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PLANTWIDE CONTROL STRUCTURE FOR METHANOL PROCESS

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การหมุนเวียนสารและพลังงานนับเป็นปัญหาที่สำคัญในการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ ซึ่งเกี่ยวข้องกับระบบควบคุมของทั้งโรงงาน ก๊าซสังเคราะห์จากกระบวนการออกซิเดชั่นบางส่วนของชีวมวลสามารถนำมาใช้เป็นสารตั้งต้นในการผลิตเมทานอล กระบวนการเมทานอลถูกนำมาใช้ในการทดสอบการออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์ เนื่องจากเป็นกระบวนการที่มีความซับซ้อน งานวิจัยนี้ได้ทำการพัฒนาโครงสร้างการควบคุมแบบแพลนท์ไวด์ของกระบวนการเมทานอลด้วยวิธีการของวงศ์ศรี (2552) ร่วมกับโปรแกรม Aspen Plus และ Aspen Dynamics ในการจำลองกระบวนการที่สภาวะคงตัวและพลวัตรวมทั้งหมดสามโครงสร้างการควบคุม และประเมินสมรรถนะของโครงสร้างการควบคุมที่ได้ออกแบบเปรียบเทียบกับงานวิจัยของลูเบน โดยการใช้ตัวรบกวนกระบวนการทางด้านปริมาณสารในกระแสป้อนและตัวรบกวนทางด้านความร้อน พบว่า ทั้งสามโครงสร้างการควบคุมที่ได้ออกแบบด้วยวิธีของวงศ์ศรีซึ่งมีการใช้ข่ายงานแลกเปลี่ยนความร้อน สามารถกำจัดตัวแปรรบกวนได้ดี มีผลตอบสนองต่อสิ่งรบกวนใกล้เคียงกับโครงสร้างการควบคุมอ้างอิงของลูเบน โดยเปรียบเทียบจากปริพันธ์ของค่าคลาดเคลื่อนสัมบูรณ์ อีกทั้งสามารถลดการใช้พลังงานและรักษาคุณภาพของผลิตภัณฑ์ได้

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The presence of material and energy recycles poses a significant problem in the plantwide control structure design (PWCD) which involves with an entire chemical plant control system. Methanol can be produced from the synthesis gas which is made from renewable energy source (biomass) by partial oxidation in gasifier. The methanol process is selected for testing PWCD because it is a complex multi-unit process. This research focused on the development control structures for methanol process by using Wongsri's procedure (2009). A steady state and dynamics simulations are done via Aspen Plus and Aspen Dynamics respectively. Three control structures (CS1 to CS3) are designed and evaluated dynamic performance to compare with the proposed control structure of Luyben (2010) by using material and thermal disturbances. The result shows that the dynamic responses of the designed control structures and base control structure are similar as compared by integral absolute error (IAE). All designed control structures with heat integration can reduce the energy consumption, can reject disturbances, and can maintain product quality close to their specified values.

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Student's Signature ....
Advisor's Signature ....

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CHAPTER I
INTRODUCTION

1.1 Importance and reasons of research

The competitive in product quality and operating profit have resulted in most industries so the production process should have high quality and high efficiency. Part of this competitiveness has required the complexity of process to increase through attempt to recover unreacted material, reduce environmental impact, and consider safety. Chemical processes have been designed to operate explicitly at the specified design conditions, minimize energy consumption, and get desirable product. In realistic situation, as a result of external and internal factors as disturbances, the process is not operated smoothly and deviated from the design condition. All of these should be eliminated from the process so that the process stable and least deviation.

Control structure design for complete chemical plants is a challenge. A complex process contains several recycle streams, energy integration, and many different unit operations. These factors combined with the chemical component inventories. The control system of individual unit independently is no longer sufficient because of increasing interaction among the process units. As a result, the plantwide control structure has emerged because it refers to the design of control system for an entire plant. The plantwide control methodologies can be classified as a heuristics-based, mathematics-based, optimization-based, and mixed.

Methanol is an important multipurpose base chemical, a simple molecule which can be recovered from many resources such as natural gas, coal, petroleum and biomass. By tradition, methanol is principally used to produce formaldehyde, acetic acid and to use in energy applications, including Dimethyl Ether (DME), biodiesel, methanol to olefins (MTO), and fuel cells. Today, the fossil fuel resources are diminishing and the high price of oil and natural gas are increasing. Renewable sources are becoming more interesting. Biomass is an alternative energy source in feedstock for methanol process. It can be produced synthesis gas by gasification then which is converted into methanol. However the methanol process as a complex multi-unit process, the effective control structures are important to develop. In this research focused on the plantwide control structure design by using Wongsri's procedure (2009) applied to methanol process.

1.2 Research Objective

To illustrate Wongsri's plantwide control system design procedure by designed the plantwide control structure for methanol process.

1.3 Scopes of Research

1. The commercial software Aspen Plus and Aspen Dynamics are used for methanol process simulations.

2. Description of methanol process is given by William L. Luyben (2010).

3. Three new plantwide control structures for methanol process are designed using Wongsri's procedure (2009).

4. The new design control structures are compared with the work proposed by William L. Luyben (2010).

1.4 Contributions of Research

1. Steady state and dynamic models of methanol process is obtained by using Aspen Plus and Aspen Dynamics respectively.

2. Three new design plantwide control structures are obtained.

3. The best set of pairing of controlled variables and manipulated variables.

4. Evaluated the performance of the new design plantwide control structures.

1.5 Research Procedures

1. Study methanol process and concerned information.

2. Study of plantwide control structure theory.

3. Simulate the steady state and dynamic of methanol process.

4. Study the Wongsri's plantwide control system design procedure.

5. Design new control structures of methanol process as followed by Wongsri's procedure.

6. Simulate the dynamic of the new design plantwide control structures.

7. Evaluate the dynamic performance of the design control structures.

8. Analyze the simulation results.

9. Conclude the thesis.

1.6 Research Contents

This thesis is divided into six chapters:

Chapter I is an introduction to this research. The chapter consists of research objective, scopes of research, contributions of research, and research procedures.

Chapter II gives the literature reviews of plantwide control design procedure, heat exchanger networks (HENs), and methanol process.

Chapter III covers some background information about heat exchanger network, plantwide control of Luyben's theory and the procedure of Wongsri (2009) for new plantwide control structures design.

Chapter IV describes description of the methanol process and the design of heat exchanger network by procedure in the previous chapter.

Chapter V presents new plantwide control structures design for methanol process following Wongsri's procedure (2009) and dynamic simulation results compared with the proposed work of Luyben.

Chapter VI analyses and concludes this research and gives the recommendation for future work.

This is follow by:

References

Appendix A: Steady State & Equipments Data

Appendix B: Tuning of Control Structures

Appendix C: Fixture Point Theorem Data

CHAPTER II

LITERATURE REVIEWS

2.1 Review of Plantwide Control Structure Design

Luyben (1994) presented the snowball effect in reactor/separator process with recycle. The snowball effect could be analyzed a mathematical of the problem for several typical kinetic systems. In the case of $A \rightarrow B$, the fresh feed flow rate and fresh feed composition involve in the recycle flow rate. Two other kinetic systems are studied numerically: consecutive first-order reactions $A \rightarrow B \rightarrow C$ and second-order reaction $A + B \rightarrow C$. Results confirm the case-study that using a control structure by fixing the flow rate of one stream in liquid recycle loop can prevent the snowball effect. In processes with one recycle, the flow rate of reactor effluent can be set. In processes with two or more recycle streams, the flow rate of each recycle can be fixed.

Luyben (1996) presented the finding the number of variables (design degree of freedom) that is the one of the problems to develop a steady-state process flowsheet. This number must be specified completely in the process. The production rate, safety constraints, product qualities, and environmental limitations as all variables are subtracted to calculate the number of design optimization variables. There are many variables and equation in complex processes so it is difficult to define the correct variables and equations. The control degrees of freedom must be known for the design of a control. It is very easy to calculate the number of controlled variables because it is equal to the number of manipulated variables. This result shows in several progressively more complex recycle process case studies. The practical significance is that the error procedure of accounting for all variables and equations can be avoided and the model does not need for the design degrees of freedom.

Larsson, Govastmark, Skogestad, and Yu (2003) presented control structure selection for a simple plant with a liquid-phase reactor, a distillation column, and recycle of unreacted reactants. A definition of the operational objectives, constraints, and degrees of freedom is clearly specified. Active constraints should be controlled to optimize the economic performance. The selection of the suitable controlled variable for remaining unconstrained degree of freedom is main focus. The concept of self-optimizing control is used which is to search for a constant setpoint strategy with an acceptable economic loss. The energy costs should be minimized and the production rate should be maximized. A good feed variable is the reflux ratio L/F. This applied to single-loop control as well as multivariable model predictive control.

Konda, Reangaiah and Krishnaswamy (2005) presented methodologies of plantwide control (PWC) for chemical processes. An integrated with recycles is important for reason of safety, environmental considerations, and economics. They proposed an integrated framework of simulation and heuristics. Simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The integrated framework is successfully applied to the hydrodealkylation of toluene (HDA) process. An analysis of results shows that the proposed framework can generate a viable control system and build synergies between the powers of both the simulation and the heuristics.

Suntisrikomol (2008) presented the “Fixture Point Theorem” for Hydrodealkylation process (HDA) to select appropriate the set of controlled variables from a large number of candidate output. The fixture point control theorem states that the most sensitive points must be satisfactorily controlled by giving them consideration before other controlled variables. The maximum (scaled) gain is used to selecting and paring the set of controlled variables and manipulated variables. The set of first rank of controlled variables are same as reference control structure. The second and third rank from fixture point and five control structures were designed and compared are selected.

In order to illustrate the dynamic behaviors of the control structures when disturbance load occur (such as change in methane composition in fresh feed gas and quencher outlet temperature), the performance of designed control structures were presented in the integral absolute error (IAE) value and compared with reference structure. The designed structures are fast response and the most effective on compared with reference control structure.

Detjareansri (2009) proposed the control structures for alkylation process using new design procedure of Wongsri. The designed control structures are evaluated the dynamic performance compared with the base control structure by two types of disturbances: material and thermal disturbances. The eight-step of Wongsri is used to design plantwide control structure. All the designed control structures have a good performance because it handle disturbances entering the process and can maintain product quality The Wongsri's procedure is a useful design procedure for complex industrial process that leads to a good performance plantwide control system.

2.2 Heat Exchanger Networks (HENs)

Linhoff and Hindmarsh (1983) presented a novel pinch design method for heat exchanger networks. The method divides a heat exchanger network problem into subproblem at the pinch temperature. It features the highest degree of freedom recovery possible with low cost solutions for best design. The pinch method is simple to be used by hand with near certainty to identify "best" designs. Moreover, the network patterns deal with a good controllability and safety. In state of the art flowsheet, the improved heat exchanger network design can be saved the energy about 20-30%. The task involves the placement of process and utility heat exchangers to heat and cool process streams from specified supply to specified target temperatures.

Linhoff, Dunford and Smith (1983) studied heat integration of distillation column. It has a good integration when the crossing of heat recovery pinch does not occur. In column, either the reboiler or the condenser can be integrated with the process. This heat integration leads to reduce the utility cost in distillation column. If these criteria can be met, energy cost for distillation can effectively be zero.

Saboo and Morari (1983) presented flexible heat exchanger network. Two classes of HENs (Class I and Class II) are classified by the kind and magnitude of disturbances. For the temperature variation, the maximum energy recovery (MER) is a function of stream supply and target conditions. This problem is Class I, i.e. the small changes in inlet temperatures do not impact on the pinch temperature location. In contrast, if an explicit function of MER does not exist for over the disturbances, the problem is class II. For example, the large variations in inlet temperature cause the discrete changes in pinch temperature locations.

Calandranis and Stephanopoulos (1988) proposed a new approach to address the following problems: design the configuration of control loops in a network of heat exchangers and sequence the control action of the loops, to accommodate set point changes and reject load disturbances. The approach proposed the structure characteristics of a HEN by identifying routes through the HEN configuration that can share load of disturbances to coolers or heaters. The variety of design issues are discussed such as the placement of bypass lines and the restrictions imposed by the existence of a process pinch. A real-time planning of control actions is the essence of implementation strategies generated by an expert controller, which selects path through the HEN is to be used for each entering disturbance or set point change, and what loops should be activated (and in what sequence) to carry the associated load (disturbance or set point change) to a utility unit.

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

Panyai (2008) designed plantwide control structures of butane isomerization plant for reversible reaction case with heat integration schemes. There are 4 alternatives of heat integrated and they are simulated using Wongsri's disturbance propagation method to achieve dynamic maximum energy recovery. Energy saving can be saved about 15.11-22.09% compared with base case (Luyben, 1998). Changing thermal and flow rate are disturbances for testing dynamic performances of all structures. CS2 and CS3 as proper control structures with heat integrated process can be handled all disturbances and RHEN-1 is better than RHEN-2 and RHEN-3.

Gayapan (2008) designed heat exchanger networks for natural gas expander plant. The resilient heat exchanger networks (HENs) are designed using the disturbance load propagation method (Wongsri, 1990) and the control structures of HENs using the heat pathway heuristics. Nine alternatives were designed with no pinch temperature. The CS3 control structure can reject disturbances better than other control structures. The designed control structure is evaluated based on the rigorous dynamic simulation.

2.3 Methanol process

Luyben (2005) presented the selection of an effective control structure for a binary distillation column producing high-purity products. This selection depended on the feed composition. The binary distillation of methanol/water is used as a case study. For either low or high feed compositions, the single-temperature control should be selected, but dual-temperature control appropriated for intermediate feed compositions. Separation of the methanol/water should be used the reflux-to-feed ratio control throughout the range of feed compositions. At low feed compositions, it has the high reflux ratio so the reflux is used to control the reflux-drum level. An alternative control structure is proposed that it is difficult to control the reflux drum level and a tray temperature by manipulating reboiler heat input and distillate flow rate, respectively. The control structure with a fixed reflux can maintain the product purities in the feed composition changes.

Theophilus (2010) designed control structure for methanol process which natural gas as the raw material. This designing is based on the self-optimizing control method proposed by Skogestad. Two types of disturbance, changing feed flow rate and feed composition, were studied for the evaluated dynamic performance. The carbon efficiency is a significant operating parameter. It indicates as the measure of how much carbon in the feed is converted to methanol product. For this reason, the operational objective function was the carbon efficiency. The pressure and split ratio between the recycle flow to methanol reactor and the purge stream lead to the implement error in .the methanol synthesis section. The best set of control variable was to control the methanol reactor pressure by manipulating the work of compressor and control the flow rate of the purge gas. He suggested that the reactor outlet temperature should be controlled by controlling the temperature of the steam.

Luyben (2010) developed the economically optimum design of a methanol reactor/distillation column system with three gas recycle streams to produce high purity methanol from synthesis gas. Design optimization variables have impacted on the economics. The capital costs, energy costs, the value of the methanol product, and the heating value of a vent stream that is necessary for purging off inert components entering in the feed are considered. A developed plantwide control structure can be handled large disturbances in the production rate and synthesis gas composition. This control structure has permitting the reactor pressure to vary as conditions change. In the synthesis gas feed stream, the stoichiometry of the reactants is imbalances so a high pressure override controller is needed.

CHAPTER III

THEORY

The summarization of heuristic approach in heat pathway view point, match classification and patterns of heat exchanger networks (HEN), and the plantwide control fundamentals to design control structure entire plant consisting of many interconnected unit operations are presented in this chapter.

3.1 Basic Knowledge for Pinch Technology

3.1.1 Pinch Technology

Pinch technology is a rigorous, structured approach that used to tackle a wide range of improvements related to process such as reducing operating costs, improving efficiency, and reducing and planning capital investment. It has been developed for more than two decades and now provides a systematic methodology for analysis chemical processes and surrounding utility systems. The concept was first developed by two independent research groups (Flower and Linnhoff, 1978; Umeda et al., 1979) based on an applied thermodynamics point of view.

3.1.2 Basic Pinch Analysis Concept

The pinch analysis concept is originated to design the heat recovery in network for a specified design task. Starting with do calculate heat and material balance of the process obtained after the core process, i.e. reaction and separation system, has been designed. By using thermal data from the process, we can set the target for energy saving prior to the design of the heat exchanger networks. The necessary data is source, target temperature and heat capacity flow rate for each stream as shown in Table 3.1

Table 3.1 Thermal data for process streams (Linnhoff and Hindmarsh, 1983).

Stream No.	Stream type	Start Temperature (Ts), °C	Target Temperature (Tt), °C	Heat capacity flow rate (CP), kW/°C
1	Hot	150	60	2
2	Hot	90	60	8
3	Cold	20	125	2.5
4	Cold	25	100	3

Here the hot streams are referred to the streams that required cooling, i.e. the source temperature is higher than that of the target. While the cold streams are referred to those required heating, i.e. the target temperature is higher than the supply. Heat capacity flow rate is defined as the multiple between specific heat capacity and mass flow rate as shown below.

$$CP = Cp * F \tag{3.1}$$

Where: CP is heat capacity flow rate (kW/°C).
Cp is specific heat capacity of the stream (kJ/°C.kg).
F is mass flow rate of stream (kg/s).

The data used here is based on assumption that the heat capacity flow rate is constant. In practice, this assumption is valid because every streams with or without phase change can easily be described in terms of linearization temperature-enthalpy data (i.e. CP is constant). The location of pinch and minimum utility requirement can be calculated by using the problem table algorithm (Flower and Linnhoff, 1979) for a specified minimum temperature different, ΔT_{min}. In the case of ΔT_{min} = 20°C, the results obtained from this method are shown in Table 3.2.

Table 3.2 The problem table for data given in Table 3.1.

W				T hot (°C)	T cold (°C)	$\sum W$ (kW/°C)	ΔT (°C)	Required Heat (kW)	Interval (kW)	Cascade Heat (kW)	Sum Interval (kW)
H1	H2	C1	C2								
0	0	0	0	150	130	0		Qh		-105	
2	0	0	0	145	125	2	5	107.5	10	2.5	10
2	0	2.5	0	120	100	-0.5	25	117.5	-12.5	12.5	-2.5
2	0	2.5	3	90	70	-3.5	30	105	-105	0	-107.5
2	8	2.5	3	60	40	4.5	30	0	135	-105	27.5
0	0	2.5	3	45	25	-5.5	15	135	-82.5	30	-55
0	0	2.5	0	40	20	-2.5	5	52.5	-12.5	-52.5	-67.5
										Qc	

At the temperature where cascade heat equals to zero, we call this the pinch temperature. The point where ΔT_{min} is observed is known as the “Pinch” and recognizing its implications allows energy targets to be realized in practice. Once the pinch has been identified, it is possible to consider the process as two separate systems: one above and one below the pinch.

Thermodynamic regions, namely, hot end and cold end are separated for the pinch problem. The hot end is the region comprising all streams or part of stream above the pinch temperature. The system above the pinch requires only hot utility. In contrast to the hot end, the cold end is the region comprising all streams or part of stream below the pinch temperature and only cold utility is instead desired regardless the hot utility. It is important to note that heat must not be transferred across the pinch therefore the minimum utility requirement for process is achieved.

Additionally, Saboo and Morari (1983) classified flexible HENs into two classes according to the kind and magnitude of disturbances that affect the pinch location. For the temperature variation, they show that if the MER can be expressed explicitly as a function of the stream supply and target conditions the problem belongs to Class I, i.e. the case where small variations in inlet temperatures do not affect the pinch temperature location. If the explicit function for the minimum utility requirement valid over the whole disturbance range does not exist, the problem is of Class II, i.e. the case where large changes inlet temperatures or flow rate variations cause the discrete changes in pinch temperature locations.

3.2 Heat Exchanger Networks

Energy conservation has always been important in process design. Heat Exchanger Network (HEN) is generally accepted that an optimal network must feature a minimum number of units that reflects on a capital cost and minimum utility consumption that reflects on operating costs. A good engineering design must exhibit minimum capital and operating costs. For Heat Exchanger Network synthesis, other features that are usually considered in design are operability, reliability, safety, etc. in recent years the attention in HEN synthesis has been focused on the operability features of a HEN, e.g. the ability of a HEN to tolerate unwanted changes in operating conditions. It has been learned that considering only a cost objective in synthesis may lead to a worse network, i.e. a minimum cost network may not be operable at some neighboring operating conditions. The design must not only feature minimum cost, but also be able cope with a fluctuation or changes in operating conditions. The ability of a HEN to tolerate unwanted changes is called resiliency. It should be note that the ability of a HEN to tolerate wanted changes is called flexibility.

The resiliency property of a design becomes an important feature to be accounted for when the extent of integration of a design introduces significant interactions among process components. The energy integration of a HEN generates a quite complex interaction of process streams, despite the fact that transfer of heat from hot to cold process streams to their target temperatures by using most of their heating and cooling availability and a minimum of heating and cooling utilities. The process streams in the network may affect the performances of many heat exchanges and the conditions of several process streams. Since resiliency is a property of a network structure.

3.2.1 Definition of HEN Resiliency

In the literature, resiliency and flexibility have been used synonymously to describe the property of HEN to satisfactorily handle variations in operating conditions. These two terms have difference in meaning.

The resiliency of HEN is defined as the ability of a network to tolerate or remain feasible for disturbances in operating conditions (e.g. fluctuations of input temperatures, heat capacity flow rate, etc.). As mentioned before, HEN flexibility is closed in meaning to HEN resiliency, but HEN flexibility usually refers to the wanted changes of process conditions, e.g. different nominal operating conditions, different feed stocks, etc. That is, HEN flexibility refers to the preservation of satisfactory performance despite varying conditions, while flexibility is the capability to handle alternate (desirable) operating conditions.

A further distinction between resiliency and flexibility is suggested by Colberg et al. (1989). Flexibility deals with planed, desirable changes that often have a discrete set of values; resilience deal with unplanned, undesirable changes that naturally are continuous values. Thus a flexibility is a ‘multiple period’ type of problem. A resilience problem should be a problem with a continuous range of operating conditions in the neighborhood of nominal operating points.

In order to make Alternative 6 of hydrodealkylation process more economically appealing, the minimum number of auxiliary utilities is identified using the proposed design scheme adapted from Wongsri's RHEN (for resilient heat exchanger network) design method.

3.2.2 Heuristics for HEN Synthesis

Several HEN matching rules with minimum energy and investment costs have been presented (Masso and Rudd, 1969, Ponton and Donalson, 1974, Rathore and Powers, 1975, Linnhoff and Hindmarsh, 1983, Jezowski and Hahne, 1986 etc.).

The following are heuristics from the literature classified according to the design criteria.

The heuristics to minimize the capital cost (the number of heat exchangers):

Heuristic C1. To generate a network featuring the minimum number of heat exchanger units, let each match eliminate at least one of the two streams; a tick-off rule (Hohmann, 1971).

Heuristic C2. Prefer the matches that will leave a residual stream at the cold end for a heating problem, or its hot end for a cooling problem. A match of this type will feature the maximum temperature difference.

Heuristic C3. Prefer matching large heat load streams together. The significance of this rule is that the control problem (a capital cost) of a match of this type (whether it is implemented by one or many heat exchangers) should be less than that of heating or cooling a large stream with many small streams.

The heuristics to minimize the energy cost (the minimum utility requirement):

<u>Heuristic E1.</u> Divide the problem at the pinch into subproblems, one a heat sink (heating subproblem or hot end problem) and the other a heat source (cooling subproblem or cold end problem), and solve them separately (Linnhoff and Hindmarsh, 1983).

<u>Heuristic E2.</u> Do not transfer heat across the pinch.

<u>Heuristic E3.</u> Do not cool above the pinch.

<u>Heuristic E4.</u> Do not heat below the pinch.

The laws of thermodynamics:

<u>Heuristic T1.</u> In a heating problem, if a supply temperature of a cold stream is less than a target temperature of a hot stream by ΔT_{min} or more and the heat capacity flow rate of a hot stream is less than or equal to the heat capacity flow rate of a cold stream, the match between these two streams is feasible. (Immediately above the pinch temperature, the heat capacity flow rate of a cold stream must be greater than or equal to that of a hot stream.)

<u>Heuristic T2.</u> In a cooling problem, if a supply temperature of a hot stream is grater than a target temperature of a cold stream by ΔT_{min} or more and the heat capacity flow rate of a hot stream is greater than equal to the heat capacity flow rate of a cold stream, the match between these two streams is feasible. (Immediately below the pinch temperature, the heat capacity flow rate of a hot stream must be greater than or equal to that of a cold stream.).

Heuristic T3. For a situation different from the above rule, a match feasibility must be determined by checking whether the minimum temperature difference of a match violates the minimum approach, ΔT_{min} specific by the design.

3.2.3 Match Classification

In order to make use of the heuristics we must classify matches. The following criteria are considered important in this research:

1. **Position of a Match.** One heuristic prefers a match at the cold end and another prefers a match at the hot end. Pinch heuristics prefers a match at the cold end in a heating subproblem and a match at the hot end in a cooling subproblem. However, there are other possibilities. By using the tick-off heuristic, there are four ways that two streams can match. This leads to the basic four match patterns (Wongsri, 1990).
2. **Heat capacity flow rate** (between hot and cold streams). See Heuristic T.1 and T.2.
3. **Heat Load** (between hot and cold streams). The heuristic that concerns heat load state that one must match large heat load hot and cold streams first. This leads to two additional heuristic:

Heuristic N1. For a heating subproblem, a match where the heat load of a cold stream is greater than that of a hot stream should be given higher priority than the other. The reason is that the net heat load heating subproblem is in deficit. The sum of heat loads of cold streams is greater than of hot streams. The purposed match will likely be part of a solution (Wongsri, 1990).

Heuristic N2. Conversely, we prefer a match where the heat load of a hot stream is greater than that of a cold in a cooling subproblem (Wongsri, 1990).

4. Residual Heat Load. No heuristics for this quantity have thus far appeared in the literature. Two new heuristics are introduced.

For a match in a cooling subproblem that satisfies the heat load preference or heuristics N2:

Heuristic N4. We prefer a match where the residual heat load is less than or equal to the minimum cooling requirement, (Wongsri, 1990).

The reason behind the above two heuristics N3 and N4 is that the residual may be matched to a utility stream. One has the possibility of eliminating two streams at once.

