S2**	**Compressor work K4**

Table 9 Controlled variable (CV) and Manipulated variable (MV) for methanol process control in CS0, CS1, and CS2 (Continued)

Unit	CS0		CS1 and CS2	
	CV	**MV**	**CV**	**MV**
Distillation column C1	Reflux drum level	C1 Distillate flow rate	Reflux drum level	C1 Distillate flow rate
	Reboiler level	C1 Bottoms flow rate	Reboiler level	C1 Bottoms flow rate
	Column pressure	Condenser heat removal in column	Column pressure	Condenser heat removal in column
	Reflux to feed ratio (R/F)	**Reflux flow rate**	**Reflux ratio (RR) for CS1 and Reflux to feed ratio (R/F) for CS2**	**Reflux flow rate**
	Flow rate of recycle gas from reflux drum	Compressor work K5	Flow rate of recycle gas from reflux drum	Compressor work K5
	Temperature at tray 39	Reboiler duty	Temperature at tray 39	Reboiler duty

Table 10 Summation of the application of Wongsri's plantwide control structure design procedure

No.	Stage 1: Plant Information and Analysis								Stage 2: Fixture Plant and Disturbance Management						
	Independent Stream	Controlled variable	2.2	2.3	2.4	2.5	2.6	2.7	Step 3: Establishing Fixture Plant				Step 4: Executing Disturbances Management		
									3.1	3.2	3.4	3.5	4.1.1	4.1.2	4.2
1	Compressor duty K1	Synthesis gas feed flow						✓	✓						
2	Cooler duty HX1	Temperature of stream entering K2	✓										✓		
3	Reactor preheater duty HX3	Reactor inlet temperature	✓										✓		
4	Reactor cooling rate	Reactor temperature				✓						✓			
5	Cooler duty HX4	Temperature of stream entering S1	✓										✓		
6	Compressor duty K3	Recycle from S1 to synthesis gas feed ratio							✓						
7	Vent flow	CH4 composition from S1, Pressure in S1			✓					✓	✓				
8	Compressor duty K4	S2 Recycle flow							✓						

Table 10 Summation of the application of Wongsri's plantwide control structure design procedure (Continued)

No.	Stage 1: Plant Information and Analysis								Stage 2: Fixture Plant and Disturbance Management						
	Independent Stream	Controlled variable	2.2	2.3	2.4	2.5	2.6	2.7	Step 3: Establishing Fixture Plant				Step 4: Executing Disturbances Management		
									3.1	3.2	3.4	3.5	4.1.1	4.1.2	4.2
9	Column C1 distillate flow	C1 Reflux drum level (CH3OH)			✓					✓					
10	Column C1 reflux flow	Reflux to feed (R/F) for CS2 and Reflux ratio (RR) for CS1					✓								✓
11	Compressor duty K5	Column C1 recycle flow							✓						
12	Column C1 bottom flow	C1 Reboiler level (H2O)			✓					✓					
13	Column C1 Reboiler duty	Column temperature at tray 39	✓											✓	

Table 10 Summation of the application of Wongsri's plantwide control structure design procedure (Continued)

No.	Independent Stream	Controlled variable	**Stage 3: Unit Level Design**		**Stage 4: Energy Management and Optimization**	**Stage 5: Design Validation**
			5.1	5.2	7	8
14	Compressor duty K2	Pressure of stream entering K2	✓			
15	Bypass valve of FEHE	Reactor inlet temperature			✓	
16	S1 Bottoms flow	S1 level	✓			
17	S2 Bottoms flow	S2 lelvel	✓			
18	Column C1 condenser duty	Column pressure	✓			

CHAPTER VI

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

The new design procedure has been applied in this article to design the plantwide control structure of methanol process. Plantwide control structures (CS1 and CS2) designed by Wongsri's procedure are compared with the base-case control structure (CS0) proposed by Luyben (2010). Owing to establishing a fixture plant for having a material-balanced with stable operation and disturbance management for product quality as well as altering the process design for improving control performance, the control structures in the recycle, C1 column, and reactor feed of both design procedure are different as shown in Table 9. The new control structures give better responses in significant plant condition upon changes in synthesis gas feed and CH4 composition in feed than Luyben's structure, the plant condition are held much closer to their specifications. For instance, the product purity streams are closer specified value than the ones of Luyben's and the responses of most cases also perform more smoothly than the ones of Luyben's on account of creating fixture plant and disturbance management that support to reduce the disturbance propagation throughout the entire plant. The application of Wongsri's plantwide control structure design procedure is summarized in Table 10. The procedure is detailed, instructive, simple, and easy to apply for novice

6.2 Recommendation

Control design procedure of Wongsri (2012) is able to be applied to other process.

REFERENCES

Arthur, T. "Control Structure Design for Methanol Process." *Norwegian University of Science and Technology*, (2010).

Buckley, P. S. "Technique of Process Control." *University of Michigan. Wiley*, (1984).

de Andrade, G.V.N. and Lima, E.L. "Control Structure Design for an Ethanol Production Plant." *10th International Symposium on Process Systems Engineering*, (2009).

Husnil, Y.A., Yeo, G.C. and Lee, M. "Plant-Wide Control for the Economic Operation of Modified Single Mixed Refrigerant Process for an Offshore Natural Gas Liquefaction Plant." *CHERD*, (2013): 1415.

Konda, N.V.S.N. M., Rangaiah, G.P. and Krishnaswamy, P.R. "Plantwide Control of Industrial Processes: An Integrate Framework of Simulation and Heuristics." *Ind. Eng. Chem. Res.* 44, (2005): 8300-8313.

Konda, N.V.S.N. M., Rangaiah, G.P. and Krishnaswamy, P.R. "Simulation Based Heuristics Methodology for Plant-Wide Control of Industrial Processes." *Proceeding of the 16 th IFAC World Congress* 16, (2005): Part 1.

Konda, N.V.S.N. M., Rangaiah, G.P. and Krishnaswamy, P.R. "A Simple and Effective Procedure for Control Degree of Freedom." *Chem. Eng. Sci.* 61, (2006): 1184-1194.

Konda, N.V.S.N. M., Rangaiah, G.P. and Lim, D.K.H. "Optimal Process Design and Effective Plantwide Control of Industrial Processes by a Simulation-Based Heuristic Approach." *Ind. Eng. Chem. Res.* 45, (2006): 5955-5970.

Larsson, T., Govatsmark, M.S., Skogestad, S. and Yu C.C. "Control Structure Selection for Reactor, Separator and Recycle Process." *Ind. Eng. Chem. Res.*, (2003).

Luppi, P.A., Zumoffen, D.A.R. and Basualdo, M.S. "Decentralized Plantwide Control Strategy for Large-Scale Processes. Case Study: Pulp Mill Benchmark Problem." *Comp. Chem. Eng.* 52, (2013): 272-285.

Luyben, W. L. "Snowball Effects in Reactor/Separator Processes with Recycle." *Ind. Eng. Chem. Res.* 33, (1994): 299-305.

Luyben, W. L. "Design and Control Degree of Freedom." *Ind. Eng. Chem. Res.* 35, (1996): 2204-2214.

Luyben, W. L. "Design and Control of a Methanol Reactor/Column Process." *Ind. Eng. Chem. Res.* 49, (2010): 6150–6163.

Luyben, W. L., Tyréus, B. D. and Luyben, M. L. "Plantwide Control Design Procedure." *AIChE Journal* 43, (1997): 3161-3174.

Luyben, W. L., Tyréus, B. D. and Luyben, W. L. "Plantwide Process Control." *New York. McGraw-Hill*, (1998).

Luyben, W.L. "Design and Control of the Ethyl Benzene Process." *AIChE Journal* 57, (2010): 655-670.