3.2.4 Match Patterns

HEN synthesis is usually considered as a combinatorial matching problem. For a HEN in which a design property is regarded as a network property, or a structural property, we need to look beyond the match level to a higher level where such a property exists, e.g. to a match structure or match pattern. Match patterns are the descriptions of the match configuration of two, and possibly more, process streams and their properties that are thermally connected with heat exchangers. Not only the match description, e.g. heat duty of an exchanger and inlet and outlet temperatures is required but also the position of a match, e.g. upstream or downstream, the magnitude of the residual heat load and the heat capacity flow rates between a pair of matched streams.

By using the ‘tick off rule’ there are four match patterns for a pair of hot and cold streams according to the match position and the length (heat load) of streams. The four patterns are considered to the basic match pattern classes. The members of these classes are the patterns where other configurations and properties are specified. The four match pattern classes are simply called A, B, C and D and are shown in Figure

3.1, 3.2, 3.3, and 3.4 respectively. Any eligible match must belong to one of the four match pattern classes.

Definition 3.1 Class A Match Pattern: The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the cold end of the cold stream. The residual heat load is on the hot portion of the cold stream. (See Figure 3.1)

A match of this class is a first type match at cold end position and the heat load of the cold stream is greater than that of the hot stream. This is an upstream match. For a heating subproblem, a Class A match is favored, because it leaves a cold process stream at the hot end (Heuristic N1) and follows the pinch heuristics. (See Table 3.3)

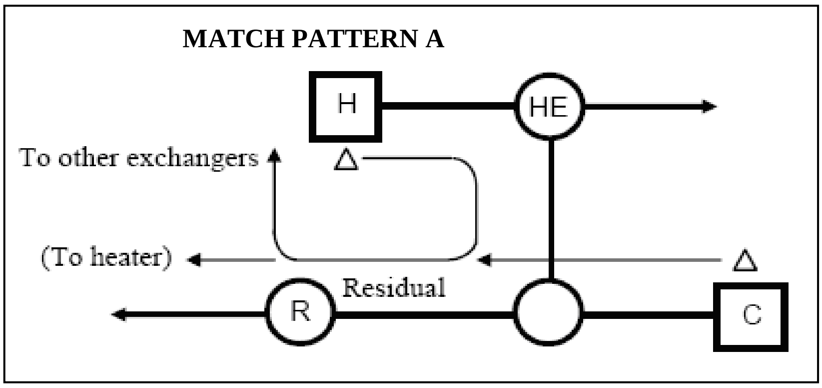


Figure 3.1 Class A Match Pattern

Definition 3.2 Class B Match Pattern: The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the hot end of the hot stream. The residual heat load is on the cold portion of the hot stream. (See Figure 3.2)

A match of this class is a second type match; a hot end match and the heat load of the hot stream greater than that the cold stream. This is an upstream match.

For a cooling subproblem, a Class B match is favored, because it leaves a hot process stream at the cold end (Heuristic N2) and also follows the pinch heuristics. (See Table 3.3)

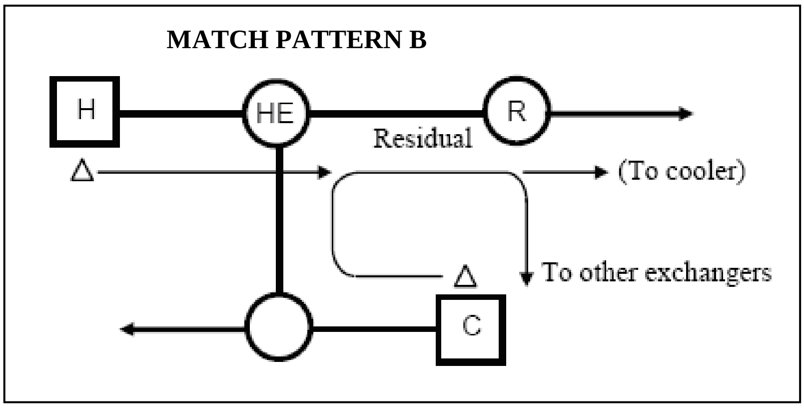


Figure 3.2 Class B Match Pattern

Definition 3.3 Class C Match Pattern: The heat load of a hot stream is greater than the heat load of cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the cold end of the hot stream. The residual heat load is on the hot portion of the hot stream. (See Figure 3.3)

A match of this class is a first type match; a cold end match and the heat load of the hot stream greater than that of the cold stream. This is a downstream match. (See Table 3.4)

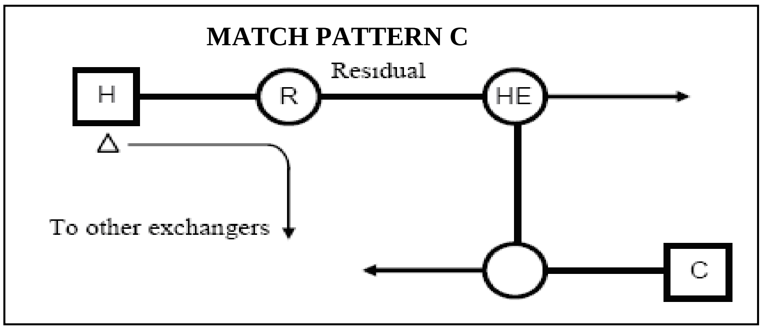


Figure 3.3 Class C Match Pattern

Definition 3.4 Class D Match Pattern: The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the hot end of the cold stream. The residual heat load is on the cold portion of the cold stream. (See Figure 3.4)

A match of this class is a second type match; a hot end match and the heat load of the cold stream greater than that of the hot stream. This is a downstream match. (See Table 3.4)

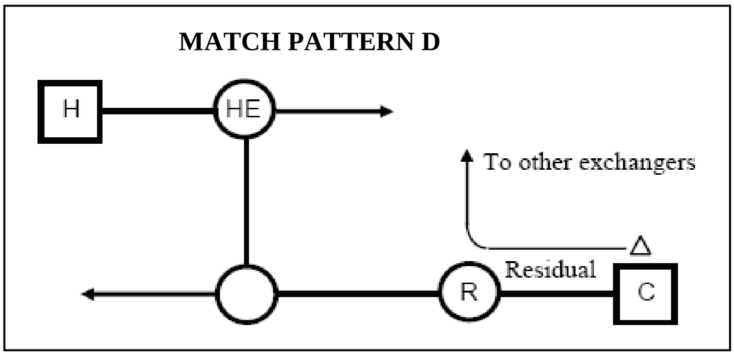


Figure 3.4 Class D Match Pattern

When the residual heat load in a match pattern is matched to a utility stream, it is closed or completed pattern. Otherwise, it is an open or incomplete pattern. It can be seen that if the heat load of the residual stream is less than the minimum heating or cooling requirement then the chances that the match pattern will be matched to a utility stream is high. So we give a match pattern which it's residual less than the minimum heating or cooling requirement a high priority in match pattern.

A match of Class A or Class C will leave a residual at the hot end, while a match of Class B or D will leave a residual at the cold end. Heuristics N3 and N4 will be use heuristics to further subclassify matches of Class A and B into matches of high priority.

Subclass AH. A match of this subclass is a member of Class A, a heating problem where the residual is less than or equal to the minimum heating requirement. (A letter H in the subclass name denotes that the residual is matched to heating utility.)

Subclass BK. A match of this subclass is a member of Class B, a cooling problem where the residual is less than or equal to the minimum cooling requirement. (A letter K in the subclass name denotes that the residual is matched to a cooling utility.)

As it might be expected, we give a match of subclasses AH in a heating subproblem and BK in cooling subproblem the highest priorities. See Table 3.4.

We further discriminate match patterns according to heat capacity flowrate. By following pinch heuristics, in a heating problem, we prefer a match where the heat capacity flowrate of a cold stream is greater than or equal to that of a hot stream. For example, A[H]H is a match in which the heat capacity flowrate of the cold stream is greater than that of the hot stream and the residual of the cold stream is matched to the heating utility.

Table 3.3 Match Pattern Operators of Class A and B

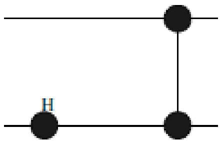
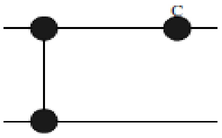
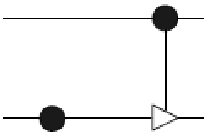
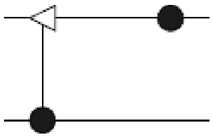
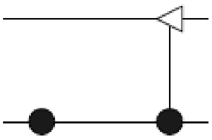
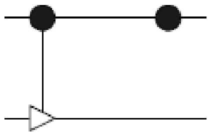
Match Operators	Conditions	Actions
 Pattern AH	$T_H^{s*} \geq T_C^{t**}$ $L_H \leq L_C$ $T_H^s \geq T_C^s + L_H W_C^{-1}$ $L_C - L_H \leq Q_{min}^{heating}$	Match H and C Status of H $\Leftarrow$ Matched*** $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern BK	$T_H^s \geq T_C^t$ $L_C \leq L_H$ $T_C^s \geq T_H^s - L_C W_H^{-1}$ $L_H - L_C \leq Q_{min}^{cooling}$	Match H and C Status of C $\Leftarrow$ Matched $T_H^s \Leftarrow T_H^s + L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$

Table 3.3(Continued) Match Pattern Operators of Class A and B

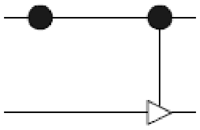
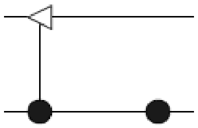
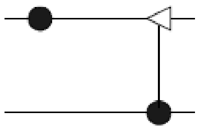
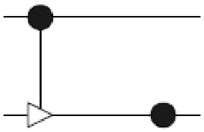
Match Operators	Conditions	Actions
 Pattern [AH]	$T_H^t \geq T_C^s$ $L_H \leq L_C$ $W_C \geq W_H$	Match H and C Status of C ⇐ Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern B[C]	$T_H^t \geq T_C^s$ $L_H \leq L_C$ $W_C \geq W_H$	Match H and C Status of C ⇐ Matched $T_H^s \Leftarrow T_H^s + L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern A[C]	$T_H^t \geq T_C^s$ $L_H \leq L_C$ $W_C < W_H$ $T_H^s \geq T_C^s + L_H W_C^{-1}$	Match H and C Status of H ⇐ Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern B[H]	$T_H^s \geq T_C^t$ $L_C \leq L_H$ $W_H < W_C$ $T_C^s \geq T_H^s - L_C W_H^{-1}$	Match H and C Status of C ⇐ Matched $T_H^s \Leftarrow T_H^s + L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$

*T^t = target temp, T^s = supply temp, W = heat capacity flowrate, L, Q=heat load.

** Cold stream temperatures are shifted up by ΔT_{min}.

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set process streams to be selected next.

Table 3.4 Match Pattern Operators of Class C and D

Match Operators	Conditions	Actions
 Pattern C[H]	$T_H^{t*} \geq T_C^{s**}$ $L_H > L_C$ $W_H \leq W_C$	Match H and C Status of C $\Leftarrow$ Matched*** $T_H^t \Leftarrow T_H^t - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern D[C]	$T_H^s \geq T_C^t$ $L_H < L_C$ $W_H \geq W_C$	Match H and C Status of H $\Leftarrow$ Matched $T_C^t \Leftarrow T_C^t + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 Pattern C[C]	$T_H^t \geq T_C^s$ $L_H > L_C$ $W_C < W_H$ $T_C^t \leq T_H^t + L_C W_H^{-1}$	Match H and C Status of C $\Leftarrow$ Matched $T_H^t \Leftarrow T_H^t - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 Pattern D[H]	$T_H^s \geq T_C^t$ $L_H \leq L_C$ $W_H < W_C$ $T_H^t \geq T_C^t - L_H W_C^{-1}$	Match H and C Status of H $\Leftarrow$ Matched $T_C^t \Leftarrow T_C^t + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$

*T^t = target temp, T^s = supply temp, W = heat capacity flowrate, L, Q=heat load.

** Cold stream temperatures are shifted up by ΔT_{min}.

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set process streams to be selected next.

Similarly in a cooling problem, we prefer a match where the heat capacity flowrate of the hot stream is greater than or equal to that of the cold stream. For example, B[C]K is a match in which the heat capacity flowrate of the hot stream is greater than that of the cold stream and the residual of the hot stream is matched to cooling utility.

In summary, the rankings of the match patterns in a heating problem are AH, A[H], B[C], A[C], B[H], C[H], D[C], C[C] and D[H]. For a cooling problem, BK, B[C], A[H], B[H], A[C], D[C], C[H], D[H] and C[C].

3.2.5 Disturbance Propagation Design Method

In order for a stream to be resilient with a specified disturbance load, the disturbance load must be transferred to heat sinks or heat sources within the network. With the use of the heuristic: To generate a heat exchanger network featuring the minimum number of heat transfer units, let each eliminate at least one of the two streams.

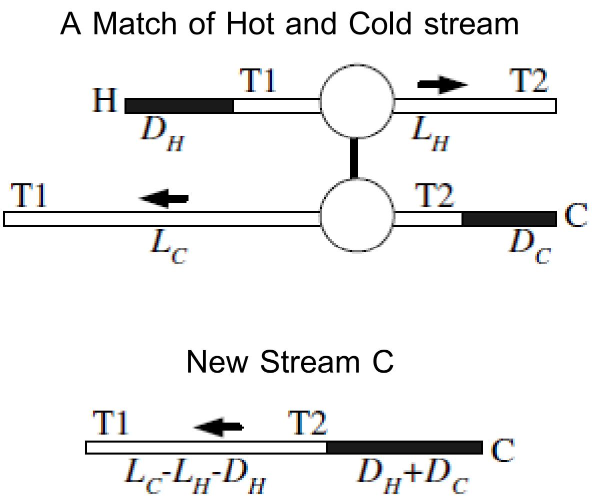
We can see that in a match of two heat load variable streams, the variation in heat load of the smaller stream S1 will cause a variation to the residual of the larger stream S2 by the same degree: in effect the disturbance load of S1 is shifted to the residual of S2. If the residual stream S2 is matched to S3 which has larger heat load, the same situation will happen. The combined disturbance load of S1 and S2 will cause the variation in the heat load to the residual S3. Hence, it is easy to see that the disturbance load and those obtained from S1 and S2. Or, if S2 is matched to a smaller heat load stream S4, the new disturbance load of residual S2 will be the sum of the disturbance loads of S1 and S4. Form this observation, in order to be resilient, a smaller process stream with specified disturbance load must be matched to be a larger stream that can tolerate its disturbance. In other words, the propagated disturbance wil not overshoot the target of the larger process stream.

However, the amount of disturbance load that can be shifted from one stream to another depends upon the type of match patterns and the residual heat load.

Hence, in design we must choose a pattern that yields the maximum resiliency. We can state that the resiliency requirement for a match pattern selection is that the entire disturbance load from a smaller heat load stream must be tolerated by a residual stream. Otherwise, the target temperature of the smaller stream will fluctuate by the unshifted disturbance. Of course, the propagated disturbance will be finally handled by utility exchangers. In short, the minimum heat load value of a larger stream must be less than a maximum heat load value of a larger stream must be less than a maximum heat load value of a smaller stream. By choosing the minimum heat load condition for the design, the new input temperature of a residual stream to its design condition according to the propagated disturbance. The propagated disturbance will proportionally cause more temperature variation in the residual stream and the range of temperature variation of the residual stream will be larger than its original range.

Definition 3.5 Propagated Disturbance. The propagated disturbance of a stream is the disturbance caused by a variation in heat load of 'up-path' streams to which such a stream is matched. Only a residual stream will have a propagated disturbance. The new disturbance load of a residual stream will be the sum of its own disturbance (if any) and the propagated disturbance. See Figure 3.5 and 3.6.

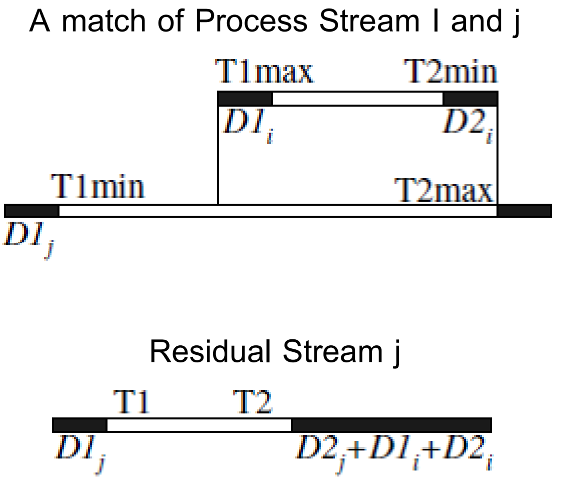
Hence, a stream with no original variation in heat load will be subjected to variation in heat load if it is matched to a stream with disturbance. Another design consideration is that the disturbance load travel path should be as short as possible, i.e. the least number of streams involved. Otherwise, the accumulated disturbance will be at high level. From the control point of view, it is difficult to achieve good control if the order of the process and the transportation lag are high. From the design viewpoint, are may not find heat sinks or sources that can handle the large amount of propagated disturbance (Wongsri, 1990).



A Match of Hot and Cold stream

New Stream C

Figure 3.5 A Concept of Propagated Disturbance



A match of Process Stream I and j

Residual Stream j

Figure 3.6 A General Concept of Propagated Disturbance

3.3 The Main Function of Control System

3.3.1 To reject disturbance

It is main function in the installation of process control system. The external disturbance is uncertain so the operator cannot monitor the changing in process. As a result, the control system must be installed to follow the process changing and manipulate the process variables to compensate for the external disturbance factors.

3.3.2 To maintain stability

Every control system must guarantee first the stability. The control system is set to improve the process stability for ensure of product quality and safety to equipment of process and plant.

3.3.3 To keep the highest performance of process

Besides the rejection of disturbance and maintaining stability, the control system can achieve the great profit because it losses less energy and raw materials during the operating. Furthermore the product will meet the desired specification and have production rate.

3.4 Plantwide Control Fundamentals

3.4.1 Integrated Processes

Figure 3.7 shows integrated process flowsheet. Three basic features of integrated chemical processes is the root of need to consider the entire plant's control system:

1) The effect of material recycle
2) The effect of energy integration
3) The need account for chemical component inventories

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

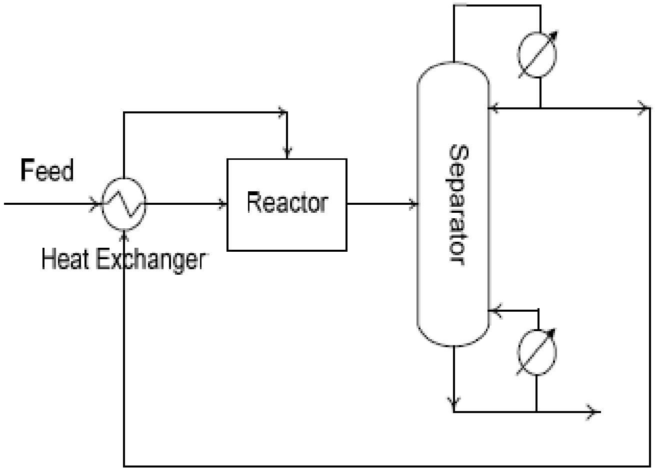


Figure 3.7 Integrated Process Flowsheet

3.4.1.1 Material Recycle

There are six basic and important reasons for material recycle.

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

2. Improve economics: In most systems it is simply cheaper to build a reactor with incomplete conversion level in one reactor or several in series. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

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

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

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

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

3.4.1.2 Energy Integration

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

3.4.1.3 Chemical Component Inventories

A plant's chemical species are divided into three types: reactants, products, and inerts. A materials balance for each of these components must be satisfied. However, the real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every mole of reactants fed into the plant must be consumed via reaction or leave as a purge or impurity. Because of their value, we prevent the leaving of reactants from process.

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

3.4.2 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex. The presence of recycle streams profoundly changes the plant's dynamic and steady state behavior. Two basic effects of recycle:

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

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

Snowball Effects

The high sensitivity of the recycle flow rates to small disturbances is called snowball effect. It is important to note that this is not a dynamic effect; it is a steady-state phenomenon. But it does have dynamic implications for inventory control and for disturbance propagation. It has nothing to do with closed-loop stability. However, this does not imply that it is independent of the plant's control structure. In contrast, the extent of the snowball effect is very strongly dependent upon the control structure used.

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

Let us consider one of the simplest recycle processes imaginable: a continuous stirred tank reactor (CSTR) and a distillation column. As shown in Figure 3.8, a fresh reactant stream is fed into reactor. Inside the reactor, a first-order isothermal irreversible reaction occurs $A \rightarrow B$. The specific reaction rates is k (h^{-1}) and the reactor hold up is V_R (moles). F_0 (moles/h) is the fresh feed flow rate and its composition is z_0 (mole fraction component A). The system is binary with only two components: reactant A and product B. The composition in the reactor is z (mole fraction A). The flow rate effluent reactor, F (moles/h), is fed into a distillation column that separates unreacted A from product B.

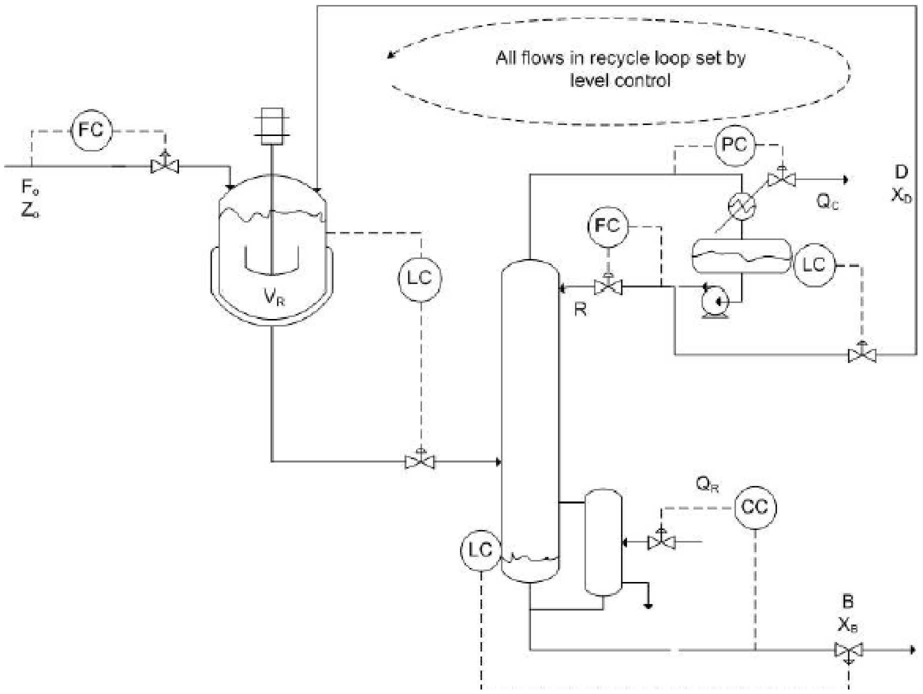


Figure 3.8 Conventional control structure with fixed reactor holdup

The relative volatile of A is more volatile than B, so the bottom from the column is the product stream. Its flow rate is B (moles/h) and its composition is x_B (mole fraction A). The amount of A impurity in this product stream is an important control objective and must be maintained at some specified level to satisfy the product quality requirements of the customer.

The overhead distillate stream from the column contains almost all of component A that leaves the reactor because of the purity specification on the bottom stream. It is recycled back to the reactor at a flow rate D and with a composition x_D (mole fraction A). The column has N_T trays and the feed tray is N_F (counting from the bottom). The reflux flow rate is R and the vapor boilup is V (moles/h).

Conventional control structure, as shown in Figure 3.6, the following control loops are chosen:

1. Fresh feed flow is controlled.
2. Reactor level is controlled by manipulating reactor effluent flow.
3. Bottoms product purity is controlled by manipulating heat input to the reboiler.
4. Distillate purity is controlled by manipulating reflux flow. Note that dual composition control (controlling both distillate and bottom purities) have been chosen to use in the distillate column, but there is no a priori reason for holding the composition of the recycle stream constant since it does not leave the process. It may be useful to control the composition of this recycle stream for reactor yield purposes or for improved dynamic response. The "best" recycle purity levels in both the design and operation of the plant are been often free to find.
5. Reflux drum level is held by distillate flow (recycle).
6. Base level is held by bottoms flow.
7. Column pressure is controlled by manipulating coolant flow rate to the condenser.

This control scheme is probably what most engineers would devise if given the problem of designing a control structure for this simple plant. Our tendency is to start with settling the flow of the fresh reactant feed stream as the means to regulate plant production rate, and then work downstream from there as if looking at a steady-state flowsheet and simply connect the recycle stream back to the reactor based upon a standard control strategy for the column.

However, this strategy is no flow controller anywhere in the recycle loop. The flows around the loop are set based upon level control in the reactor and reflux drum. This control structure is expected to find that exhibiting the snowball effect. By writing the various overall steady-state mass and component balances around the whole process and around the reactor and column, the flow of the recycle stream can be calculated at steady state for any given fresh reactant feed flow and composition.

With the control structure in Figure 3.8 and the base case fresh feed flow and composition, the recycle flow rate is normally 260.5 moles/h. However, the recycle flow must decrease to 330 moles/h when the fresh feed composition changes to pure A. Thus a 25 percent change in the disturbance (fresh feed composition) results in a 60 percent change in recycle flow. With this same control structure and the base case fresh reactant feed composition, the recycle flow drops to 187 moles/h if the fresh feed flow rate is changes to 265 moles/h. Thus a 23 percent change in fresh feed flow rate results in a 94 percent change in recycle flow rate. These snowball effects are typical for many recycle systems when control structure such as that show in Figure 3.8 are used and there is no flow controller somewhere in the recycle loop.

Variable reactant holdup structure, an alternative control structure is shown in Figure 3.9. This strategy differs from the previous one in two simple but important ways.

1. Reactor effluent flow is controlled.

2. Reactor holdup is controlled by manipulating the fresh reactant feed flow rate.

All other control loops are the same. The production rate cannot change directly by manipulating the fresh feed flow, because it is used to control reactor level. However, the plant throughput can achieve indirectly in this scheme by changing the setpoint of the reactor level controller. Using the same numerical case considered previously, the recycle flow rate does not change at all when the fresh feed composition changes. To alter production rate from 215 moles/h to 265 moles/h (a 23 percent change), the reactor holdup must be change from 1030 moles/h to 1520 moles/h (a 48 percent change), Recycle flow also changes, but only from 285 to 235 moles/h. This is an 18 percent change in recycle flow compared with 94 percent in the alternative strategy.

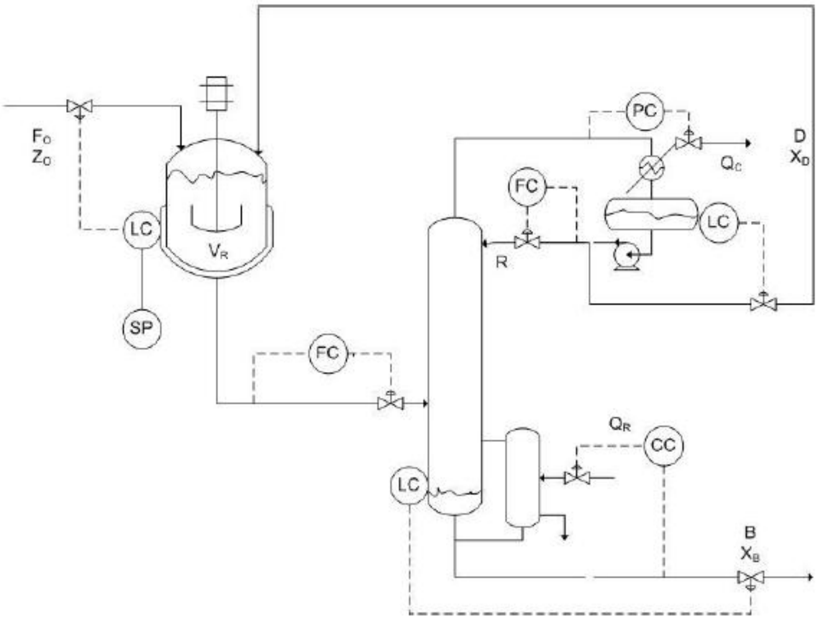


Figure 3.9 Control structure with variable reactor hold

3.4.3 Reaction/Separation Section Interaction

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

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

If the tuning of the reactor level controller in the conventional structure (Figure 3.9) is modified from normal PI to P only, then changes in production rate also produce changes in reactor holdup. This tends to compensate somewhat for the required changes in overall reaction rate and lessens the impact on the separation section. So both control system structure and the algorithm used in the inventory controller of the reactor affect the amount of this snowball phenomenon.

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

From this simple binary system, a very useful generation conclusion can be applied to more complex processes: changes in production rate can be achieved only by changing conditions in the reactor. This means something that affects reaction rate in the reactor must vary: hold up in liquid phase reactor, pressure in gas phase reactor, temperature, concentrations of reactants, and catalyst activity or initiator addition rate. Variable with a large effect are called dominant. By controlling the dominant variables in a process, partial control is achieved. The term partial control arises because it typically has fewer available manipulators than variables that would like to control. The setpoints of the partial control loops are the manipulated to hold the important economic objectives in the desire ranges.

The plantwide control implication of this idea is that production rate changes should preferentially be achieved by modifying the setpoint of a partial control loop in the reaction section. This means that the separation section will not be significantly disturbed. Using the control structure in Figure 3.8, changes in production rate require large changes in reactor composition, which disturb the column. Using the control structure shown in Figure 3.9, changes in production rate are achieved by altering the setpoint of a controlled dominant variable, reactor holdup, with only small changes in reactor composition. This means that the column is not disturbed as much as with the alternative control scheme.

3.5 The Plantwide Process Control

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

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

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

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

The goals for an effective plantwide process control system include:

1) Safe and smooth process operation
2) Tight control of product quality in the face off disturbance
3) Avoidance of unsafe process conditions
4) A control system run in automatic, not manual, requiring minimal operator attention
5) Rapid rate and product quality transitions
6) Zero unexpected environmental releases

3.6 Basic Concepts of Plantwide Control

Buckley Basics

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

Douglas doctrines

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Douglas points out the costs of raw materials and the value of the products. This leads to two Douglas doctrines.

a. Minimize losses of reactants and products.
b. Maximize flowrates through gas recycle systems.

The first idea implies that the tight control of stream compositions exiting the process is needs to avoid losses of reactants and products. The second rests on the principle that yield is worth more than energy.

Downs drill

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

Luyben laws

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

1. All recycle loops should be flow controlled to prevent the snowball effect.

2. A fresh reactant feed stream cannot be flow controlled unless there is essentially complete one-pass conversion of one of the reactants.

3. If final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). If the feed is saturated liquid, changes in feed flowrate or feed composition have less of dynamic effect on distillate composition than they do on bottoms composition.

Richardson rule

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

Shinskey schemes

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

Tyreus tuning

The P-only controller is used for liquid levels and sets the controller gain equal to 1.67. This will have the valve wide open when the level ia at 80 percent and the valve shut when the level is at 20 percent.

For PI controllers, the relay- feedback test is a simple and fast way to obtain the ultimate gain (K_u) and ultimate period (P_u). Either the Ziegler-Nichlos settings or the Tyerus-Luyben (1992) settings can be used:

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

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

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

3.7 Steps of Plantwide Process Control Design Procedure

In this section, each step of the design procedure is discussed in detail.

Step 1: Establish control objectives

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

This is probably the most important aspect of the problem because different control objectives lead to different control structures. These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine control degrees of freedom

Count the number of control valves available.

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to setpoint. The placement of these control valves can sometimes be made to improve dynamic performance, but often there is no choice in their location.

Most of these valves will be used to achieve basic regulatory control of the process: set production rate, maintain gas and liquid inventories, control product qualities, and avoid safety and environmental constraints. Any valves that remain after these vital tasks have been accomplished can be utilized to enhance steady state economic objectives or dynamic controllability.

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.

The term of energy management is used to describe two functions:

1) A control system must to remove exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used other unit operations in the process.

2) If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled.

Heat removal in exothermic reactors is crucial because of the potential for thermal runaways. In exothermic reactor is running adiabatically, the control system must prevent excessive temperature rise through reactor.

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. And this can be accomplished by raising temperature, increasing reactor holdup, increasing reactant concentrations, or increasing reactor pressure. 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.

Whatever variable we choose, we would like it to provide smooth and stable production rate transitions and to reject disturbances. The selected variable has the least effect on the separation section but also has a rapid and direct effect on reaction rate in reactor.

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.

For economic and operational reasons, we should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constant and deadtimes and large steady-state gains.

The product quality is more important compared with material balance. Hence it should be considered the product quality loops first, before the material balance control structure.

Step 6: Fix a flow in every recycle loop and control inventories (pressures and levels)

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

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent large changes in recycle flows that can occur if all flows in the recycle loop are controlled by level. Flow controlling a stream somewhere in all recycle loops is an important for any plantwide control strategy. So we determine what valve should be used to control each inventory variable. An inventory variable should be controlled with the manipulated variable that has the largest effect on it within that unit (Richardson rule).

Step 7: Check component balances

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

Component balances are important in processes with recycle streams. We must identify the specific mechanism or control loop to guarantee that there will be no uncontrollable buildup of any chemical component within the process (Downs drill)

The reactant components should be prevented to leave in the product streams. So we are limited to the use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. The purge rate is adjusted to control the inert composition stream in the recycle stream.

Step 8: Control individual unit operations

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

A tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flow rate to a furnace supplying energy to the reactor.

Step 9: Optimize economics or improve dynamic controllability

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

After satisfying all of the basic regulatory requirements, 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 utilized either to optimize steady-state economic process performance or to improve dynamic response.

3.8 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provide we can independently manipulate the two inlet flow rates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom fairy easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Figure 3.10 (a). It is possible to combine the P/P exchanger with a utility exchanger as in Figure 3.10 (b).

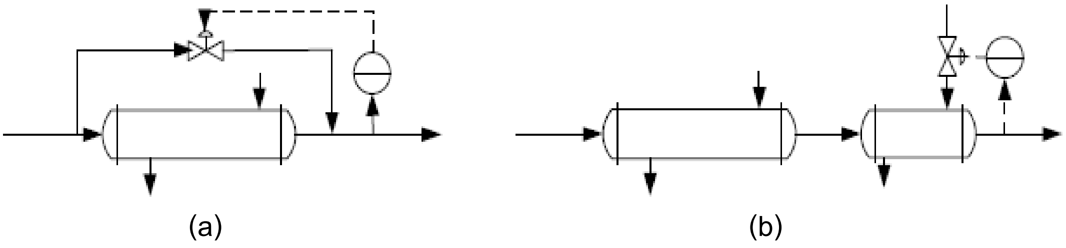


Figure 3.10 Control of P/P heat exchangers:

(a) Use of bypass; (b) use of auxiliary utility exchanger

3.8.1 Use of Bypass Control

When the bypass method is used for unit operation control, we have several choices about the bypass location and the control point. Figure 3.10 (b) shows the most common alternatives. For choosing the beat option, it depends on how we define the best. Design consideration might suggest, we measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high-temperature service. Cost consideration would also suggest a small bypass flow to minimize the exchanger and control valve sizes.

From a control standpoint, we should measure the most important stream, regardless of temperature, and bypass on the same side as well we control (see Figure 3.11 (a) and (b)). This minimizes the effects of exchanger dynamics in the loop. We should also want to bypass a large fraction of the controlled stream since it improves the control range. This requires a large fraction of the controlled stream since it improves the control range. This requires a large heat exchanger. There are several general heuristic guidelines for heat exchanger bypass streams. We typically want to bypass the flow of the stream whose temperature we want to control. The bypass should be about 5 to 10 percent of the flow to be able to handle disturbances. Finally, we must carefully consider the fluid mechanics of the bypass design for the pressure drops through the control valves and heat exchanger.

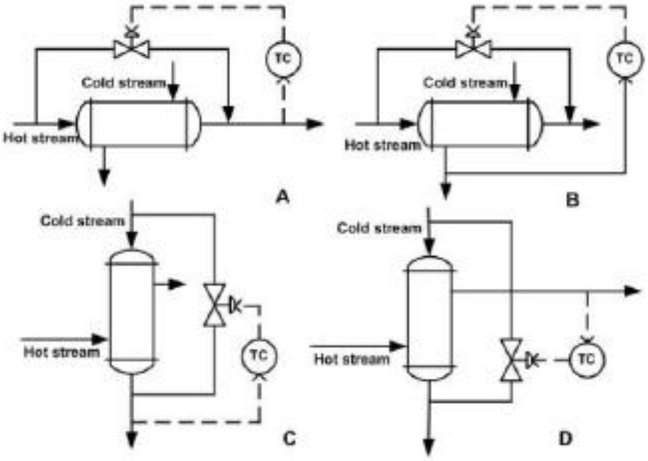


Figure 3.11 Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

3.9 New Plantwide Control Design Procedure

Luyben et al. (1998) proposed a 9-step heuristics procedure to design the plantwide control structure. This procedure is widely studied and used the plantwide process control community. Although the heuristic methodologies are easier to understand and implement but they just need the basic understanding of the process along with some experience. Thereby the structural design procedure is given explicitly. The designer's process engineering insight is necessity to pair CVs and MVs. Skogestad (2004) presented the new design procedure based on mathematical analysis. First, the operational objectives and the dynamic and steady state degree of freedom are identified. Then the set of primary controlled variables are selected. They basically are the active constraints and variables that must be maintained to achieve minimal economic loss when disturbances or implement error occur. Then the production rate is set based on the optimization resulted in the previous step. The secondary controlled variables are selected and the pairing of the choose sets of MVs and CVs are done hierarchically: regulatory control, supervisory control and optimization layers. In these steps, several analysis tools are utilized, e.g. pole vector analysis, RGA, CLDG analysis, linear and nonlinear optimization. This procedure does not discuss about the precedence of control variables and how to handle the disturbances.

New design procedure of Wongsri (2010) established the precedence of control variables. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the thermal disturbance propagation method (Wongsri, 1990) to cover the materials disturbances. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

Wongsri's plantwide control system design procedure:

Step 1: Establishment of control objectives

Step 2: Selected controlled variables to maintain product quality and to satisfy safety operational and environmental constrains and to setting the production rate. The selected CVs are ranked using the Fixture Point theorem.

Step 3: Selected manipulated variables and measurements via degree of freedom analysis.

Step 4: Energy management via heat exchanger network.

Step 5: Selection of control configuration using various tools available.

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

Step 7: Selection of controller type

Step 8: Validation via rigorous dynamic simulation.

3.10 Fixture Point Theorem

Hagglund (1995) present the real-time oscillation detection by calculates the integrated absolute error (IAE) between successive zero crossing of controller error signal. Its motivation is automatic monitoring of control-loop performance. The concept of material and energy disturbance propagation controls lead to fixture point theorem.

Fixture point theorem analysis:

1. The process is considered at dynamic mode (we run the process until the process responses are at the steady state).

2. Controlled variable can be arranged to follow the most sensibility of the process variable by step change of the manipulated variable in open loop control (change only one MV, the other should be fixed then alternate to other until complete).

3. Study the magnitude of integral absolute error (IAE) of all process variables that deviates from steady state.

4. Select controlled variable (CV) by considering CV that gave the most deviation from steady state (high value score).

CHAPTER IV
METHANOL PROCESS

4.1 Process Description

Methanol, also known as methyl alcohol or wood alcohol, is a volatile, colorless, flammable, and water-soluble liquid with mild alcoholic odor. It has a melting point of -97.7 °C, boiling point of 64.6 °C and density of 791 kg/m^3. It is polar, acid-base neutral, and generally considered non-corrosive.

The methanol process was proposed by Luyben (2010). It is a complex multi-unit process. There are three recycle streams, several unit operations, and many control loops to achieve the final goal of producing high product quality. The methanol process consists of three parts: synthesis gas compression, the methanol synthesis, and methanol separation.

4.1.1 Compression and Reactor Preheating

A fixed amount of synthesis gas is fed into the process. It is a mixture of carbon monoxide, carbon dioxide, hydrogen, methane, nitrogen, and water that can be produced from the gasification of biomass. A two-stage compression system is used for compressed the synthesis gas at 51.2 bar to 110 bar. The fresh feed flow rate is 11,450 kmol/h with composition 67.46 mol% hydrogen, 22.97 mol% carbon monoxide, 6.86 mol% carbon dioxide, 2.17 mol% methane, 0.3 mol% nitrogen, and 0.23 mol% water.

Three recycle gas streams are added, and the total gas stream enters a feed effluent heat exchanger (FEHE). The hot reactor effluent transfers heat into cold stream. The FEHE required area is 2,157 m^2 using an overall heat transfer coefficient of 144 kcal/h·m^2·K. Then the gas is heated to 150°C by a reactor pre-heater (H-102).

4.1.2 Methanol Synthesis

In this section, chemical reactions and kinetics parameters involved in methanol production are presented. The methanol synthesis takes place according to the reactions:

$$\begin{aligned} &CO + 2H_2 \leftrightarrow CH_3OH \\ &CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \end{aligned} \qquad (1)$$

The kinetic rate expressions are given by Vander Bussche and Froment (1996) in the following form by using the water gas shift reaction:

$$\begin{aligned} &CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \\ &CO_2 + H_2 \leftrightarrow CO + H_2O \end{aligned} \qquad (2)$$

Table 4.1 gives the kinetic and adsorption parameters (Luyben, 2010). The kinetic rate expressions are described by LHHW-type equations (Langmuir-Hinshelwood-Hougen-Watson). The unit of pressures and reaction rates use in bar and kmol/min/kg catalyst respectively. These must be transformed to use Pascals. The LHHW kinetic structure has the form:

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

The gas-phase exothermic reactions are conducted in a packed tubular reactor. The reaction used $Cu/ZnO/Al_2O_3$ as a solid catalyst. The reaction rate for the first reaction for the production of methanol from carbon dioxide is given in equation 4.

$$R_1 = (k_4 p_{CO_2} p_{H_2}) \frac{\left[1 - \frac{1}{K_{E1}}\left(\frac{p_{CH_3OH} p_{H_2O}}{p_{CO_2} p_{H_2}^3}\right)\right]}{\left[1 + k_3\left(\frac{p_{H_2O}}{p_{H_2}}\right) + K_{H_2}\sqrt{p_{H_2}} + K_{H_2O} p_{H_2O}\right]^3} \tag{4}$$

The reaction rate for the water gas shift reaction is given in equation 5.

$$R_2 = (k_5 p_{CO_2}) \frac{\left[1 - \frac{1}{K_{E2}}\left(\frac{p_{CO} p_{H_2O}}{p_{CO_2} p_{H_2}}\right)\right]}{\left[1 + k_3\left(\frac{p_{H_2O}}{p_{H_2}}\right) + K_{H_2}\sqrt{p_{H_2}} + K_{H_2O} p_{H_2O}\right]} \tag{5}$$

In which rate constant, adsorption coefficient and equilibrium constant are provided by Vander Bussche and Froment (1996).

For a type of reactor, the packed tubular reactor is selected. It has 8,000 tubes with length 12.2 m and diameter 0.03675 m. The heat transfer rate for coolant process stream is 244 kcal/h·m^2·K. The catalyst has a density of 2,000 kg/m^3, and the reactor bed void is 0.5. The temperature effluent reactor is cooled by FEHE and then a water-cooled heat exchanger (H-103) is used to cool it to 38°C before fed into the separator as shown in Figure 4.1.

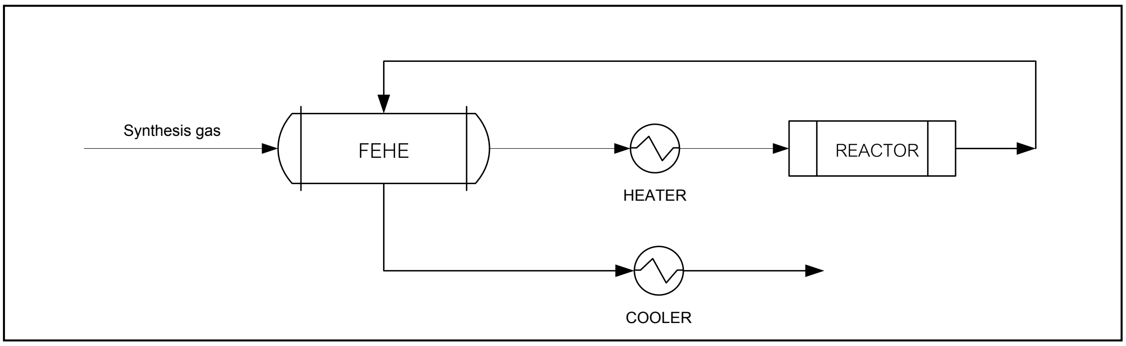


Figure 4.1 Methanol synthesis

Table 4.1 Kinetic LHHW Parameters (Luyben, 2010)

R_1: $CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$	
kinetic factor	k = 1.07 x 10^{-3} , E = 36 696 kJ/kmol
Driving-force expressions	
term 1: conc. exponents for reactants:	CO_2 = 1; H_2 = 1
conc. exponents for products:	CH_3OH = 0; H_2O = 0
coefficients:	A = -23.02581; B = C = D = 0
term 2: conc. exponents for reactants:	CO_2 = 0; H_2 = -2
conc. exponents for products:	CH_3OH = 1; H_2O = 1
coefficients:	A = 24.388981; B = -7059.7258; C = D = 0
Adsorption expression	
adsorption term exponent:	3
concentration exponents:	
term 1:	H_2 = 0; H_2O = 0
term 2:	H_2 = -1; H_2O = 1
adsorption constants:	
term 1:	A = 0, B = 0, C = 0, D = 0
term 2:	A = 8.1471087, B = C = D =0

Table 4.1(Continued) Kinetic LHHW Parameters (Luyben, 2010)

R_2: CO_2+ H_2 ↔ CO + H_2O	
kinetic factor	k = 1.07 x 10^{-3} ,E = 36 696 kJ/kmol
Driving-force expressions	
term 1: conc. exponents for reactants:	CO_2 = 1; H_2 = 1
conc. exponents for products:	CH_3OH = 0; H_2O = 0
coefficients:	A = -23.02581; B = C = D = 0
term 2: conc. exponents for reactants:	CO_2 = 0; H_2 = -2
conc. exponents for products:	CH_3OH = 1; H_2O = 1
coefficients:	A = 24.388981; B = -7059.7258; C = D = 0
Adsorption expression	
adsorption term exponent:	3
concentration exponents:	
term 1:	H_2 = 0; H_2O = 0
term 2:	H_2 = -1; H_2O = 1
adsorption constants:	
term 1:	A = 0, B = 0, C = 0, D = 0
term 2:	A = 8.1471087, B = C = D =0

4.1.3 Methanol Separation

The separator operates at 106.46 bar and 38°C. Most of vapor stream is compressed back up to 110 bar and recycled with compressor work (K3). The inert components (methane and nitrogen) must be purge out of the system. A split fraction (0.022) is vented off. The concentrations of methane and nitrogen in the vent stream are 28.5 mol% and 4 mol%, respectively.

Because of high pressure in the separator, the liquid from this unit contains amounts of light components. Therefore, a flash tank is used to remove most of the light components before feeding into distillation column. The flash tank is operated at 2 bar. The gas is compressed to 110 bar and recycled with compressor work (KFLASH).

In methanol distillation, liquid from flash tank is pumped into a column on stage 27. This column has 42 trays (including reboiler and condenser) and operates at 1 bar. A small vapor stream from the top of reflux drum recycles the small amounts of inert components entering the distillation column. The compressor K4 compresses this small vapor stream (0.669 kmol/h) to 110 bar. The distillation stream with a purity of 98.9 mol% methanol removes the water from system. The final flowsheet shows in Figure 4.2.

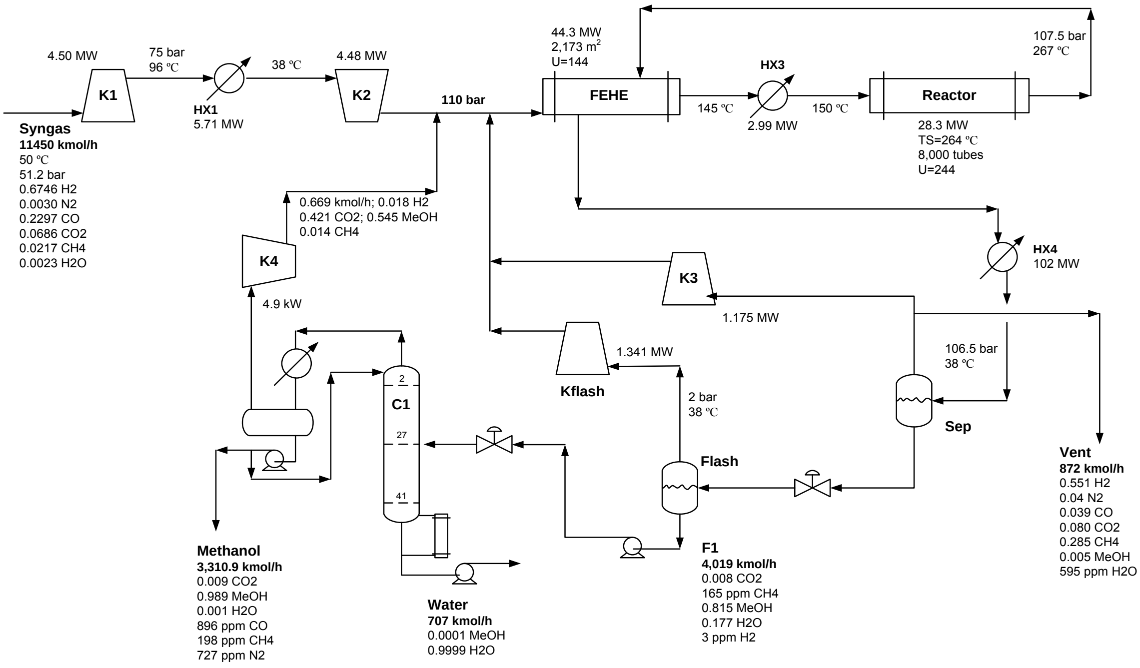


Figure 4.2 Methanol Process Flowsheet

4.2 Design of Heat Exchanger Networks

From previous chapter, the design procedures and definition of Heat Exchanger Networks (HENs) are used to design for methanol process. The Problem Table Method is applied to find pinch temperature. The information for design is shown in Table 4.2 (a) and (b).

Table 4.2(a): The information of the methanol process

Stream Name	Tin (°C)	Tout (°C)	W (MW/°C)	Duty (MW)
H1: Product Stream of Methanol Reactor	266.60	38.00	0.491	112.40
C1: Stream total	52.90	144.50	0.485	44.44
C2: Reboiler	109.60	109.82	239.981	52.79

Table 4.2(b): The information of the methanol process

Stream	W (MW/C)	Supply Temp (°C)			Target Temp (°C)
		Nom	Min	Max	
H1	0.491	266.60	261.60	271.60	38.00
C1	0.485	52.90	47.90	57.90	150.00
C2	239.981	109.60	104.60	109.60	109.82

There is no pinch temperature when we use pinch method, which use the minimum temperature difference, equal to 10°C. However, we can find the minimum cold utilities requirements which equal to 12.91 MW.

4.2.1 HEN Base Case

Figure 4.3 shows Heat Exchanger Network (HEN) of methanol process (Base case) followed by a task of Luyben (2010).

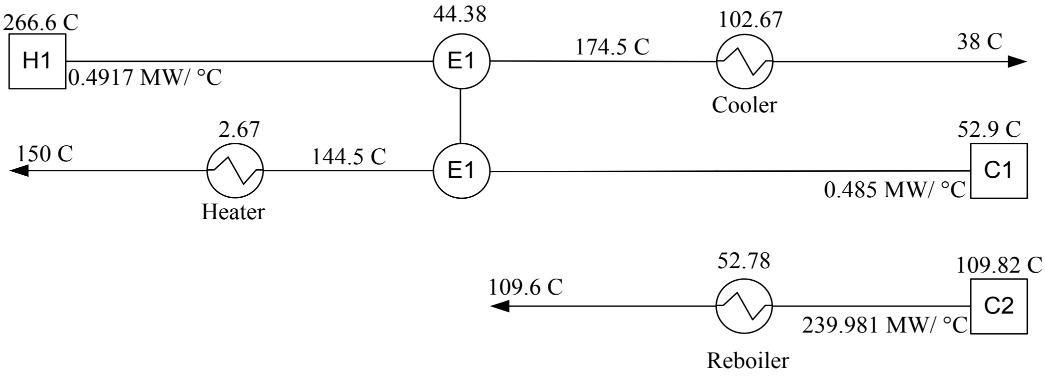


Figure 4.3 The heat exchanger network, Base case.