Ng, C.S. and Stephanopoulos, G. "Synthesis of Control Systems for Chemical Plants." *Comp. Chem. Eng.* 20, (1996): 999-1004.

Price, R. M. and Georgakis, C. "Plantwide Regulatory Control Design Procedure Using a Tiered Framework." *Ind. Eng. Chem. Res.* 32, (1993): 2693-2705.

Price, R. M., Lyman, P.R. and Georgakis, C. "Throughput Manipulation in Plantwide Control Structures." *Ind. Eng. Chem. Res.* 33, (1994): 1197-1207.

Rodríguez, M. and Gayoso, J.A. "Degrees of Freedom Analysis for Process Control." *16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering*, (2006).

Seki, H. and Naka, Y. "Control Structure Design for a Reactor/Separator Process with Two Recycles." *8th International IFAC Symposium on Dynamics and Control of Process Systems* 2, (2007).

Skogestad, S. "Control Structure Design for Complete Chemical Plants." *Comp. Chem. Eng.* 28, (2004): 219-234.

Skogestad, S. and Larsson, T. "Plantwide Control – a Review and a New Design Procedure." *Modeling, Identification and Control* 21, (2000): 209-240.

APPENDICES

APPENDIX A

EQUIPMENT DATA

Table A. 1 Equipment size for dynamic simulation of methanol process

Equipment	Specifications	
Plug flow reactor	Tube diameter (m)	0.03675
	Tube length (m)	12.2
	Void volume	0.5
	Number of tubes	8000
	Density of catalyst (kg/m^3)	2000
Distillation column (C1)	Number of trays	42
	Feed stage	27
	Diameter (m)	6.5
	Reflux ratio	1.03
Separator (S1)	Diameter (m)	6.5
Flash separator (S2)	Diameter (m)	2.8

APPENDIX B

CONTROLLER DATA

Table B. 1 Controller data for based control structure CS0

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor	Syngas feed flow rate	Compressor work K1	PI	Reverse	11450 kmol/h	6000-18000 kmol/h	0-10 MW	0.5	0.5	-
	Temperature of stream going into the compressor K2	Cooler heat removal HX1	PI	Direct	40 ^oC	0-80 ^oC	0-12 MW	0.3	0.1	-
	Pressure of stream going into the compressor K2	Compressor work K2	PI	Direct	75 bar	50-100 bar	0-9 MW	0.5	5	-
	Reactor inlet temperature	Reactor preheater duty HX3	PI	Reverse	150 ^oC	100-200 ^oC	0-10 MW	0.5	5	-
	Reactor outlet temperature	Reactor heat removal	PI	Direct	265 ^oC	200-320 ^oC	0-50 MW	0.456	9.2	-
Separator S1	Temperature of stream leaving the reactor	Condenser heat removal HX4	PI	Direct	38 ^oC	0-76 ^oC	0-200 MW	0.1	3	-
	CH_4 composition from separator S1	Vent flow rate	PI	Direct	0.3182	0-0.6	0-100 %	5	56	-
	Pressure in separator S1	Vent flow rate	P	Direct	130 bar	120-140 bar	0-100 %	5	-	-

Table B. 1 Controller data for based control structure CS0 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Separator S1	Liquid level in the separator S1	Liquid flow rate leaving bottoms of S1	P	Direct	50 %	0-100 %	0-100 %	2	-	-
Flash separator S2	Liquid level in the separator S2	Liquid flow rate leaving bottoms of S2	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Pressure in separator S2	Compressor work K4	PI	Direct	2 bar	0-4 bar	0-3.2 MW	2	30	-
Distillation column C1	Reflux drum level	C1 Distillate flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Reboiler level	C1 Bottoms flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Column pressure	Condenser heat removal in column	PI	Direct	1.014 bar	0.5-1.5 bar	0-150 MW	2	20	-
	Reflux to feed ratio (R/F)	Reflux flow rate	PI	Reverse	0.8450	2000-4500 (PV1) and 3000-5000 (PV2) kmol/h	2000-4500 kmol/h	0.165	0. 5	-