4.2.2 HEN using the disturbance propagation method

The disturbance propagation method and match pattern are applied for design heat exchanger network as shown in Table 4.3. In the network of the methanol process has only one hot stream (H1) and two cold streams. This design can be simply translated to a heat exchanger network for methanol process in Figure 4.4 and 4.5.

Table 4.3 Synthesis table for methanol process

Stream	Load	W	T1	T2	D1	D2	DT	Action
b.) State 1								
H1	109.942	0.491	261.60	38.00	4.91	0.00	4.91	Selected B[H]
C1	42.017	0.485	150.00	57.90	0.00	4.85	4.85	Selected
C2	52.795	239.981	109.82	109.60	0.00	0.00	0.00	
c.) State 2								
H1	60.403	0.491	154.22	38.00	0.00	0.00	9.768	Selected BK
C1								Matched to H1
C2	52.795	239.981	109.82	109.60	0.00	0.00	0.00	Selected
d.) State 3								
H1	52.795	0.491	145.06	38.00	0.00	0.00	9.768	To cooler
C1								Matched to H1
C2								Matched to H1

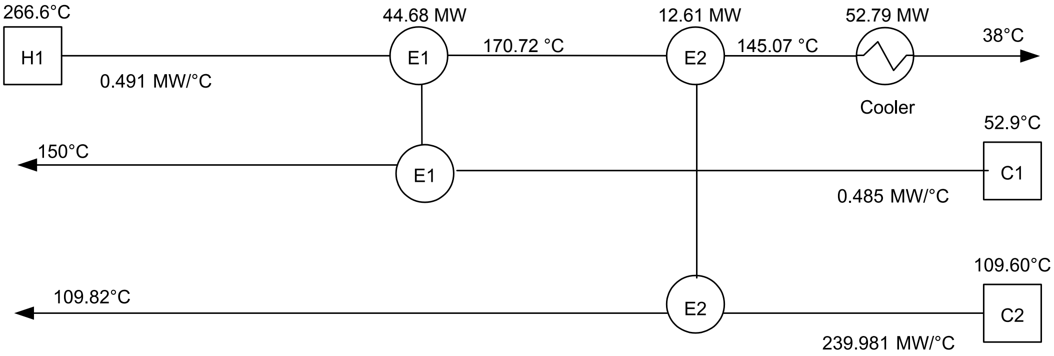


Figure 4.4 The heat exchanger network using the disturbance propagation method

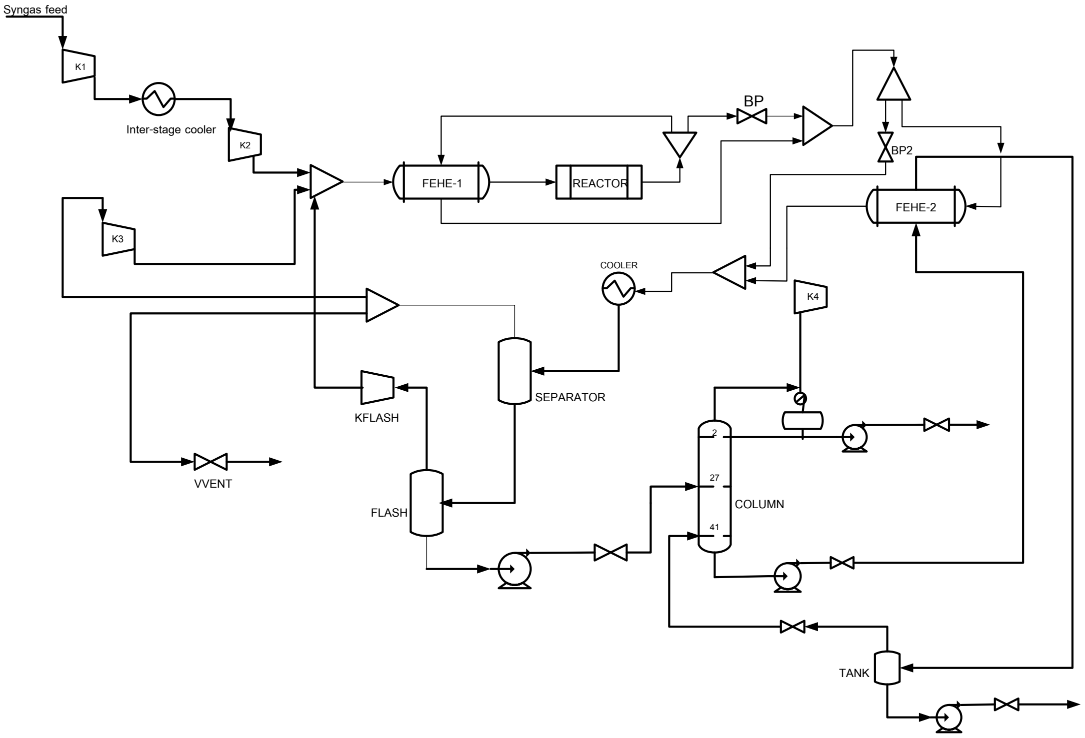


Figure 4.5 The methanol process flowsheet with resilient heat exchanger network

4.3 Steady State Simulation

Figure 4.6 and 4.7 show a steady state schematic methanol process flowsheet of the base case control structure (Luyben, 2010) and resilient heat exchanger network, respectively. It is simulated in Aspen Plus. The physical properties model “RK-Aspen” is used in all units of the process except in the distillation column which used the van Larr equations. Kinetic parameters entered into the Aspen-LHHW reaction model. A packed tubular reactor is simulated in Aspen using the RPLUG model with a constant medium temperature. There are two vapor-liquid flash separations in the process. The Aspen “Flash2” model is used in the separator block and the flash block.

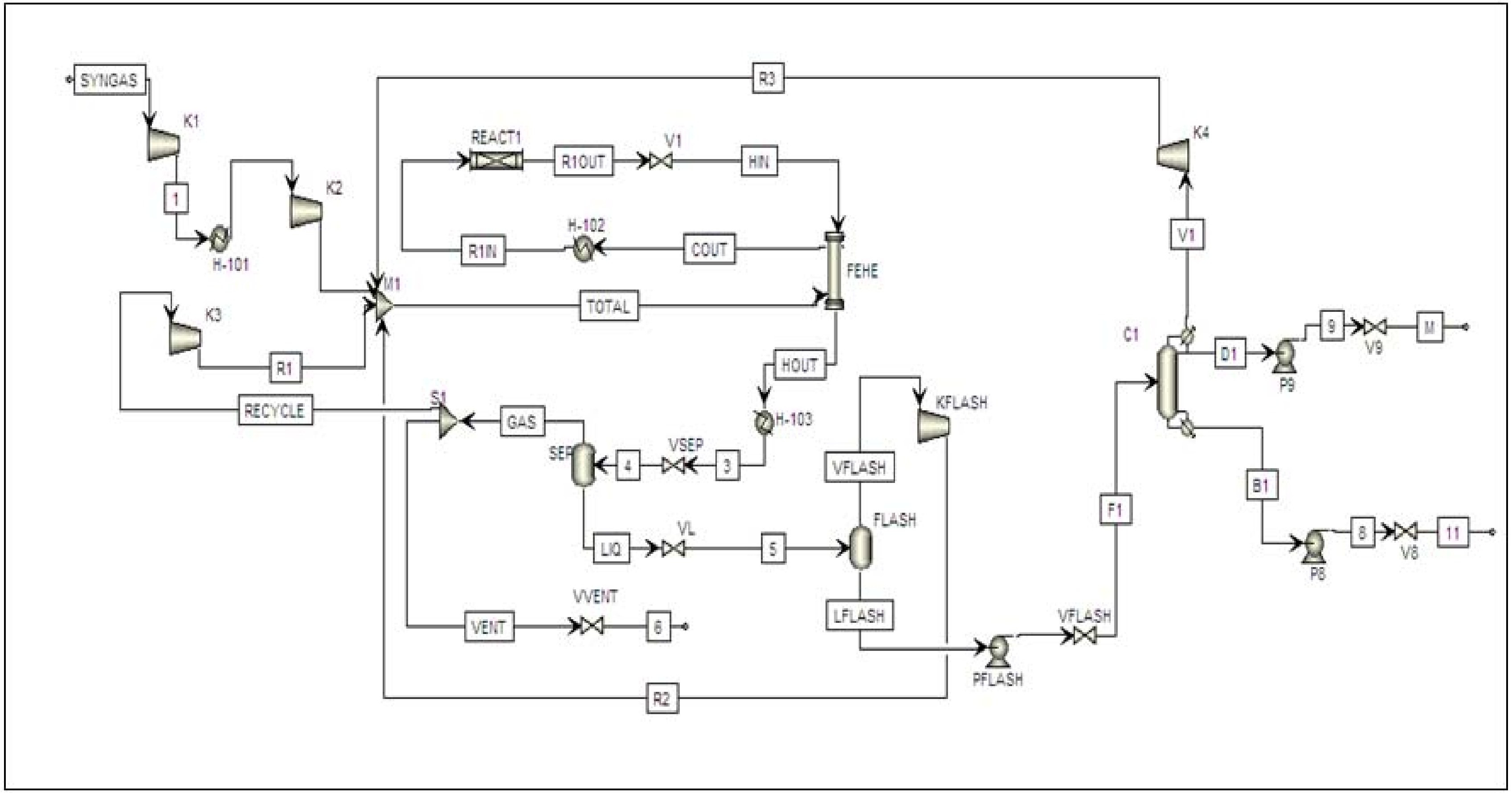


Figure 4.6 Steady state flowsheet of methanol process (Base case control structure).

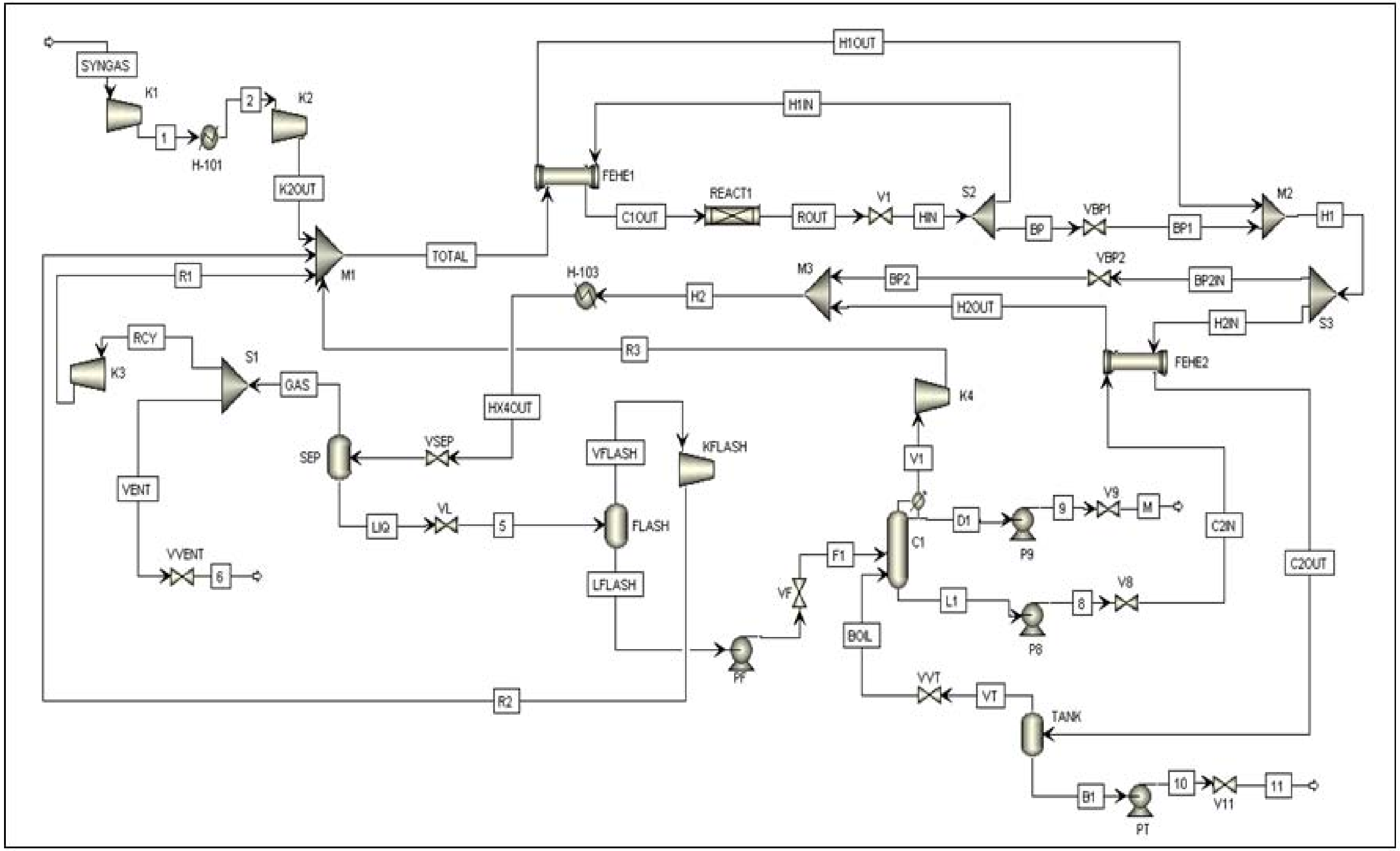


Figure 4.7 Methanol process flowsheet with resilient heat exchanger network

CHAPTER V

CONTROL STRUCTURE DESIGN AND DYNAMIC SIMULATION

Dynamic simulation is mainly used to improve unit yields, stability, safety, and controllability of plant. It is able to predict how the process changes with time and also assist in the evaluation and design of the control structures for a particular process. The essential tasks of plantwide control for a complex plant are maintaining the plant mass and energy balance when the disturbance occurs. The control system is needed to reject disturbance load and regulate process into a design condition. This chapter presents the new control structure design and compares with base case via Aspen-Dynamics version 7.0.

5.1 New Plantwide Control Structure

The proposed plantwide control structure is designed based on Wongsri's procedure and discussed below.

Step 1: Establishment of control objectives

The general objectives include reaction yield, product quality, environmental and safety restrictions. In this step, control objectives are divided into two levels: Plantwide level and Unit level.

Plantwide Level: For this process, the control objective is to maintain product purity of methanol composition at 98.9 mol%.

Unit Level: Stability and smooth operation.

Process constraints during operation:

1 The temperature reactor effluent should be 267°C.

2. The reactor inlet temperature should be 150°C.

3. The pressure in flash tank should be 2 bar.

4. The separator temperature should be 38°C.

5. The distillation column should operate at 1 bar.

Step 2: Selected controlled variables to maintain product quality and to satisfy safety operational and environmental constrains and to setting the production rate. The selected CVs are ranked using the Fixture Point theorem.

Plantwide Level: Consider material recycle loop because it causes a system to be burn “snowball effect”. Methanol process has three recycle streams. Therefore to avoid snowball effect is control the composition of methane in “RECYCLE” stream and molar flow rate of stream “V1”.

Unit Level: Use the Fixture Point method to select controlled variables from candidate all of them to maintain product quality, to satisfy safety operational, environmental constrains and to setting the production rate. The most disturbed points must be satisfactorily controlled by giving them consideration before other variables.

Table 5.1 shows the ranked controlled variables (CVs) and the integral absolute error (IAE) summation result. The candidate controlled variables are screened by using input variable change (change five percent of manipulated variables) to select appropriate controlled variables. The highest IAE summation value of the CVs is the first point to control.

Table 5.1 he ranked CVs and the IAE summation result.

Rank		Variables	SUM IAE
1	Reboiler of methanol column	Level	3.1834
2	Methanol Column	Temperature	3.0145
3	Condenser of methanol column	Level	2.2725
4	SYNGAS fresh feed stream	Flow rate	1.6525
5	Recycle stream to compressor K3	Methane composition	1.4155
6	Separator	Pressure	0.9273
7	Compressor K1 outlet stream	Pressure	0.6741
8	Separator	Temperature	0.5151
9	Condenser of methanol column	Pressure	0.4365
10	Separator	Level	0.3858
11	Methanol reactor inlet stream	Temperature	0.3399
12	Methanol reactor outlet stream	Temperature	0.2852
13	Flash tank	Pressure	0.2005
14	Flash tank	Level	0.1703
15	Inter stage cooler outlet stream	Temperature	0.1204
16	Vapor stream from methanol column	Flow rate	0.0004

Table 5.2 and Figure 5.1 show the IAE summation result of tray temperature for methanol column (C1) from Fixture Point method to select appropriate controlled variables of tray temperature for methanol column. We select the temperature on tray 35th (include reboiler and condenser stage) to control because it has maximum deviation and the most sensitive.

Table 5.2 IAE summation result of tray temperature deviation for methanol column

Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE	Tray	SUM IAE
2	0.8645	10	0.8988	18	0.8191	26	0.7106	34	2.9870
3	0.8869	11	0.8930	19	0.8047	27	0.7002	35	3.0145
4	0.9011	12	0.8861	20	0.7901	28	0.8466	36	2.7852
5	0.9084	13	0.8780	21	0.7755	29	1.0684	37	2.4648
6	0.9107	14	0.8685	22	0.7612	30	1.3396	38	2.1199
7	0.9100	15	0.8578	23	0.7474	31	1.6807	39	1.7216
8	0.9075	16	0.8459	24	0.7343	32	2.1067	40	1.2954
9	0.9037	17	0.8329	25	0.7220	33	2.6263	41	0.93330

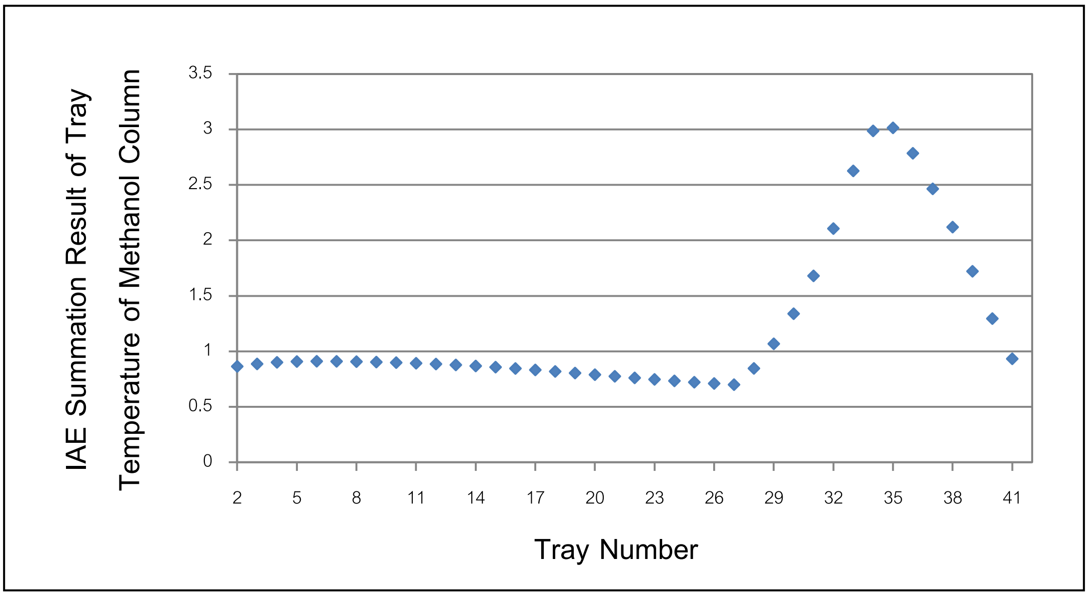


Figure 5.1 IAE summation result of tray temperature of methanol column

Figure 5.2 shows the temperature gradient for methanol column (large changes in temperature from tray to tray). The appropriate controlled variable of tray temperature from the slope value of tray temperature for methanol column at steady state condition is similar with result of Fixture Point method.

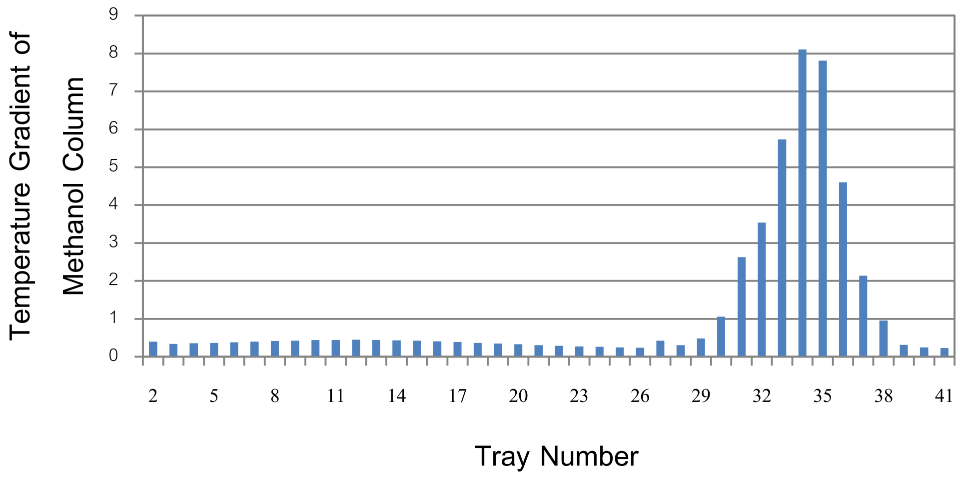


Figure 5.2 Temperature Gradient of Methanol Column

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

The manipulated variables and measurements which are selected for each designed control structures are shown in Table 5.3. The base case control structure (CS0) for methanol process has 19 degree of freedom. In the part of control structures designed with resilient heat exchanger (CS1 to CS3), the bypass valve is necessary to used as a manipulated variable so there are 22 degree of freedom.

Table 5.3 Degree of freedom of methanol process

Unit Operations	Position	degree of freedom
Compressor	Work: K1, K2, K3, K4, and KFLASH	5
Heater and Coolers	Duty: H-101, H-102, and H-103 Bypass valve (VBP1, VBP2)*	4
Methanol reactor	Reactor effluent valve (V1) and steam temperature	2
Separator	VSEP, Liquid effluent valve (VL) and vent valve (VVENT)	3
Flash tank	Liquid effluent valve (VFLASH)	1
Methanol column	Reboiler duty**, Condenser duty, Reflux flowrate, Distillate valve (V9), and Bottom valve (V8)	5
Tank*	Vapor valve (VVT), Liquid valve (V11)	2
	sum	22

Degree of freedom = 22

Note that: *the bypass valves and tank are counted and ** reboiler duty is not counted as manipulated variables for the control structure designed (CS1 to CS3).

Step 4: Energy management via heat exchanger networks

The design of heat pathways for resilient heat exchanger network is shown in Figure 5.3. In the network, hot stream (H1) is the reactor effluent stream. Cold stream (C1) is the "total" stream coming from the mixer (M1) and C2 is the cold-side stream coming from the bottoms of methanol column. Considering the hot stream H1 exchange heat with the cold stream (C1 and C2), the C1, C2 temperature is controlled using the bypass stream to maintain the inlet temperature condition of methanol reactor. Figure 5.4 presents the control configurations of resilient heat exchanger network.

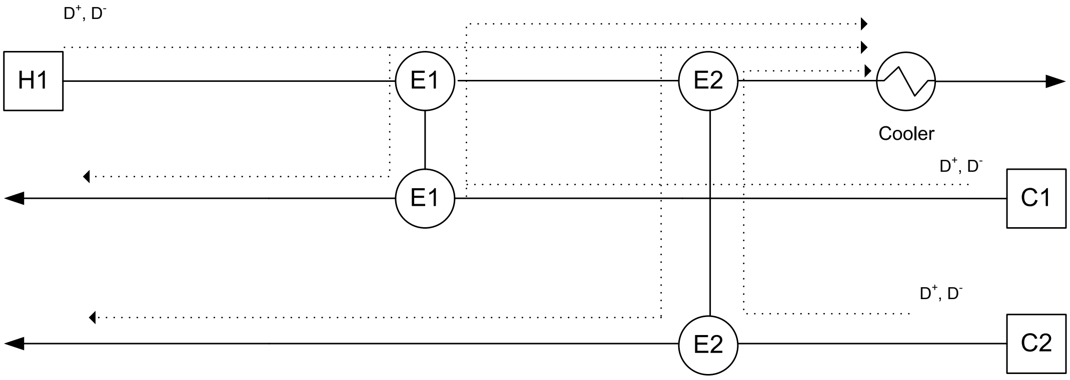


Figure 5.3 Heat pathways of resilient heat exchanger network

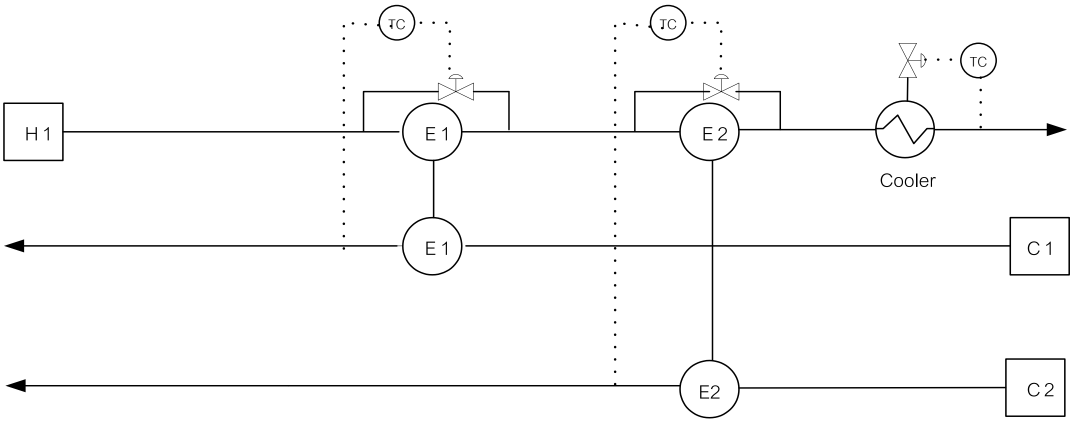


Figure 5.4 Control configurations of resilient heat exchanger network

Step 5: Selection of control configuration using various tools available

Selection of control configuration uses heuristic process knowledge. The criteria for selecting an adjustable variable include: causal relationship between the valve and controlled variable, automated valve to influence the selected flow, fast speed of response, ability to compensate for large disturbance and ability to adjust the manipulated variable rapidly and with little upset to the reminder of the plant. Table 5.4 shows the parings of controlled variables (CVs) and manipulated variables (MVs).