Table B. 1 Controller data for based control structure CS0 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Distillation column C1	Flow rate of recycle gas from reflux drum	Compressor work K5	PI	Reverse	47.48 kmol/h	0-100 kmol/h	0-0.8 MW	0.5	0.5	-
	Temperature at tray 39	Reboiler duty	PI	Reverse	101 ^{o}C	50-150 ^{o}C	0-90.77 Gcal/h	1.37	9.2	-

Table B. 2 Controller data for new control structure CS1

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor	Syngas feed flow rate	Compressor work K1	PI	Reverse	11450 kmol/h	6000-18000 kmol/h	0-10 MW	0.5	0.5	-
	Temperature of stream going into the compressor K2	Cooler heat removal HX1	PI	Direct	40 ^{o}C	0-80 ^{o}C	0-12 MW	0.3	0.1	-
	Pressure of stream going into the compressor K2	Compressor work K2	PI	Direct	75 bar	50-100 bar	0-9 MW	0.5	5	-

Table B. 2 Controller data for new control structure CS1 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor	Reactor inlet temperature	Flow rate of bypass stream at FEHE	PI	Direct	150 ^oC	100-200 ^oC	0-100%	1	0.5	-
	Reactor outlet temperature	Reactor heat removal	PI	Direct	265 ^oC	200-320 ^oC	0-50 MW	0.456	9.2	-
Separator S1	Temperature of stream leaving the reactor	Condenser heat removal HX4	PI	Direct	38 ^oC	0-76 ^oC	0-200 MW	0.1	3	-
	CH_4 composition from separator S1	Vent flow rate	PI	Direct	0.3182	0-0.6	0-100 %	5	56	-
	Pressure in separator S1	Vent flow rate	P	Direct	130 bar	120-140 bar	0-100 %	5	-	-
	Liquid level in the separator S1	Liquid flow rate leaving bottoms of S1	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Flow of recycle gas from separator S1 to synthesis gas feed flow ratio	Compressor work K3	PI	Reverse	RSP from vent	35000-51000 (PV1) and 6000-18000 (PV2) kmol/h	0-4 MW	0.1	1	-
	Vent flow rate	Compressor work K3	P	Reverse	781 kmol/h	100-1500 kmol/h	0-100 %	1.12	-	-

Table B. 2 Controller data for new control structure CS1 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Flash separator S2	Liquid level in the separator S2	Liquid flow rate leaving bottoms of S2	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Flow rate of recycle gas from separator S2	Compressor work K4	PI	Direct	320 kmol/h	200-440 kmol/h	0-3.2 MW	2	30	-
Distillation column C1	Reflux drum level	C1 Distillate flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Reboiler level	C1 Bottoms flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Column pressure	Condenser heat removal in column	PI	Direct	1.014 bar	0.5-1.5 bar	0-150 MW	2	20	-
	Reflux ratio (RR)	Reflux flow rate	PI	Reverse	1.028	2000-4500 (PV1) and 2000-5000 (PV2) kmol/h	2000-4500 kmol/h	0.165	0.5	-
	Flow rate of recycle gas from reflux drum	Compressor work K5	PI	Reverse	47.48 kmol/h	0-100 kmol/h	0-0.8 MW	0.5	0.5	-

Table B. 2 Controller data for new control structure CS1 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Distillation column C1	Temperature at tray 39	Reboiler duty	PI	Reverse	101 ^oC	50-150 ^oC	0-90.77 Gcal/h	1.37	9.2	-

Table B. 3 Controller data for new control structure CS2

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor	Syngas feed flow rate	Compressor work K1	PI	Reverse	11450 kmol/h	6000-18000 kmol/h	0-10 MW	0.5	0.5	-
	Temperature of stream going into the compressor K2	Cooler heat removal HX1	PI	Direct	40 ^oC	0-80 ^oC	0-12 MW	0.3	0.1	-
	Pressure of stream going into the compressor K2	Compressor work K2	PI	Direct	75 bar	50-100 bar	0-9 MW	0.5	5	-
	Reactor inlet temperature	Flow rate of bypass stream at FEHE	PI	Direct	150 ^oC	100-200 ^oC	0-100%	1	0.5	-

Table B. 3 Controller data for new control structure CS2 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor	Reactor outlet temperature	Reactor heat removal	PI	Direct	265 ^oC	200-320 ^oC	0-50 MW	0.456	9.2	-
Separator S1	Temperature of stream leaving the reactor	Condenser heat removal HX4	PI	Direct	38 ^oC	0-76 ^oC	0-200 MW	0.1	3	-
	CH_4 composition from separator S1	Vent flow rate	PI	Direct	0.3182	0-0.6	0-100 %	5	56	-
	Pressure in separator S1	Vent flow rate	P	Direct	130 bar	120-140 bar	0-100 %	5	-	-
	Liquid level in the separator S1	Liquid flow rate leaving bottoms of S1	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Flow of recycle gas from separator S1 to synthesis gas feed flow ratio	Compressor work K3	PI	Reverse	RSP from vent	35000-51000 (PV1) and 6000-18000 (PV2) kmol/h	0-4 MW	0.1	1	-
	Vent flow rate	Compressor work K3	P	Reverse	781 kmol/h	100-1500 kmol/h	0-100 %	1.12	-	-
Flash separator S2	Liquid level in the separator S2	Liquid flow rate leaving bottoms of S2	P	Direct	50 %	0-100 %	0-100 %	2	-	-

Table B. 3 Controller data for new control structure CS2 (Continued)

Unit	Controlled variable	Manipulated variable	Controller Type	Action	SP	PV Range	OP Range	Tuning parameter		
								K_C	τ_I	τ_D
Flash separator S2	Flow rate of recycle gas from separator S2	Compressor work K4	PI	Direct	320 kmol/h	200-440 kmol/h	0-3.2 MW	2	30	-
Distillation column C1	Reflux drum level	C1 Distillate flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Reboiler level	C1 Bottoms flow rate	P	Direct	50 %	0-100 %	0-100 %	2	-	-
	Column pressure	Condenser heat removal in column	PI	Direct	1.014 bar	0.5-1.5 bar	0-150 MW	2	20	-
	Reflux to feed ratio (R/F)	Reflux flow rate	PI	Reverse	0.8375	2000-4500 (PV1) and 3000-5000 (PV2) kmol/h	2000-4500 kmol/h	0.165	0.5	-
	Flow rate of recycle gas from reflux drum	Compressor work K5	PI	Reverse	47.48 kmol/h	0-100 kmol/h	0-0.8 MW	0.5	0.5	-
	Temperature at tray 39	Reboiler duty	PI	Reverse	101 ^oC	50-150 ^oC	0-90.77 Gcal/h	1.37	9.2	-

APPENDIX C

IAE AND ENERGY COST DATA

Control Structure Performance Evaluation

Integral absolute error is widely used and the formulation as written below:

$$IAE = \int |e(t)|\, dt \qquad (C.1)$$

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

Table C. 1 IAE's summation of dynamic performance results on changes in the set point of the synthesis gas flow controller

Control structure	Summation of IAE					
	xd	T39	yCH4	Pflash	xb	Tin
CS0 (Base case)	0.0047	1.566	**0.033**	0.29	0.000117	8.97
CS1	0.0055	**1.180**	0.047	**0.28**	**0.000111**	3.46
CS2	**0.0043**	1.292	0.046	0.31	0.000115	**2.12**

Table C. 2 IAE's summation of dynamic performance results on changes of methane impurity in synthesis gas