Table 5.4 The pairings of CVs and MVs

Unit/Stream	CVs	MVs			
		CS0	CS1	CS2	CS3
SYNGAS	F	wk1	wk1	wk1	wk1
K1OUT	P	wk2	wk2	wk2	wk2
HX1OUT	T	Qh1	Qh1	Qh1	Qh1
Reactor inlet	T	Qh2	VBP1	VBP1	VBP12
Reactor outlet	T	Tcool	Tcool	Tcool	Tcool
Separator	T	Qh3	Qh3	Qh3	Qh3
	P	VVENT	VVENT	VVENT	VVENT
	L	VL	VL	VL	VL
Flash tank	P	wkflash	wkflash	wkflash	wkflash
	L	VFLASH	VFLASH	VFLASH	VFLASH
Recycle	C	VVENT	VVENT	VVENT	VVENT
Condenser of column	P	Qcond	Qcond	Qcond	Qcond
Reflux drum	L	V9	V9	V9	Reflux
Tray 35th of column	T	Qreb	VBP2	VBP2	VBP2
Reboiler of column	L	V8	V8	V8	V8
V1 stream of column	F	wk4	wk4	wk4	wk4
Column	R/F	Reflux	Reflux	-	V8

Note: C = Composition, F = Flow rate, L = Liquid level, P = Pressure, T = Temperature, and R/F = Reflux to Feed ratio

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

Component balances are particularly important in process with recycle streams because of their integration effect. In methanol process, there are seven components: carbon dioxide (CO_2), carbon monoxide (CO), hydrogen (H_2), methanol

(CH_3OH), methane (CH_4), nitrogen (N_2) and water (H_2O). The reactant components should not be left in product stream and inert should be risked from process because of yield loss and maintain product quality. Table 5.5 shows the checking component balance of all components.

Accumulation = Input – Output + Generation – Consumption

Table 5.5 Component Balance

Component	Input	Output	Generation	Consumption	Accumulation Controlled by
CO_2	Fresh feed	0	0	Methanol synthesis	Fresh feed flow control
CO	Fresh feed	0	0	Methanol synthesis	
H_2	Fresh feed	0	0	Methanol synthesis	
CH_3OH	0	Product stream	Methanol synthesis	0	Tray temperature column control
H_2O	Fresh feed	Bottom stream	Methanol synthesis	0	
CH_4	Fresh feed	Vent stream	0	0	Composition control of recycle loop
N_2	Fresh feed	Vent stream	0	0	Fresh feed flow control

Step 7: Selection of controller type

In this research, all controller types are single loops which they consist of single loops and multiple loops. There are temperature controller, pressure controller, level controller, flow controller, and composition controller. PIs controller are used in all loops. All level loops are Proportional-only. Temperature and composition controllers as PIs are tuned using relay feedback test to obtain ultimate gains and ultimate periods and then applying Tyreus-Luyben tuning rules.

Step 8: Validation via rigorous dynamic simulation

Performance of all designed control structures is evaluated using software Aspen Dynamics and compared with base case control structure (Luyben, 2010) at dynamic simulation.

5.2 Design of Plantwide Control Structure

Wongsri's procedure (2009) is applied to design plantwide control structures for methanol process. All control structures (CS0, CS1, CS2, and CS3) the same loops are used as follows:

Plantwide level

- Compressor work of K4 is manipulated to control the vapor recycle flow rate from distillation column.
- Valve VVENT is manipulated to control the methane composition in stream "RECYCLE".

Unit level

Two-stage compressor unit

- Work of the first compressor is manipulated to control the feed flow rate.

- Work of the second compressor is manipulated to control the outlet pressure of the first compressor.

- Heat removal of inter stage cooler (H-101) is manipulated to control its outlet temperature before feed to the next stage compressor.

Reactor (REACT1) unit

- Coolant temperature is manipulated to control the reactor temperature.

Separator unit

- Heat removal (cooling water) of condenser (H-103) is manipulated to control the separator inlet temperature.

- Valve VL is manipulated to control the separator liquid level.

- Valve VVENT is manipulated to control the separator pressure.

Flash tank unit

- Compressor work of KFLASH is manipulated to control the pressure.

- Valve VFLASH is manipulated to control the liquid level.

Methanol Column (C1) unit

- Distillate valve (V9) is manipulated to control the reflux drum level.

- Condenser heat removal is manipulated to control the pressure condenser.

5.2.1 Summary of All Control Structures Design

In all of these control structures (CS0, CS1, CS2, and CS3), the different loops of each control structure are as follows:

Base case control structure (CS0)

For methanol column (C1), reflux to feed ratio control is selected and the tray 35th temperature is controlled by manipulating the reboiler heat input. The reflux drum level and base level are controlled by manipulating the distillate valve (V9) the bottom valve (V8), respectively. The pressure condenser is controlled by manipulating condenser heat removal. The inlet temperature of methanol reaction section is controlled by manipulating the heat input of the pre heater (H-102). As shown in Figure 5.5.

Control structure design I (CS1)

For methanol column (C1), the reflux to feed ratio control is selected and the tray temperature column is controlled by bypass valve (VBP2). The reflux drum level and base level are controlled by manipulating the distillate valve (V9) the bottom valve (V8), respectively. The pressure condenser is controlled by manipulating condenser heat removal. The inlet temperature of methanol reaction section is controlled by manipulating the valve bypass (VBP1). As shown in Figure 5.6.

Control structure design II (CS2)

The control structure design (CS2) lacks of reflux to feed ratio control. The tray temperature column is controlled by bypass valve (VBP2). The reflux drum level and base level are controlled by manipulating the distillate valve (V9) the bottom valve (V8), respectively. The pressure condenser is controlled by manipulating condenser heat removal. The inlet temperature of methanol reaction section is controlled by manipulating the valve bypass (VBP1). As shown in Figure 5.7.

Control structure design III (CS3)

For methanol column (C1), the reflux to feed ratio control (R/F) and the valve position control are selected for this control structure. The output from (R/F) is a setpoint of the valve position controller which has input as a reflux flowrates. The output from this controller is used to manipulate distillation valve (V9). The tray temperature is controlled by manipulating the bypass valve (VBP2). The reflux drum level is controlled by manipulating the reflux flow rate. The pressure condenser is controlled by manipulating condenser heat removal. The inlet temperature of methanol reaction section is controlled by manipulating the valve bypass (VBP1). As shown in Figure 5.8

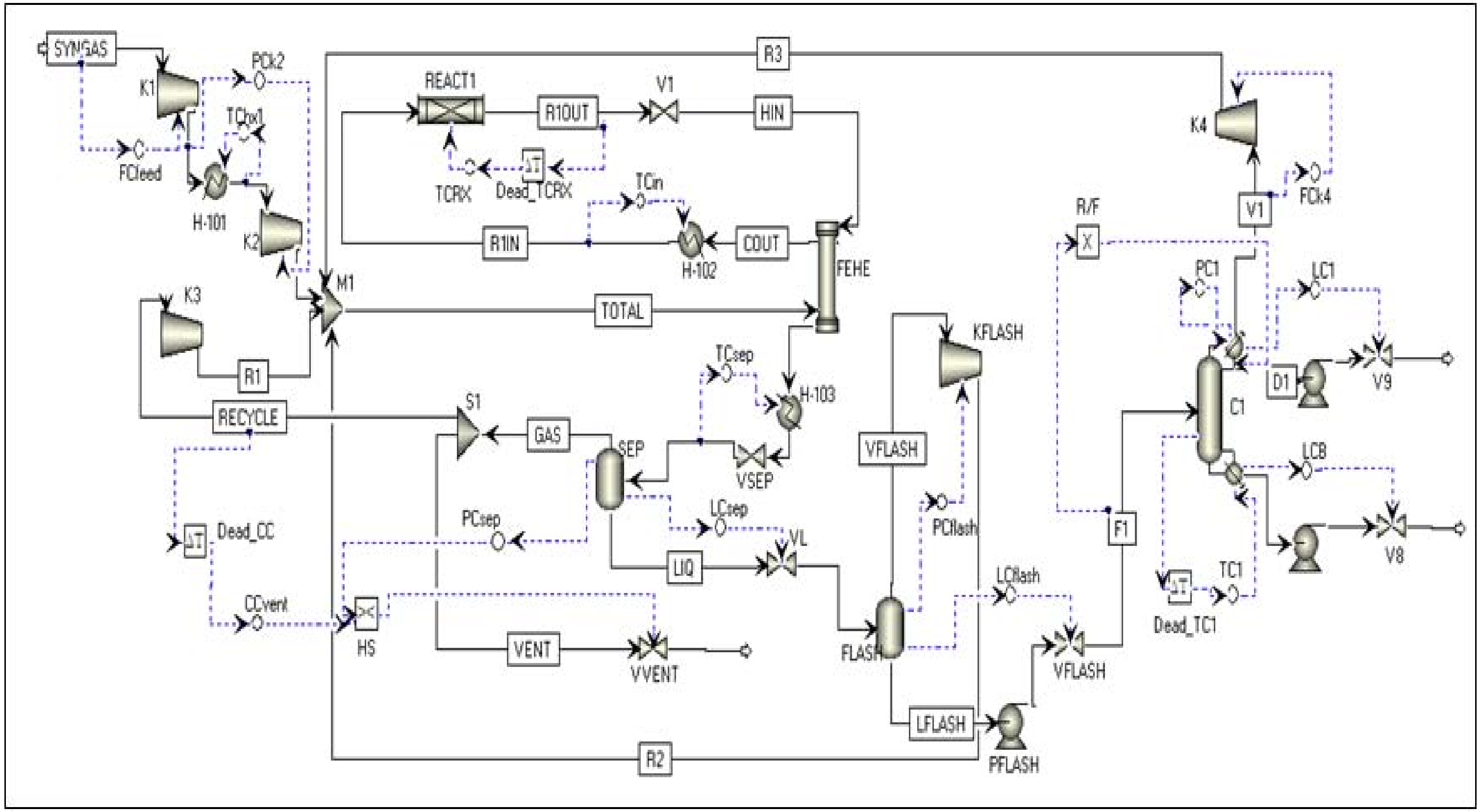


Figure 5.5 Base case control structure (CS0) for methanol process, Luyben (2010)

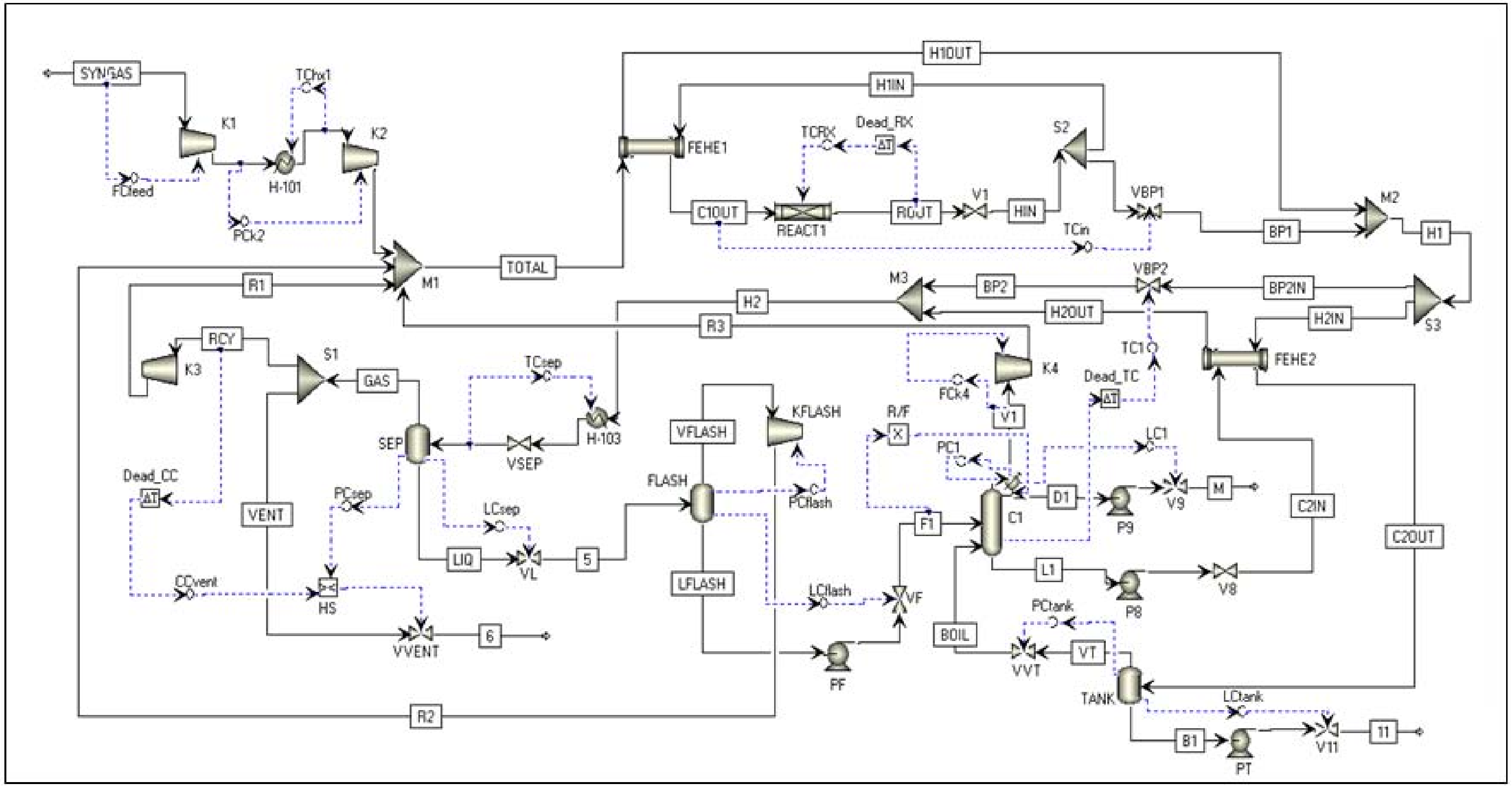


Figure 5.6 Designed control structure (CS1) for methanol process

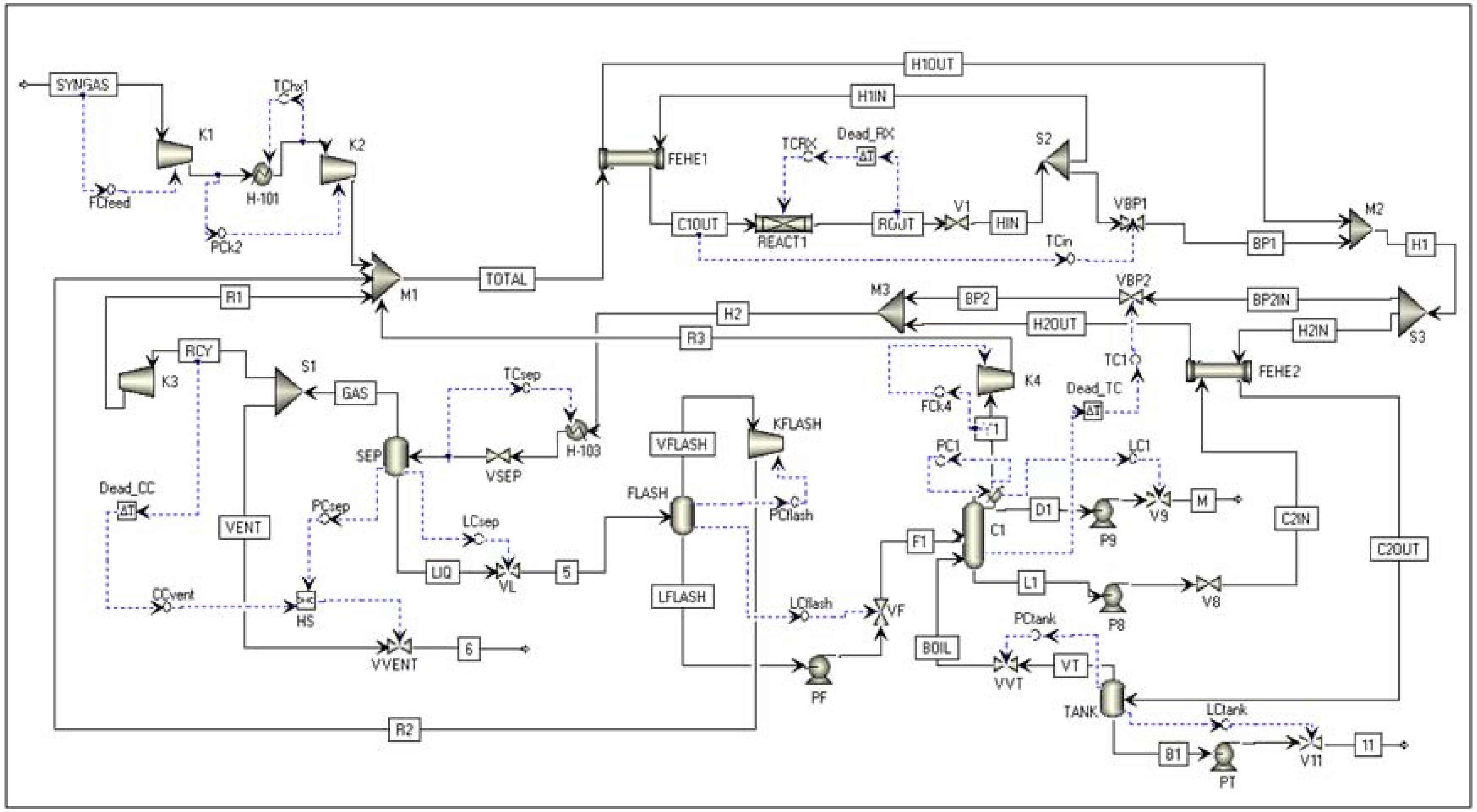


Figure 5.7 Designed control structure (CS2) for methanol process

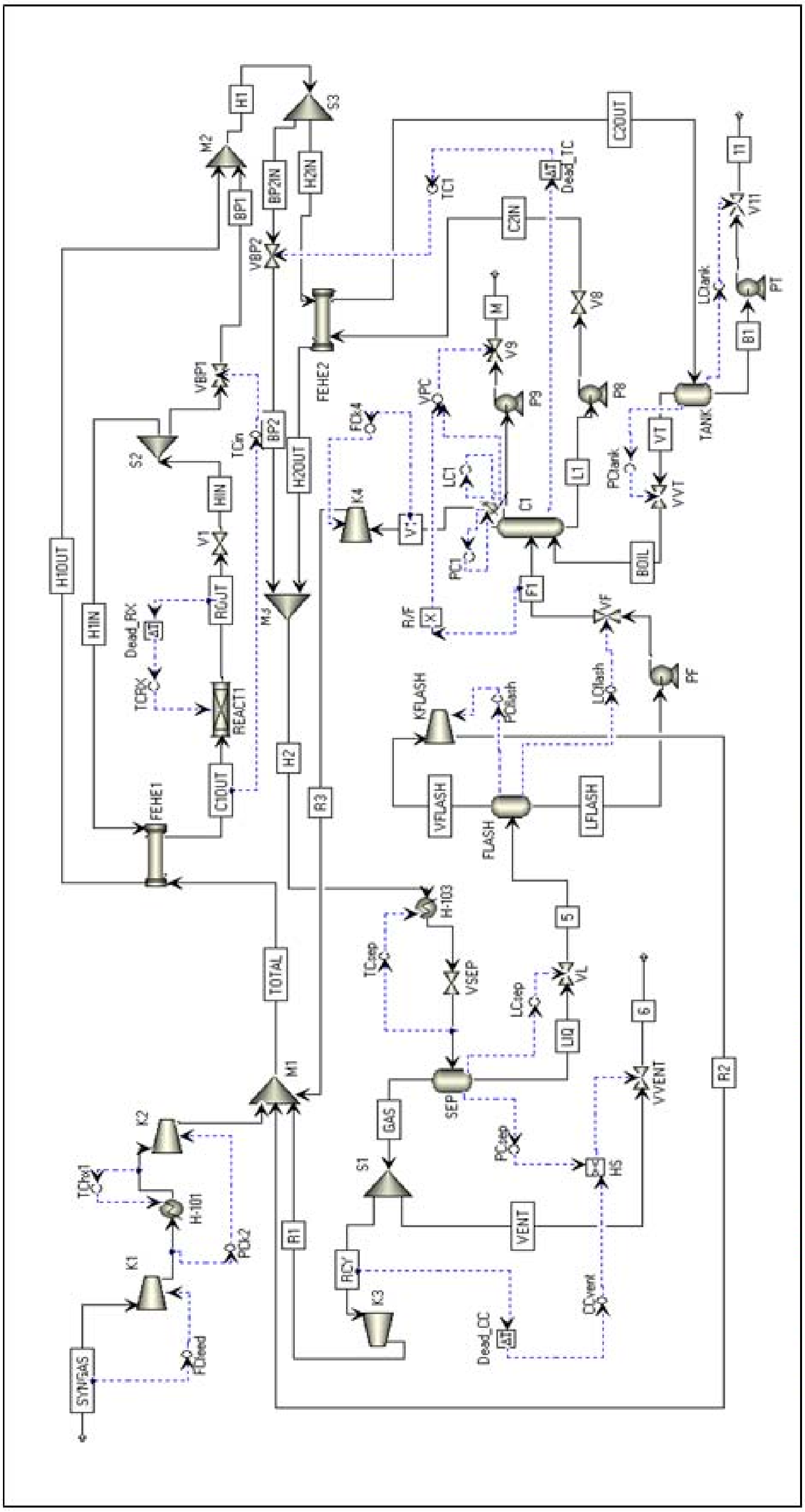


Figure 5.8 Designed control structure (CS3) for methanol process

5.3 Dynamics Simulation Results

In order to illustrate the dynamic behaviors of all control structures, the changing of the feed flow rate, reactor inlet temperature, and synthesis gas composition as disturbances were imposed on the system to test their the ability. Temperature controllers and composition controllers are PIs which are tuned using a relay-feedback. A 3 minute deadtime is used in the composition measurement lags. The reactor and column tray temperature controller have a 2 minute and 1 minute deadtime, respectively. For level, flow, and pressure controllers, their parameters are heuristics values.

5.3.1 Material Disturbances

A. Flow Rates in Synthesis Gas Feed

Figure 5.9 shows dynamic response of methanol process for 10% changes in setpoint of the synthesis gas flow controller. At time equal to 0.5 h, the feed flow rate is increased from 11450 to 12595 kmol/h and is decreased to 10305 kmol/h at time equal to 8 h.

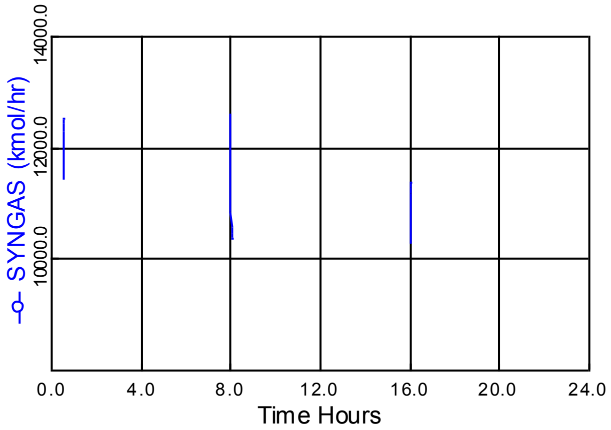


Figure 5.9 Dynamic response of methanol process by step change molar flow rate 10% in the synthesis gas feed stream.

Figure 5.10 to 5.13 give results of the dynamic responses of all control structures for change throughput disturbances, where a) is a molar flow rate of synthesis gas feed stream, b) is a reactor inlet temperature, c) is a reactor effluent temperature, d) is a coolant temperature, e) is separator pressure, f) is a methane composition in recycle stream, g) is a molar flow rate of recycle stream, h) is a molar flow rate of vent stream, i) is a pressure in flash tank, j) is the 35th tray temperature of methanol column, k) is a molar flow rate of distillate stream, l) is a methanol composition in distillate stream, m) is a molar flow rate of bottom stream, n) is a water composition in bottom stream, o) is a pressure condenser of methanol column, p) is a molar flow rate of reflux q) is a molar flow rate feed stream of methanol column, and r) is a reboiler duty.

All control structures give the same trend of dynamic responses for changing molar flow rates in synthesis gas feed stream. Designed control structures (CS1 to CS3) can be rejected this disturbances and return to their setpoint. Moreover, the process constraint variables are achieved. When the feed molar flow rate increases, the separator pressure rises up to a new setpoint, recycle, vent, distillate, and bottom flow rates increase, the reactor coolant temperature decreases to remove the heat removal from exothermal reaction. The tray temperature column of all designed control structures has a small deviation. The compositions of methanol and water leaving from column remain close to their specifications because of the reflux to feed ratio control in CS1 and CS3.

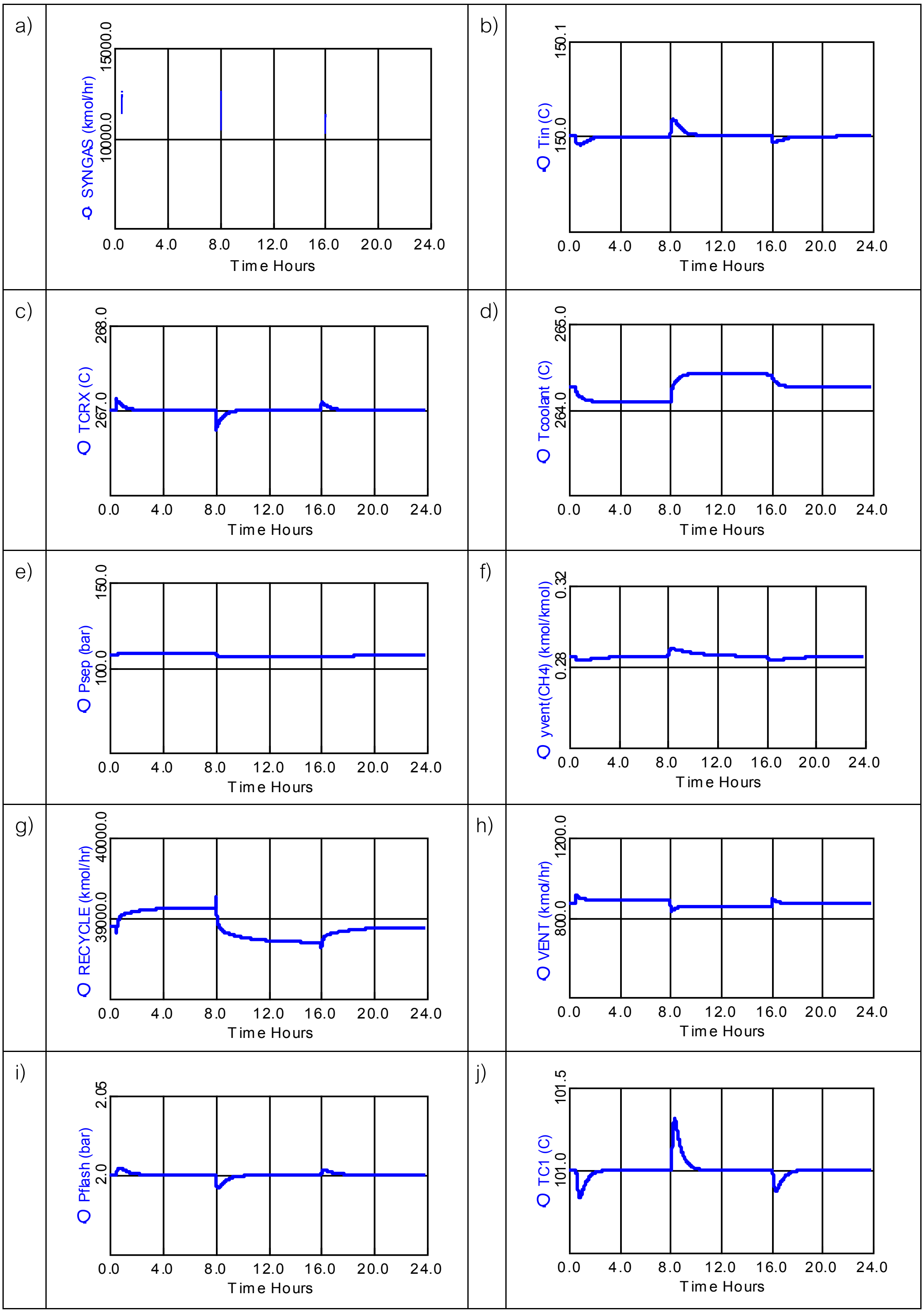


Figure 5.10 Dynamic responses of CS0 for 10% feed flow rate disturbances.

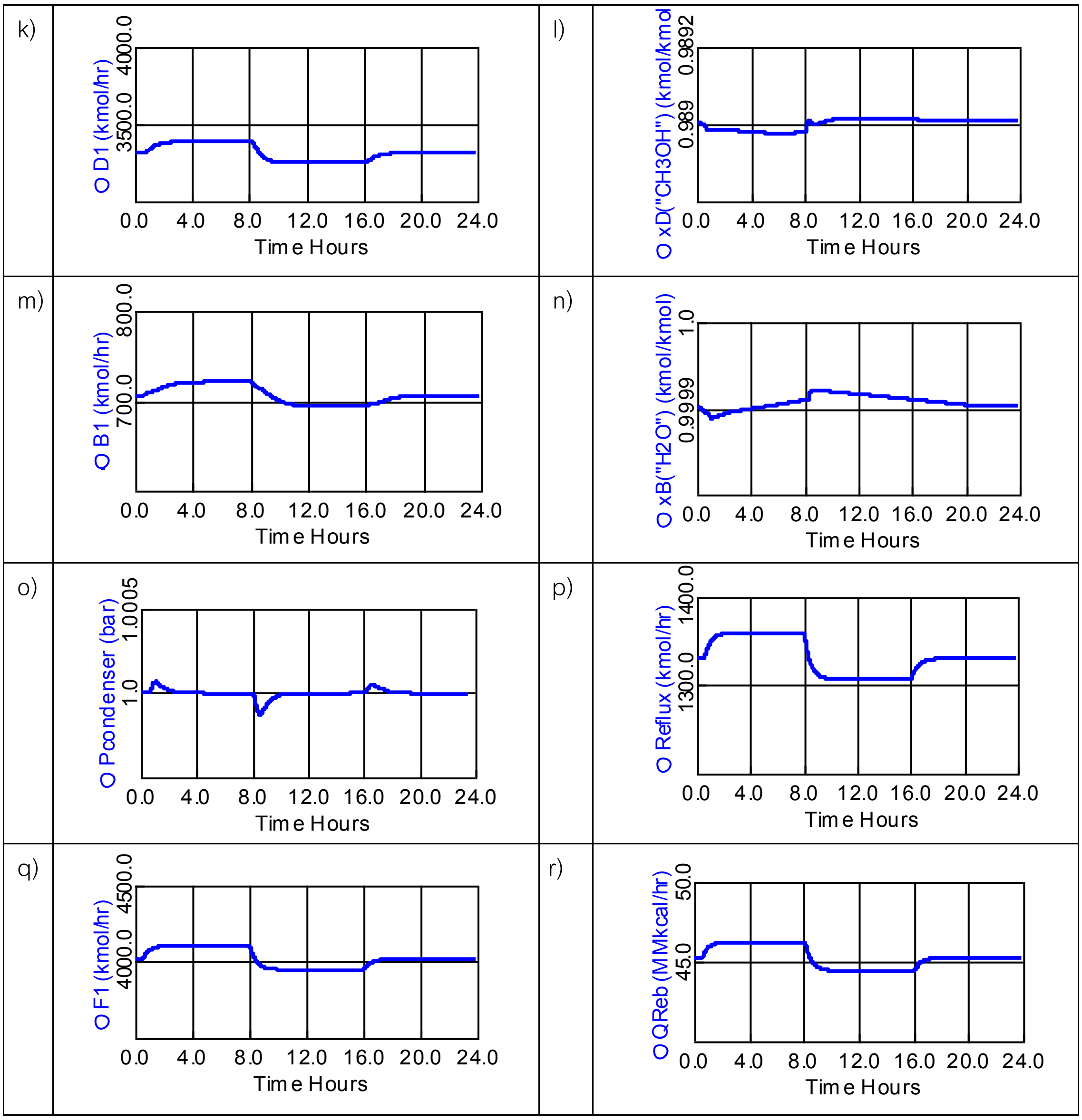


Figure 5.10 (Continued) Dynamic responses of CS0 for 10% feed flow rate disturbances.

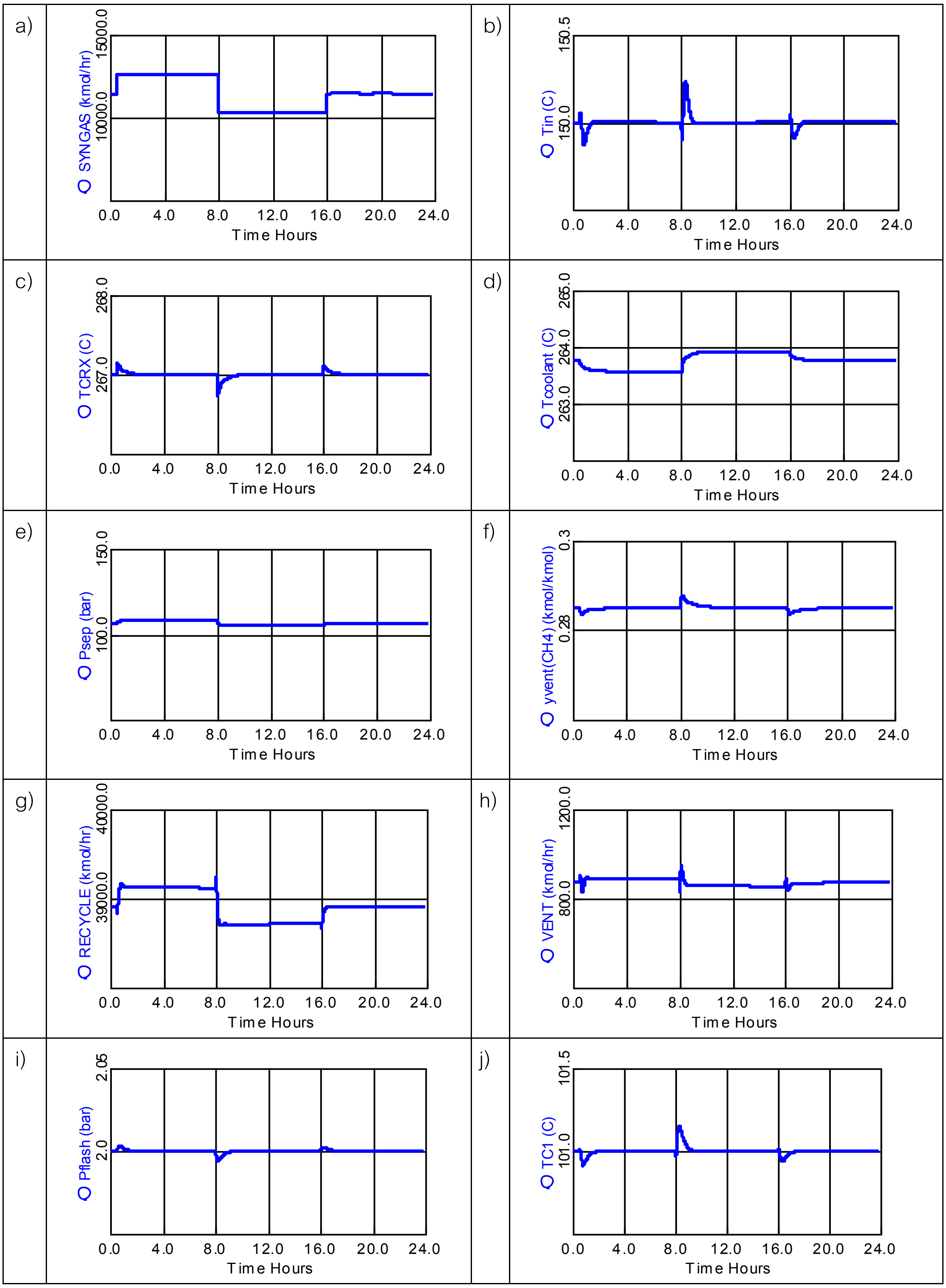


Figure 5.11 Dynamic responses of CS1 for 10% feed flow rate disturbances

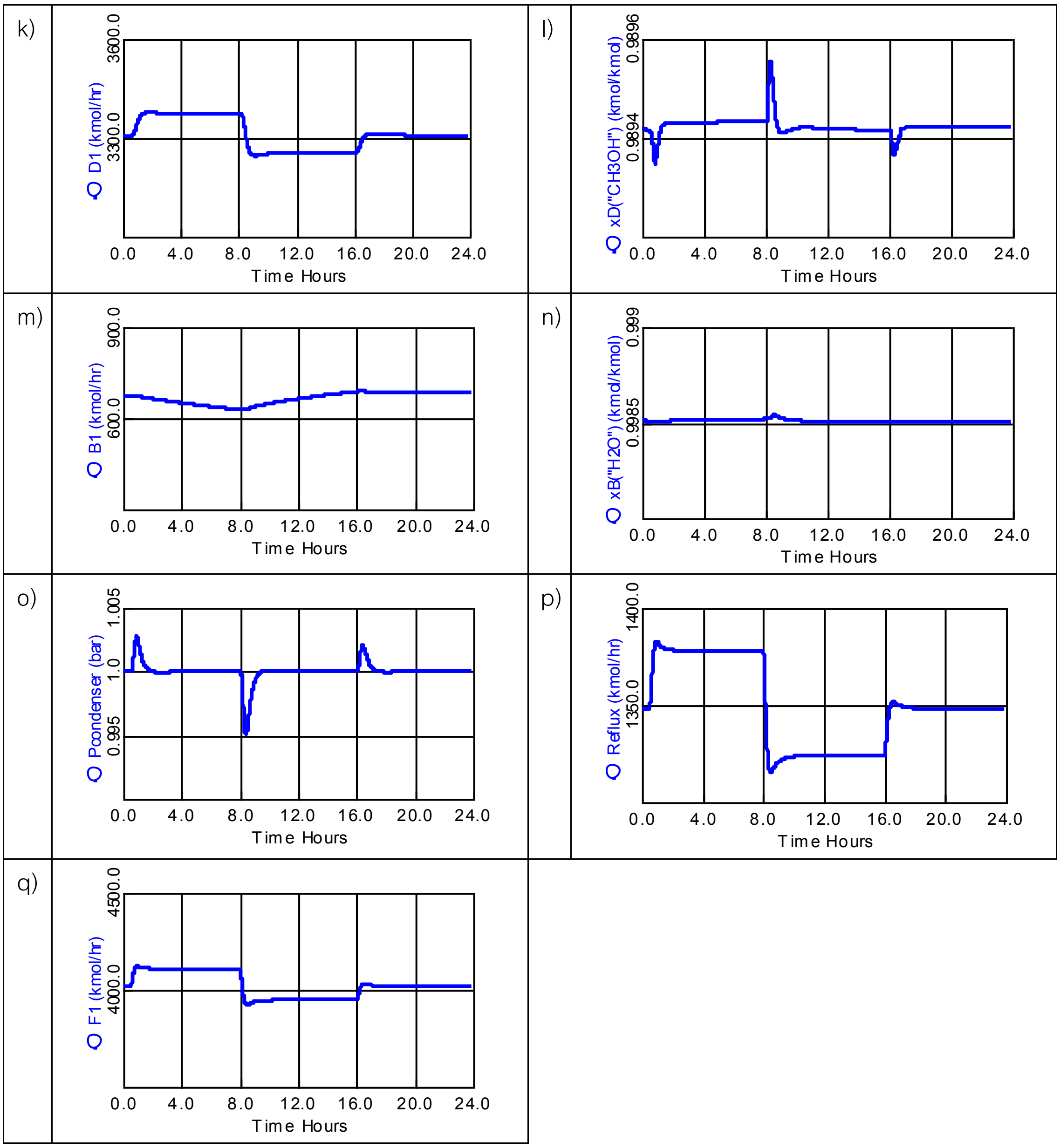


Figure 5.11 (Continued) Dynamic responses of CS1 for 10% feed flow rate disturbances

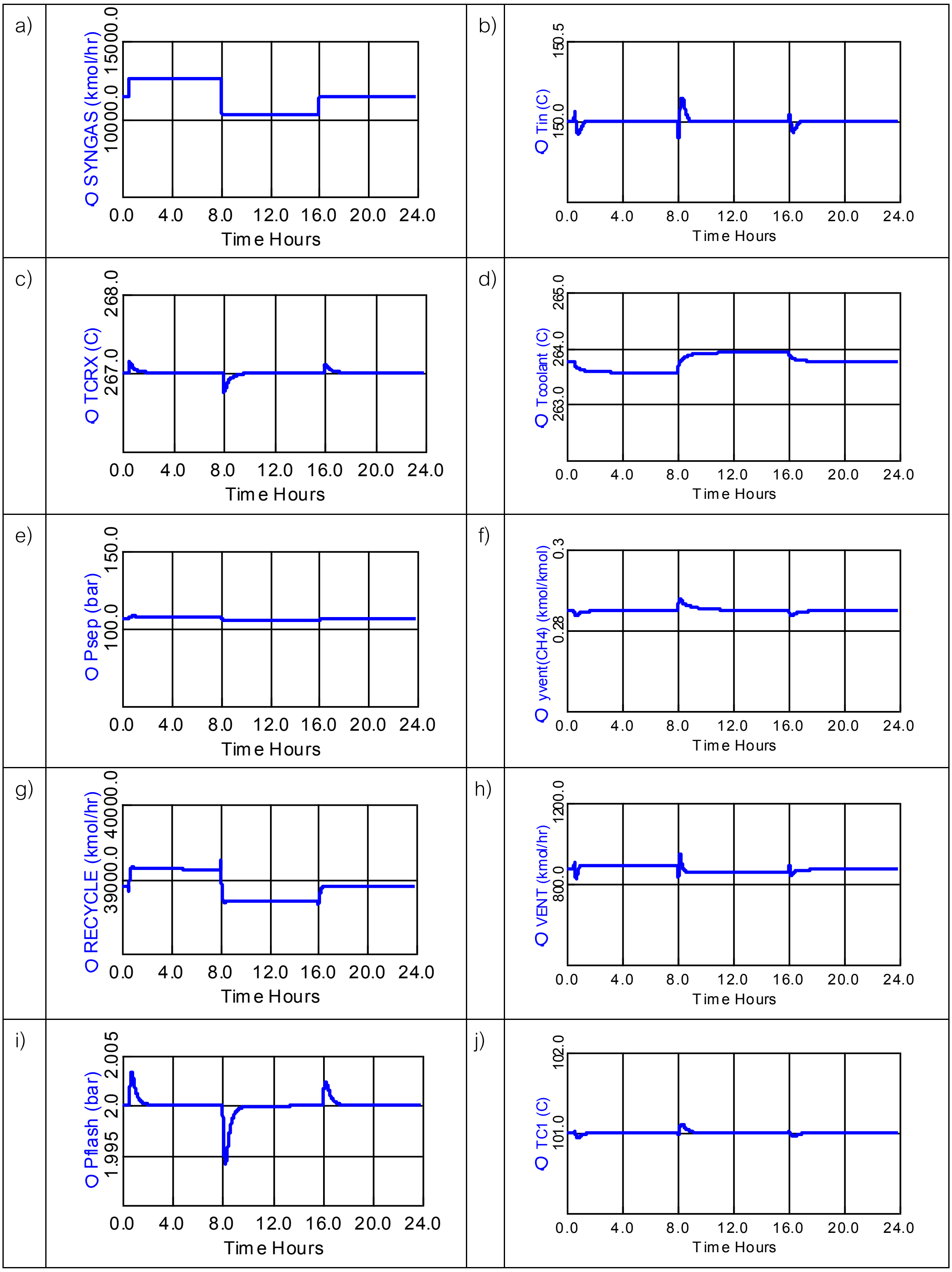


Figure 5.12 Dynamic responses of CS2 for 10% feed flow rate disturbances

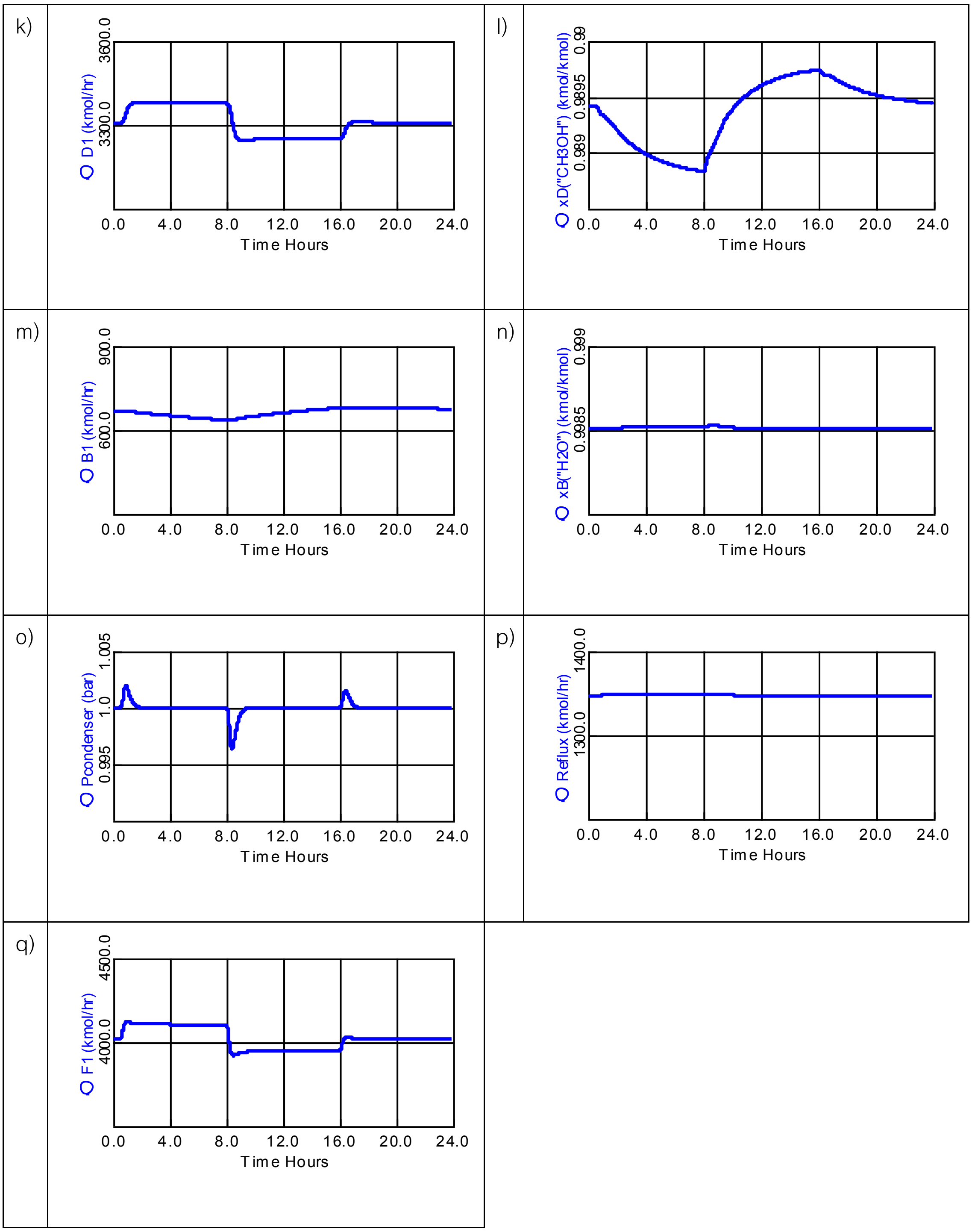


Figure 5.12 (Continued) Dynamic responses of CS2 for 10% feed flow rate disturbances

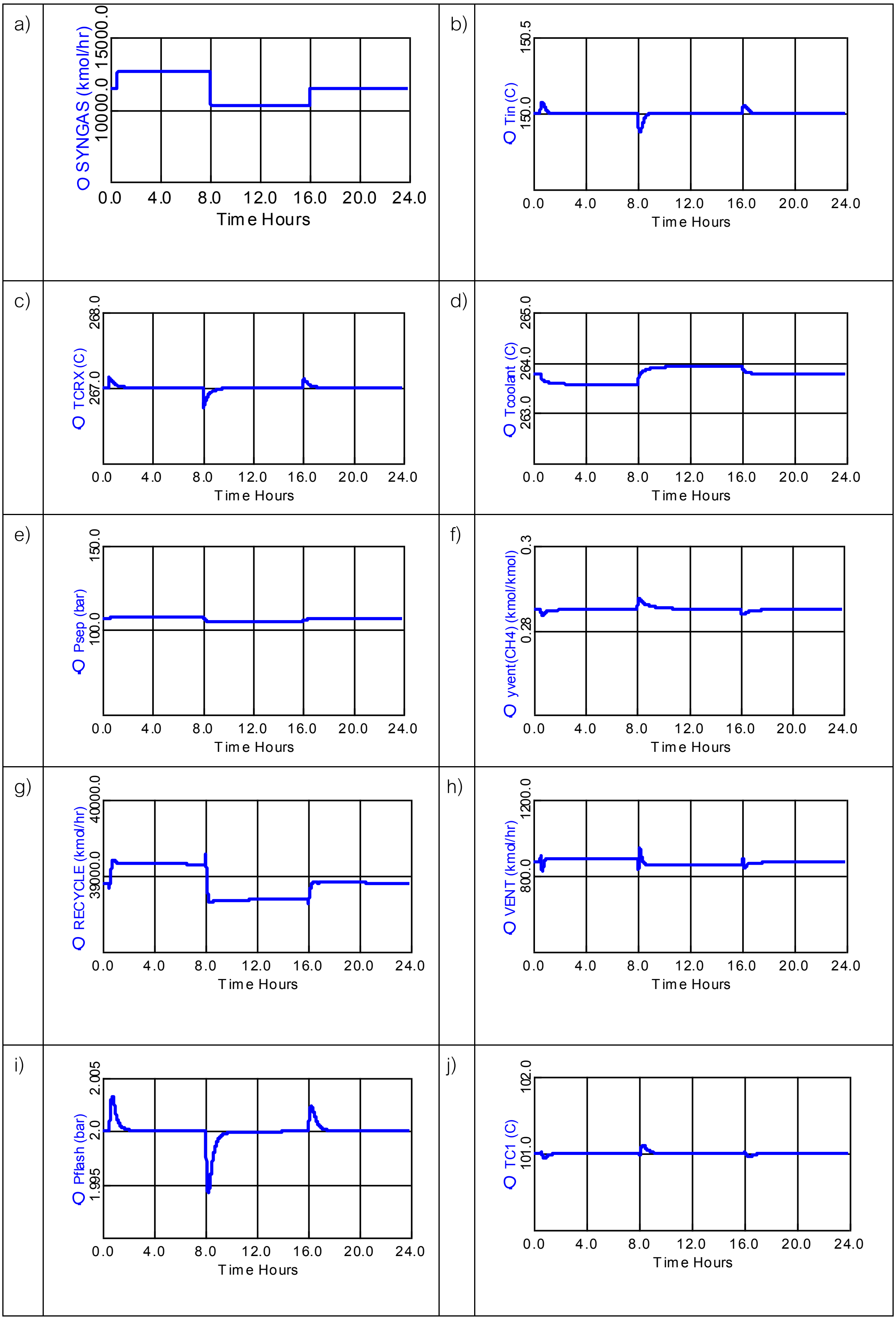


Figure 5.13 Dynamic responses of CS3 for 10% feed flow rate disturbances

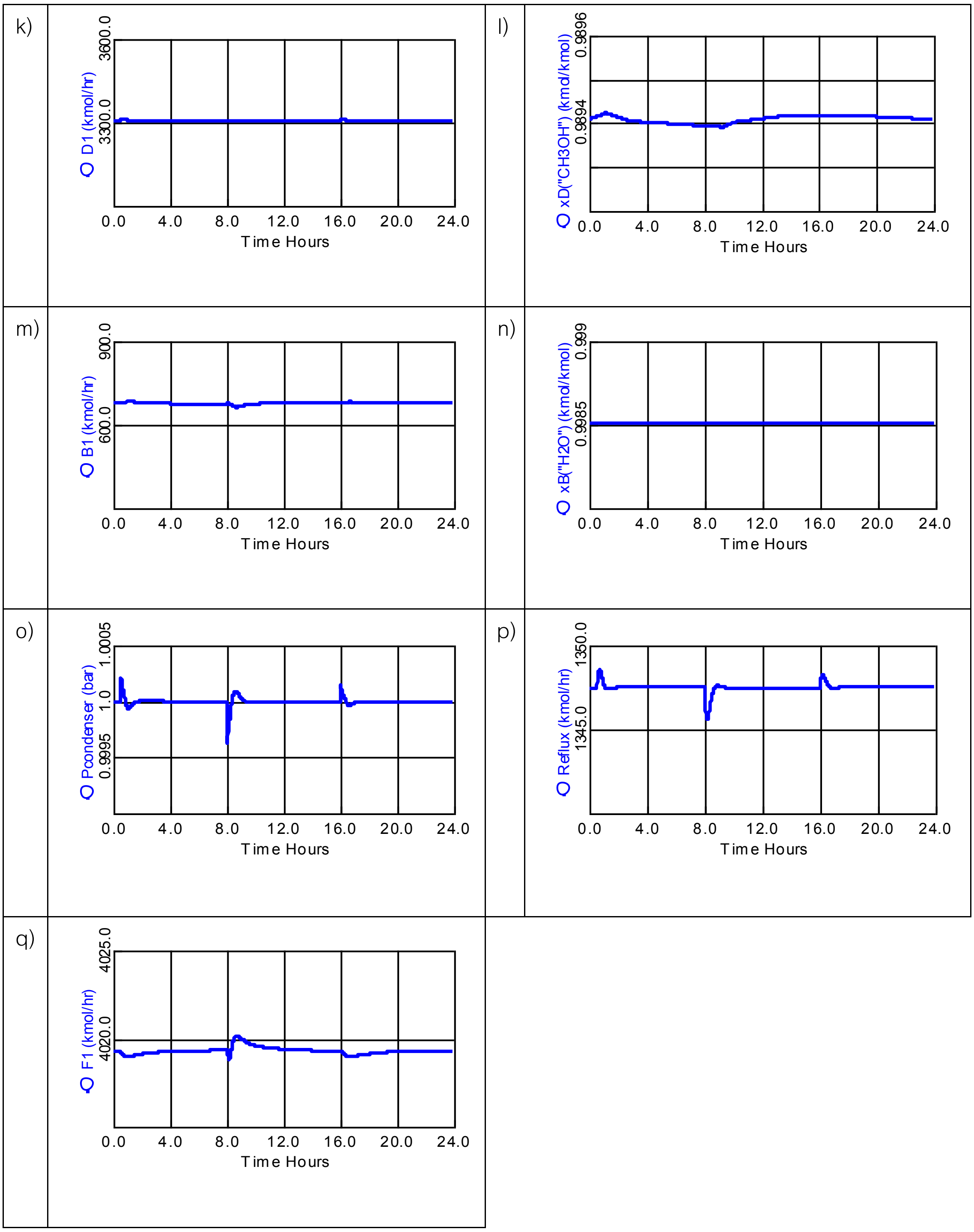


Figure 5.13 (Continued) Dynamic responses of CS3 for 10% feed flow rate disturbances