Control structure	Summation of IAE					
	xd	T39	yCH4	Pflash	xb	Tin
CS0 (Base case)	0.0056	1.209	**0.727**	0.31	0.0000388	2.51
CS1	0.0018	**0.856**	1.069	**0.20**	0.0000298	**1.35**
CS2	**0.0015**	1.008	1.432	0.47	**0.0000237**	1.85

Energy Cost Evaluation

Table C. 3 Basis of cost calculation (Luyben, 2010)

Unit	Capital cost ($)	Energy cost ($/GJ)
Distillation column	$17640(\text{diameter, m})^{1.066}(\text{length, m})^{0.802}$	-
Condenser	$7296(\text{area, m}^2)^{0.65}$	0.354
Reboiler	$7296(\text{area, m}^2)^{0.65}$	7.78
Reactor	$7296(\text{area, m}^2)^{0.65}$	6
FEHE	$7296(\text{area, m}^2)^{0.65}$	-
Preheater HX3		8.22
Compressor	$(1293)(517.3)(3.11)(\text{hp})^{0.82}/280$	16.8
Total annual cost (TAC)	capital cost /payback period + energy cost, payback period = 3 years	-

Table C. 4 Energy cost's summation for handling disturbance on changes in the set point of the synthesis gas flow controller in On-supply and On-demand mode

Operation mode	Disturbance	Energy		Work		Utility cost	Summation
		GJ/h	(m$/yr)	GJ/h	(m$/yr)	(m$/yr)	(m$/yr)
On-supply	Plus	1038.58	24.15	55.39	8.15	32.30	60.73
	Minus	938.41	21.81	45.03	6.63	28.43	
On-demand	Plus	925.47	23.58	51.38	7.56	31.15	**60.36**
	Minus	1248.47	22.57	45.17	6.65	29.22	

Table C. 5 Capital and energy costs of FEHE and Preheater HX3

Process	Unit	Duty (MW)	Area (m^2)	Capital cost ($)	Enery cost ($/yr)	TAC ($/yr)
Based case	FEHE	50.58	2494.17	1,177,842	-	1,210,066
	Preheater HX3	2.74	-	321,102	710,417	
			Total	1,498,944	710,417	
Modified case	FEHE	53.32	2906.00	1,300,849	-	**433,616**
	Preheater HX3	-	-	-	-	
			Total	1,300,849	-	

Table C. 6 Energy cost's summation for handling disturbance on changes in the set point of the synthesis gas flow controller

Control structure	Disturbance	Energy		Work		Utility cost	Summation
		GJ/h	(m$/yr)	GJ/h	(m$/yr)	(m$/yr)	(m$/yr)
CS0	Plus	1105.95	25.32	57.50	8.46	33.79	59.08
	Minus	853.02	19.90	36.71	5.40	25.30	
CS1	Plus	1035.19	23.41	57.43	8.45	31.86	**55.84**
	Minus	848.03	19.15	32.82	4.83	23.98	
CS2	Plus	1037.19	23.54	57.43	8.45	32.00	55.97
	Minus	848.03	19.15	32.82	4.83	23.98	

Table C. 7 Energy cost's summation for handling disturbance on changes of methane impurity in synthesis gas

Control structure	Disturbance	Energy		Work		Utility cost	Summation
		GJ/h	(m$/yr)	GJ/h	(m$/yr)	(m$/yr)	(m$/yr)
CS0	Plus	922.15	21.61	40.50	5.96	27.57	58.73
	Minus	1023.03	23.41	52.70	7.76	31.16	
CS1	Plus	933.82	21.07	36.63	5.39	26.46	**55.58**
	Minus	941.16	21.43	52.31	7.70	29.13	
CS2	Plus	935.82	21.20	36.63	5.39	26.59	55.72
	Minus	941.16	21.43	52.31	7.70	29.13	

VITA

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