B. Synthesis Gas Composition Disturbances

(1) Methane Impurity in Synthesis Gas Feed

Figure 5.14 to 5.17 give results of dynamic response of methanol process for changes in the methane impurity in synthesis gas. The design values of methane and hydrogen feed composition are 2.17 mol% and 67.46 mol%, respectively. All graphs show results for an increase in methane impurity to 3.17 mol% and decrease in hydrogen composition to 66.46 mol% at time equal to 0.5 h. The methane impurity is decreased to 1.17 mol% and hydrogen composition is increased to 68.46 mol% at time equal to 8 h.

The effect of increasing the methane composition in synthesis gas feed stream is an increasing in the vent flow rate, changing separator pressure, and holding product purities. In contrast, decreasing the methane impurity leads to produce more products because the vent flow rate decreases. The product purities are maintained near their specifications.

The high pressure override controller needs for this disturbance. The methane composition in recycle stream is not held at set point. It is deviated because the separator pressure in gas loop starts to increase. When the pressure is approach to 120 bar, the override controller is worked to open the vent valve for maintaining system pressure.

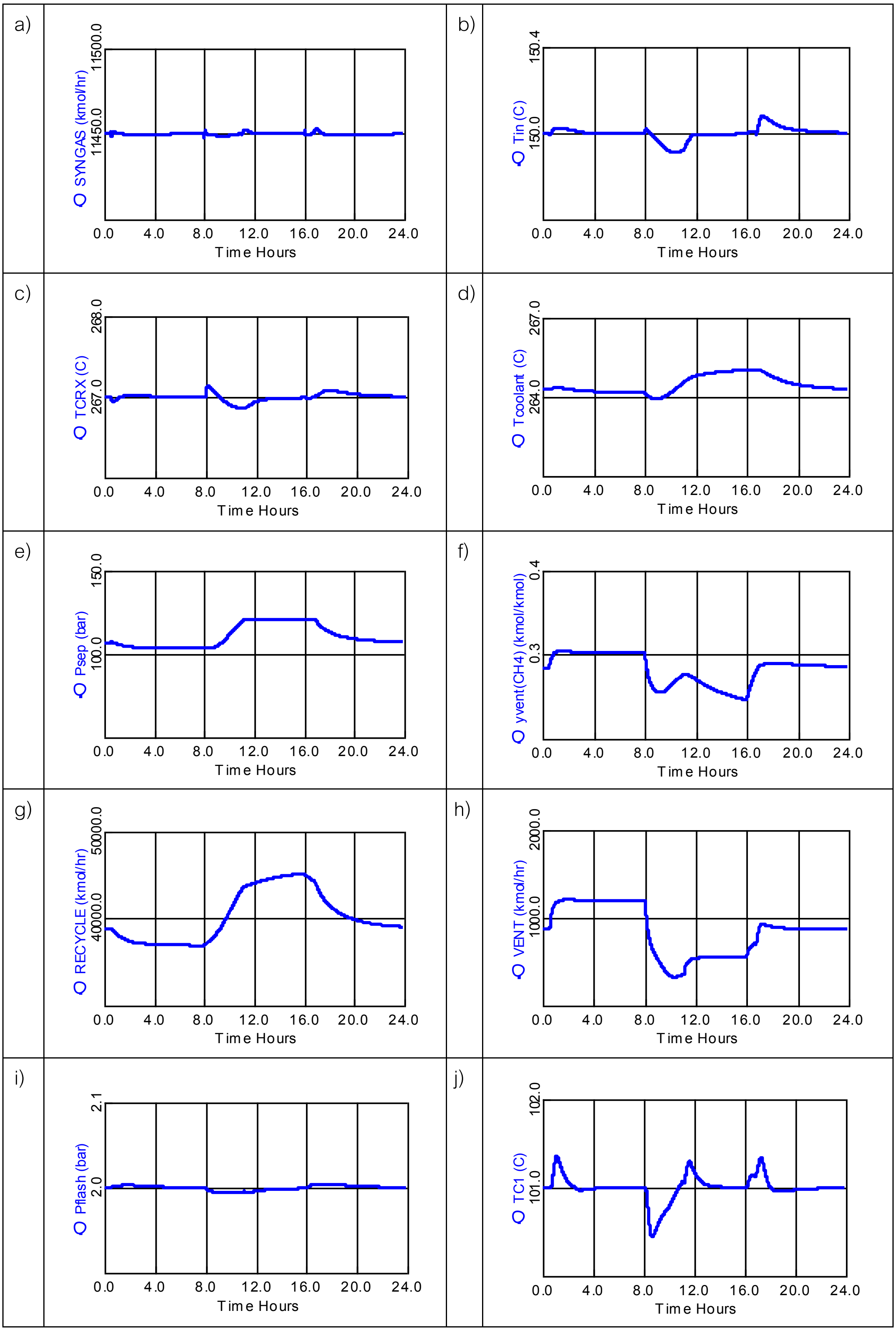


Figure 5.14 Dynamic responses of CS0 for feed methane composition disturbances

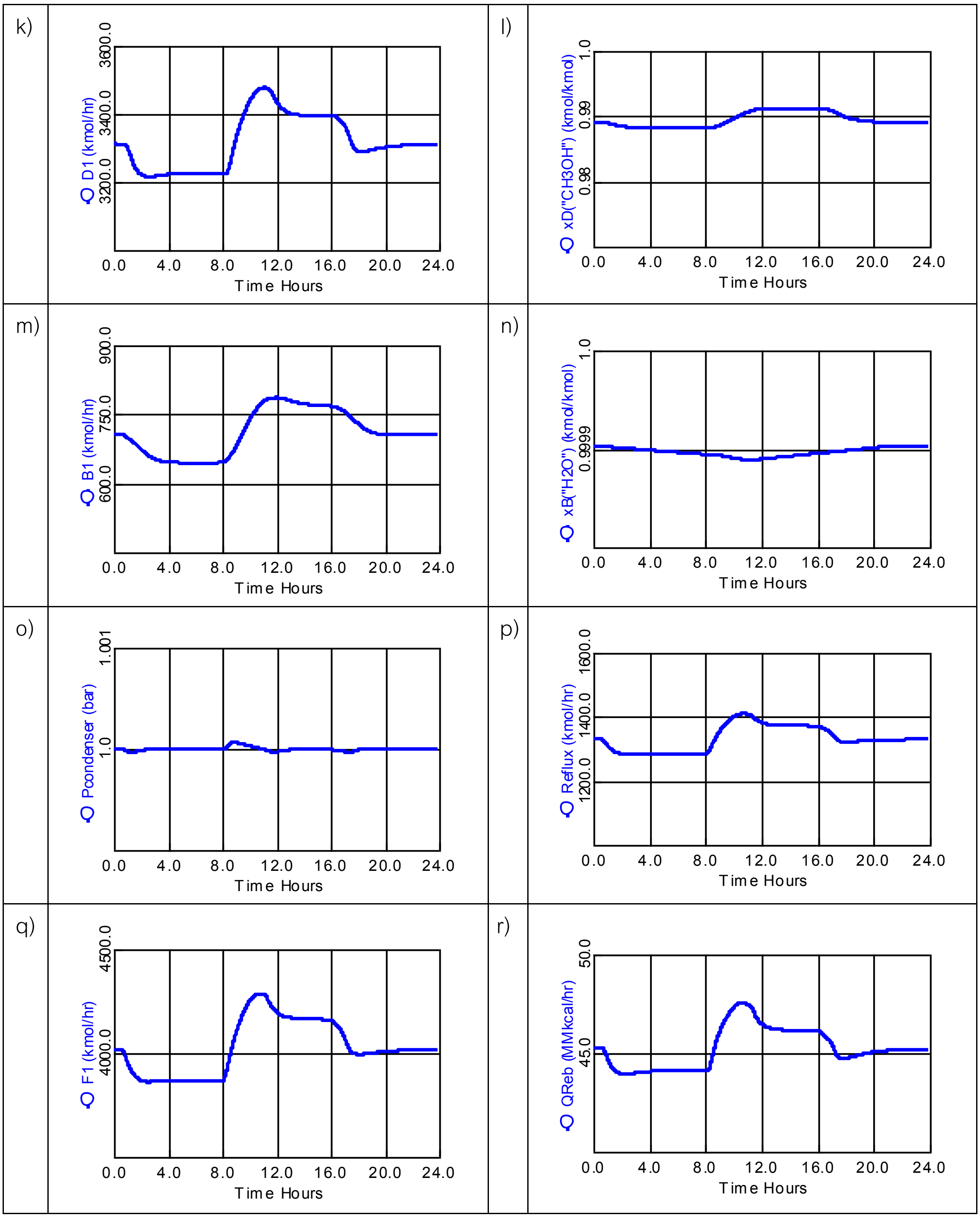


Figure 5.14 (Continued) Dynamic responses of CS0 for feed methane composition disturbances

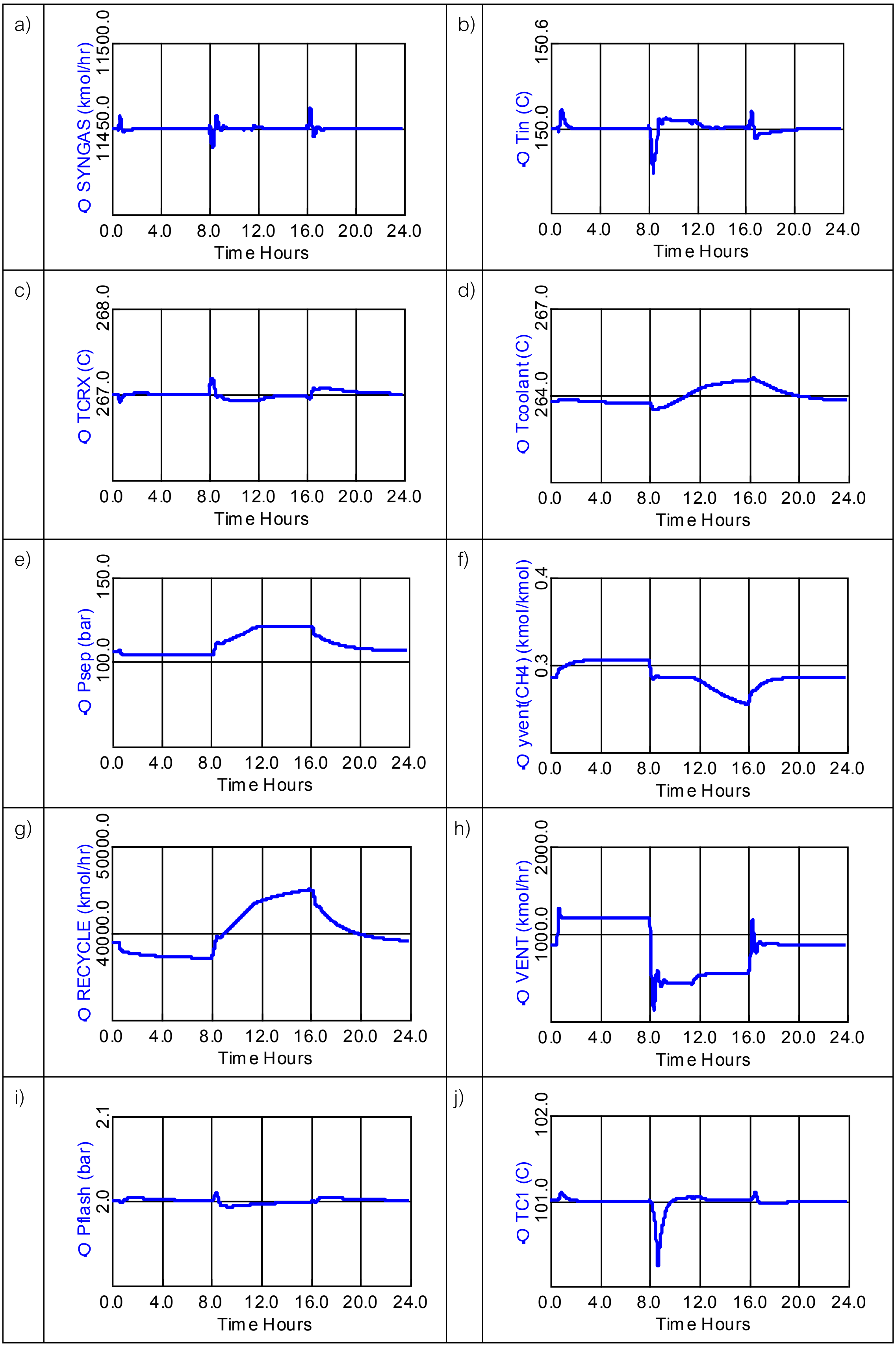


Figure 5.15 Dynamic responses of CS1 for feed methane composition disturbances

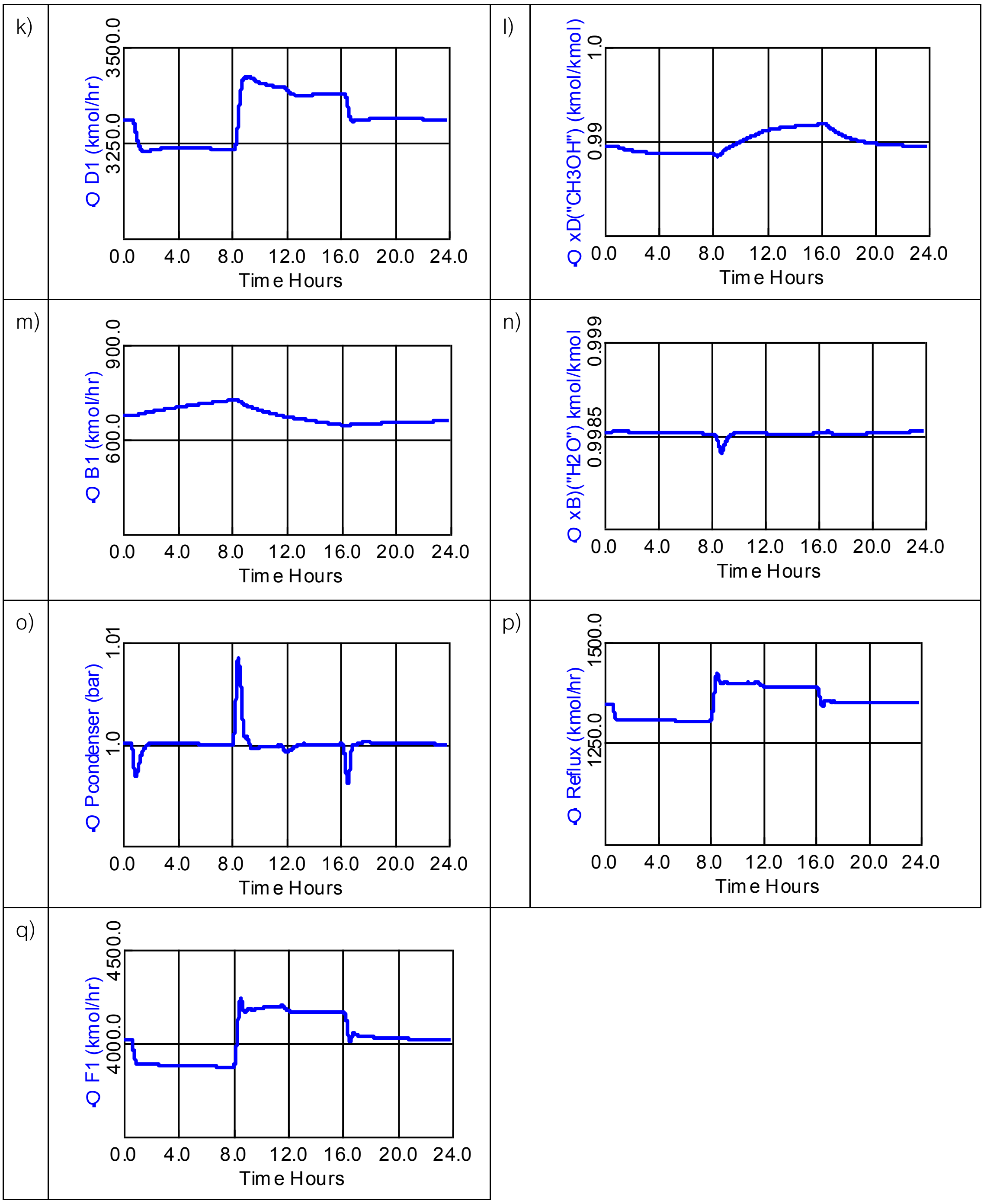


Figure 5.15 (Continued) Dynamic responses of CS1 for feed methane composition disturbances

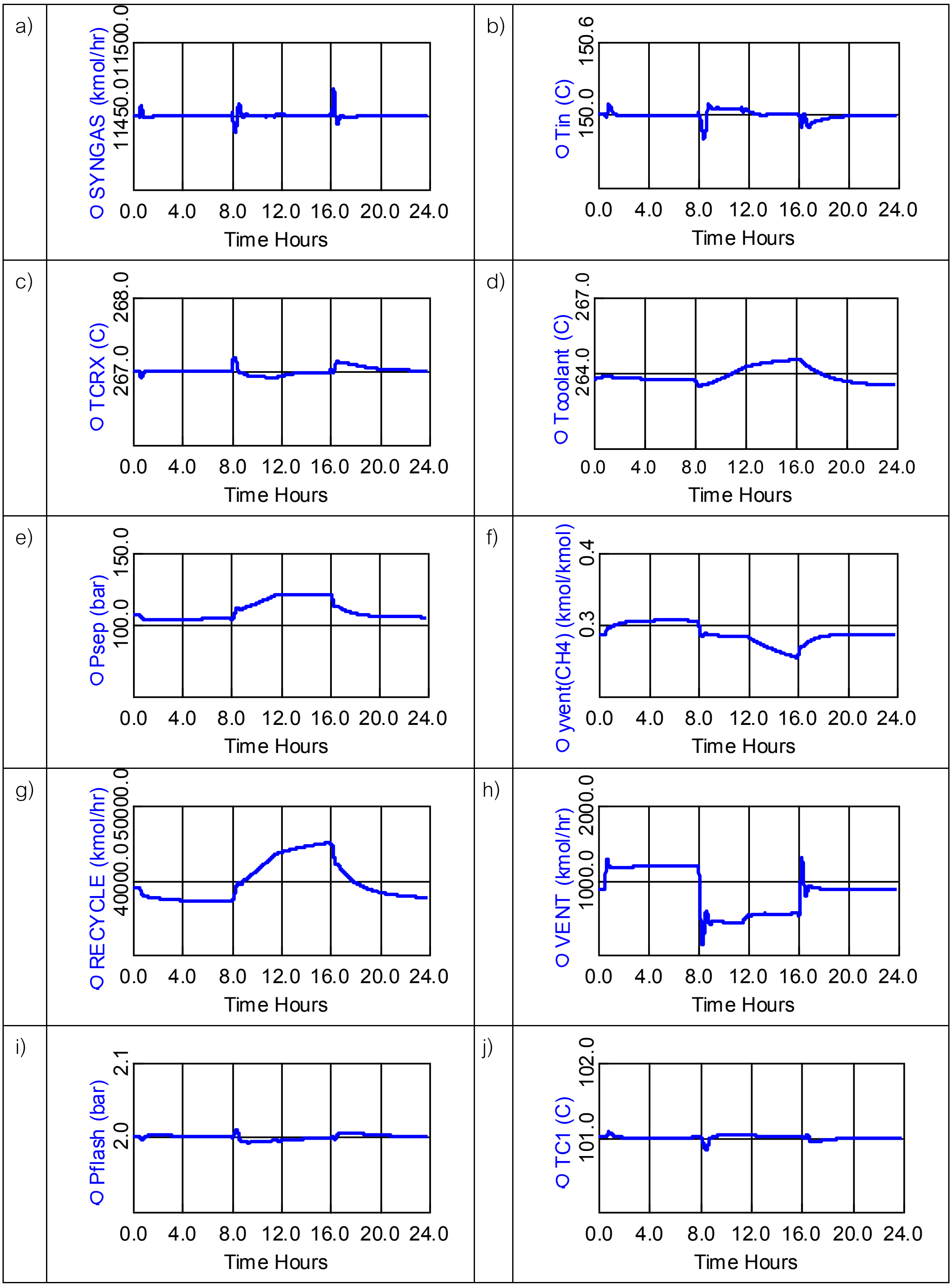


Figure 5.16 Dynamic responses of CS2 for feed methane composition disturbances

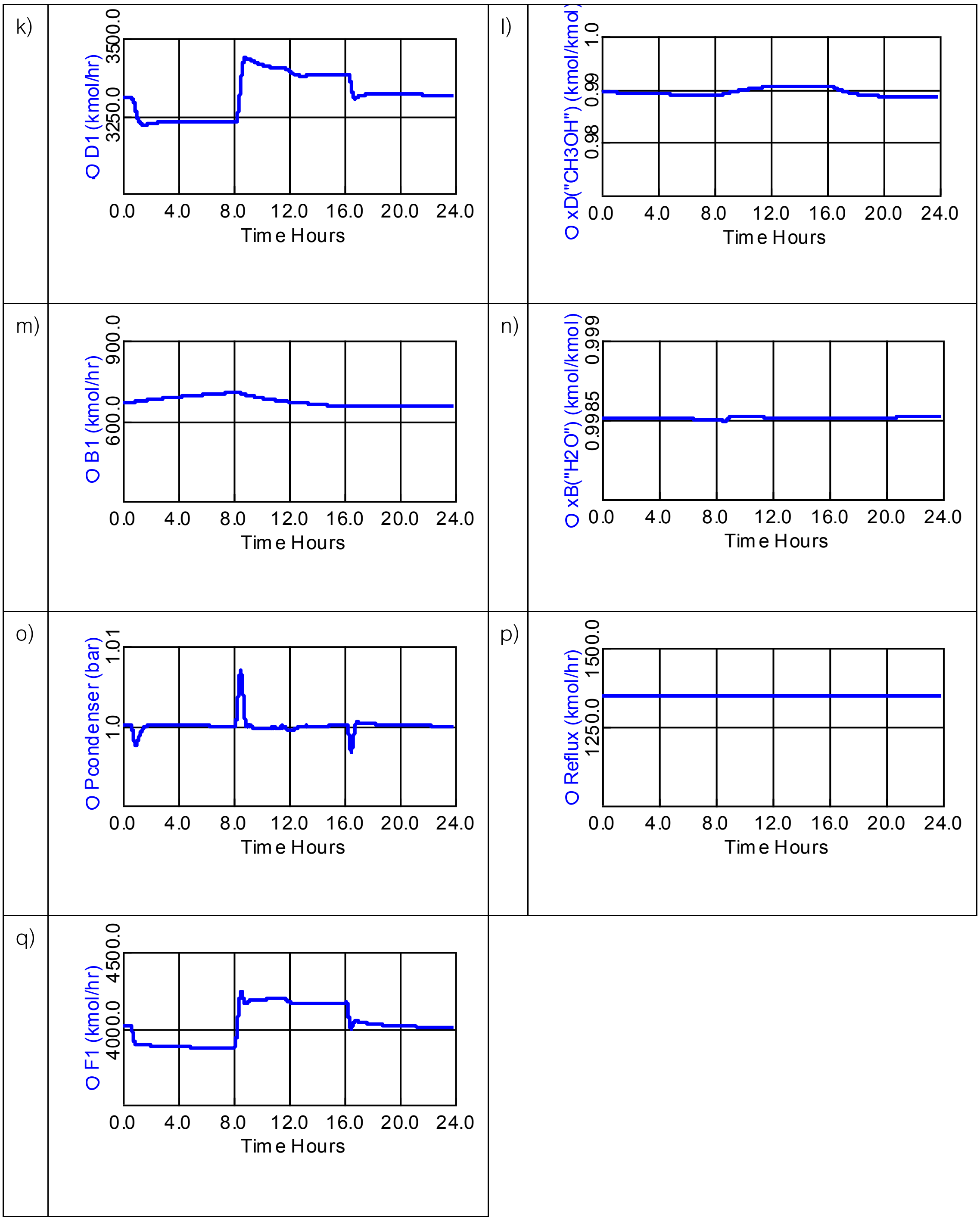


Figure 5.16 (Continued) Dynamic responses of CS2 for feed methane composition disturbances

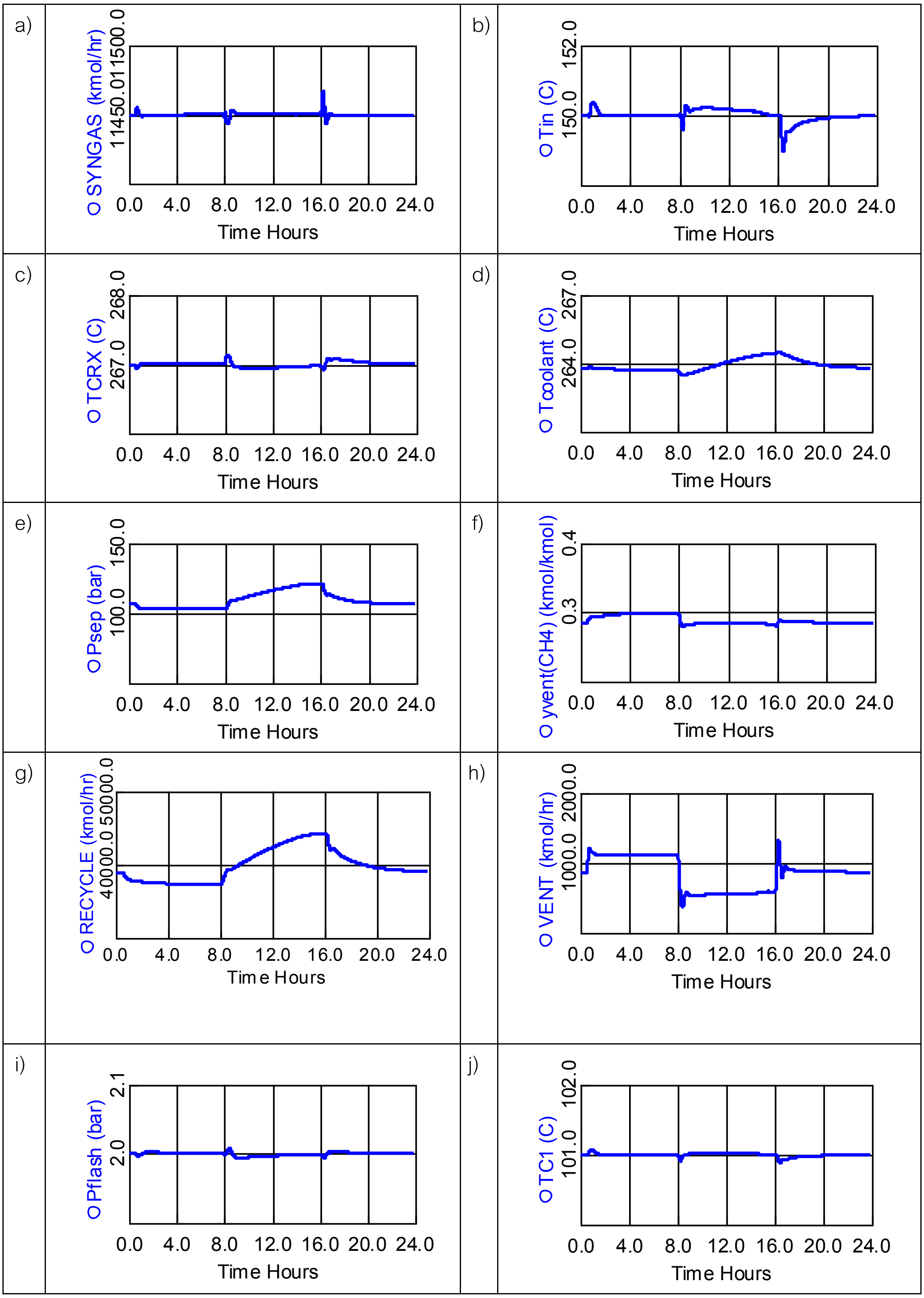


Figure 5.17 Dynamic responses of CS3 for feed methane composition disturbances

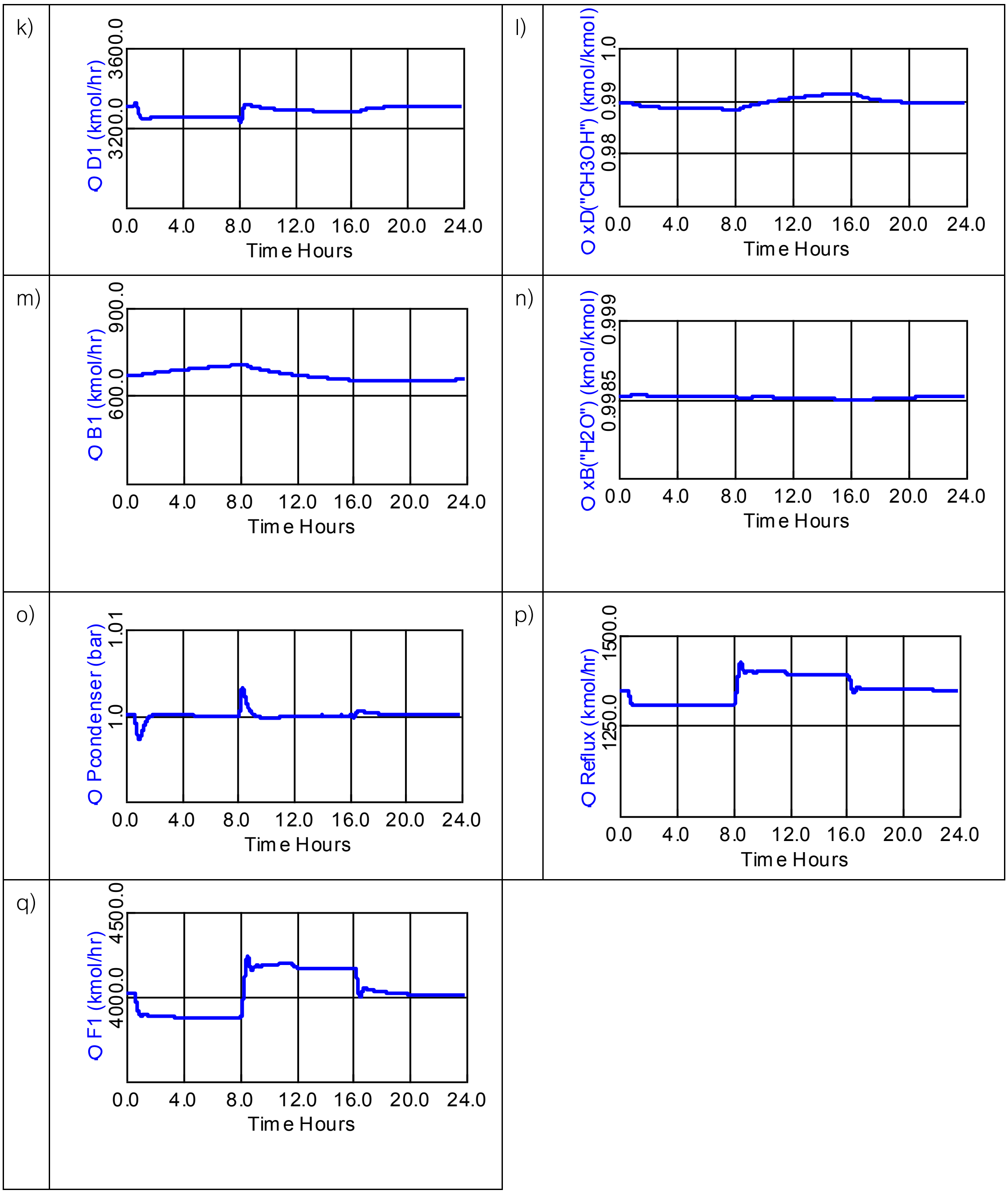


Figure 5.17 (Continued) Dynamic responses of CS3 for feed methane composition disturbances

(2) CO/CO$_2$ Ratio

The design values contain CO 6.858 mol%, CO$_2$ and 22.97 mol% Figure 5.18 to 5.21 give results of dynamic response of methanol process for change the feed carbon monoxide and carbon dioxide compositions..All graphs show results for an increase in carbon monoxide to 21.97 mol% and decrease in carbon dioxide composition to 7.858 mol% at time equal to 0.5 h. The carbon monoxide is decreased to 23.97 mol% and carbon dioxide composition is increased to 5.458 mol% at time equal to 8 h. The override controller is need for the change in the carbon monoxide (CO) and carbon dioxide (CO_2) compositions in the synthesis gas feed.

All designed control structures give the same trend of the dynamic response. The effect of increase carbon dioxide is the amount of product (methanol) in distillate stream decreases because the vent stream increases. This reason is led to more reactant losses. The separator pressure is less than 120 bar so the override controller does not take over control of the vent valve. The recycle of gas methane is held at its setpoint.

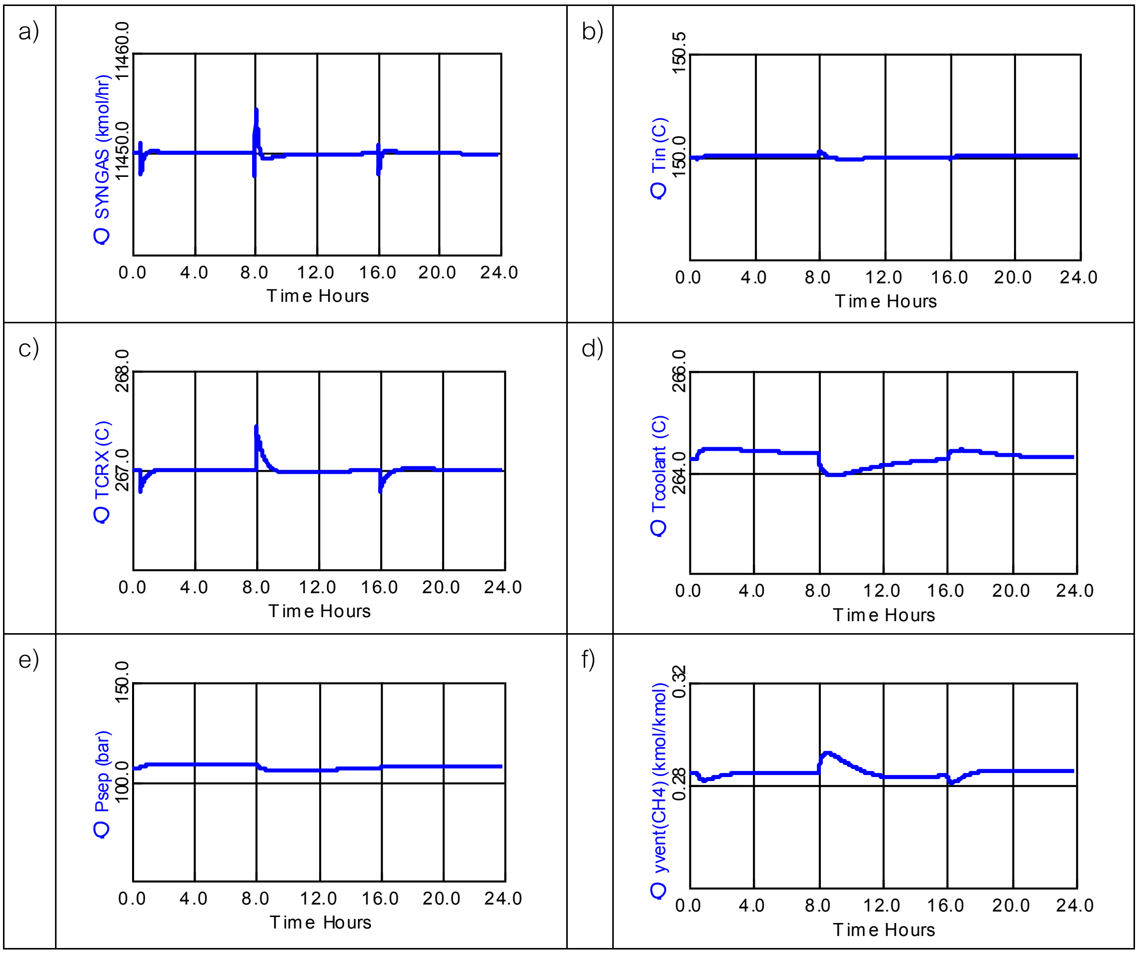


Figure 5.18 Dynamic responses of CS0 for the change CO/CO_2 ratio.

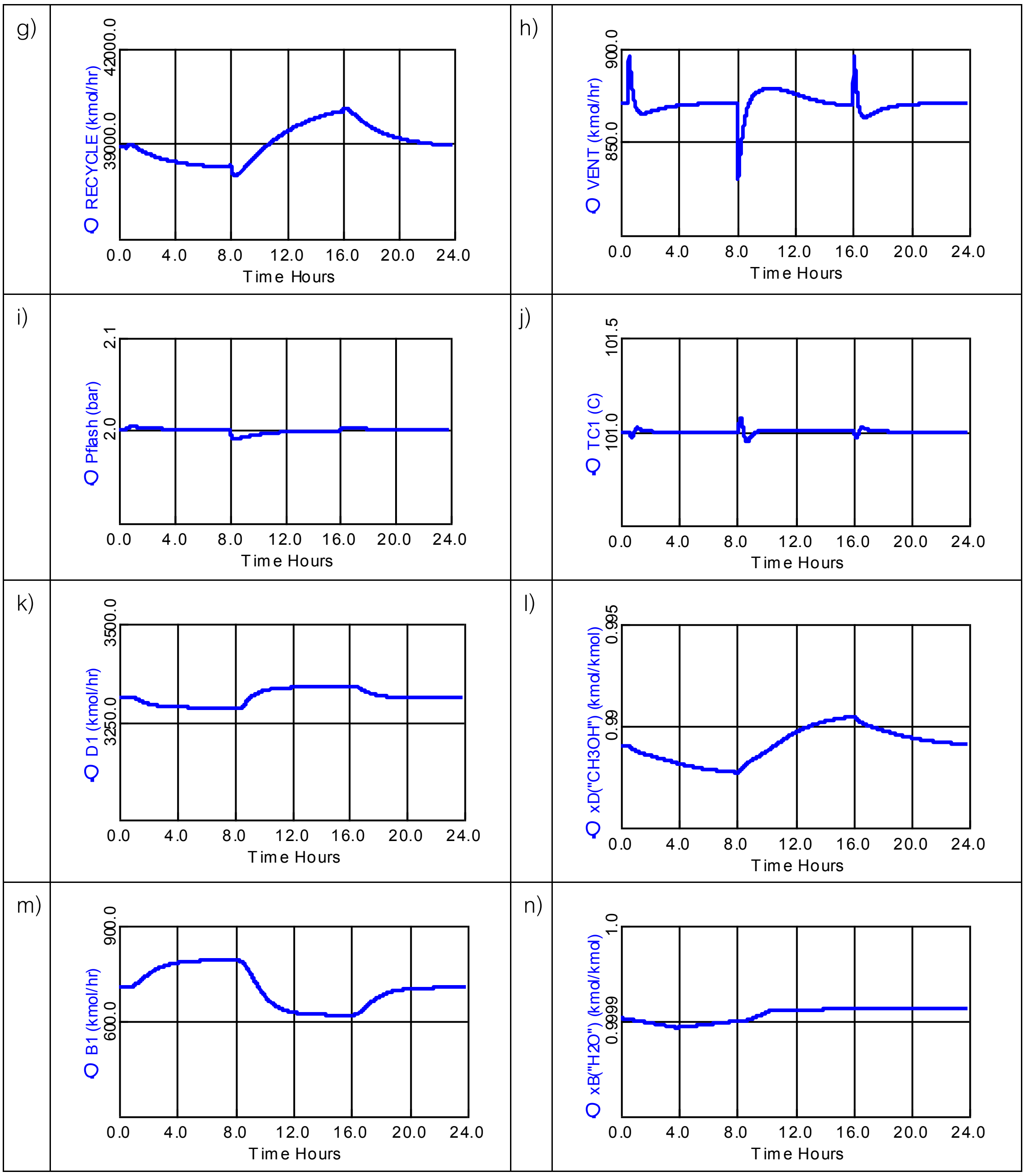


Figure 5.18 (Continued) Dynamic responses of CS0 for the change CO/CO_2 ratio.

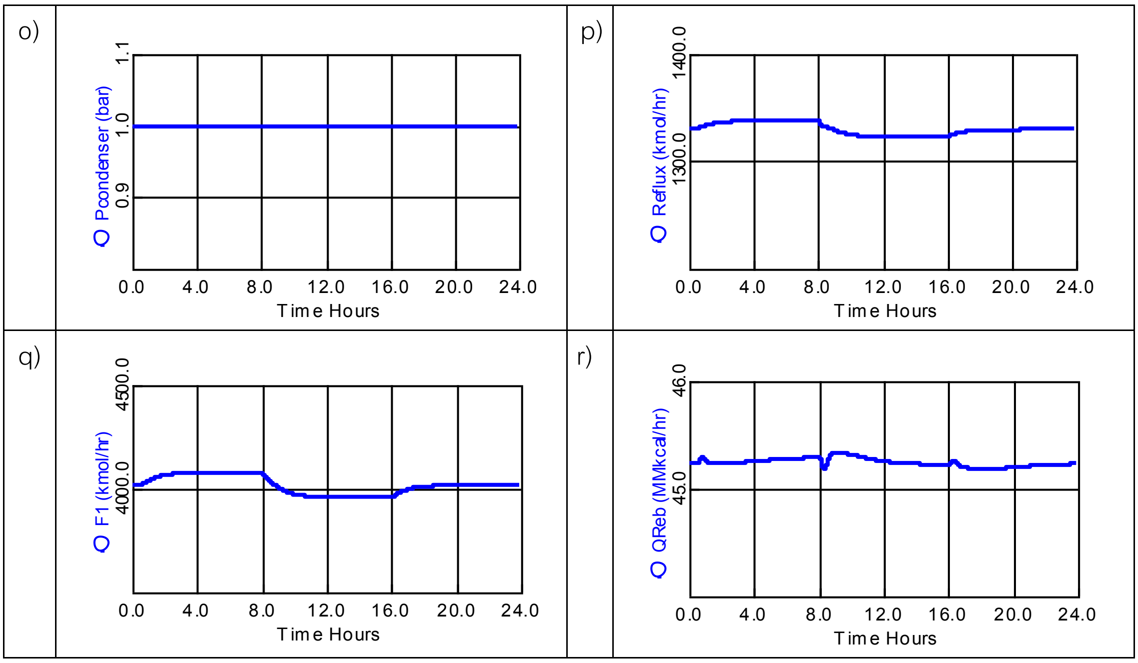


Figure 5.18 (Continued) Dynamic responses of CS0 for the change CO/CO_2 ratio.

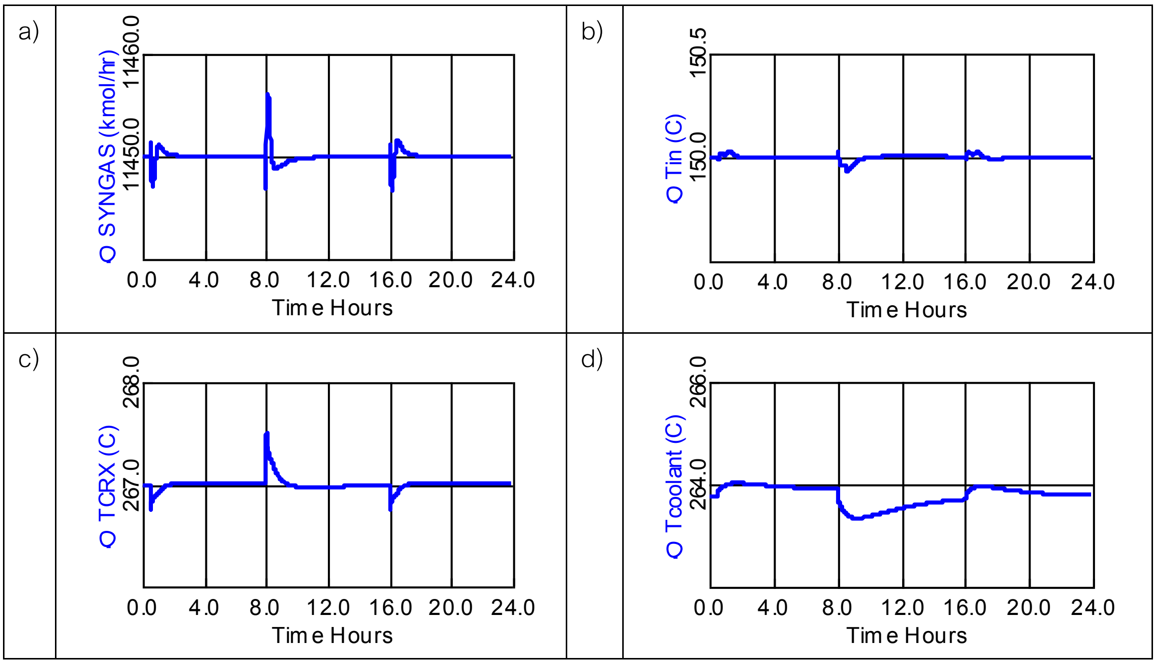


Figure 5.19 Dynamic responses of CS1 for the change CO/CO_2 ratio.

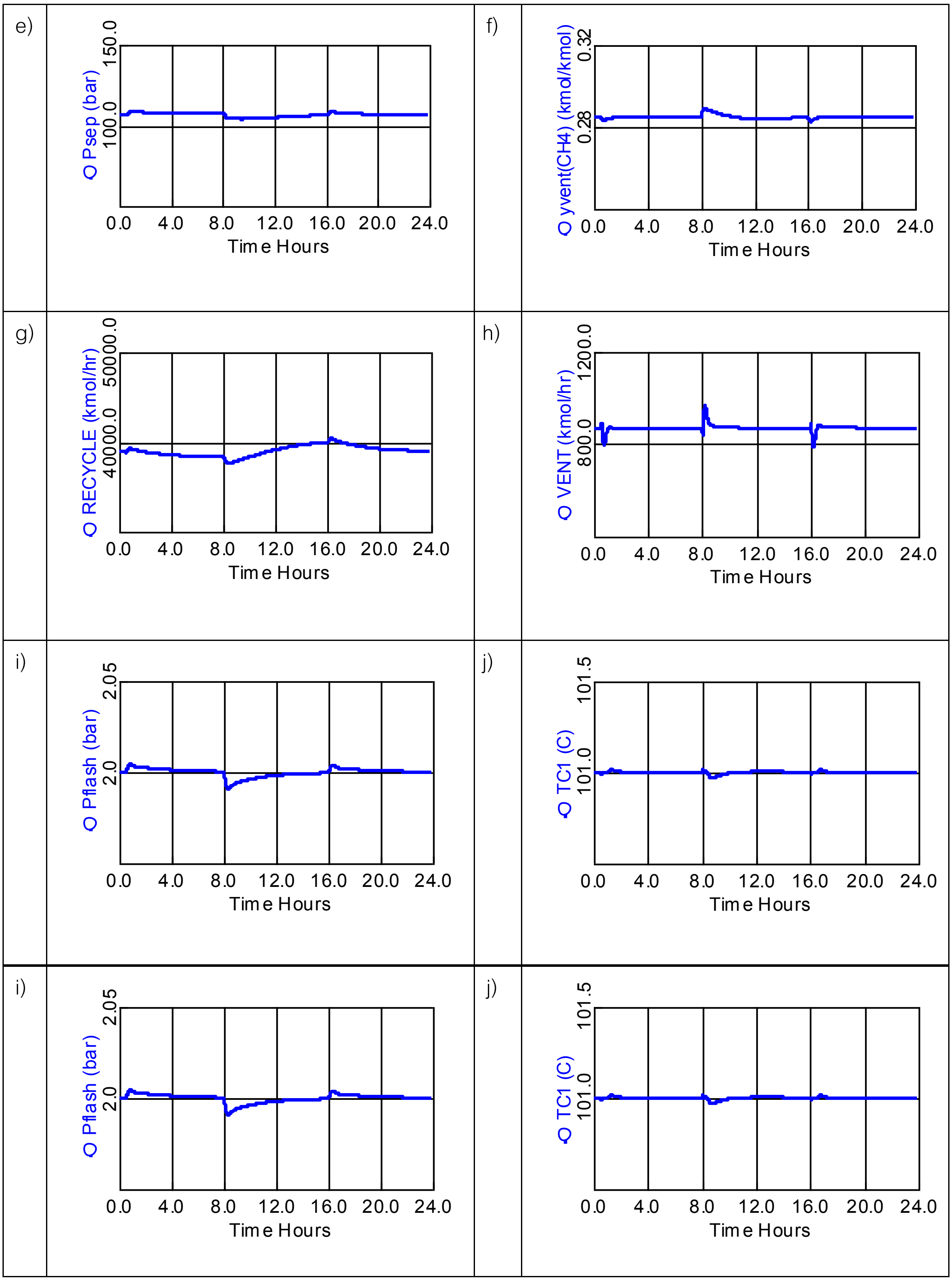


Figure 5.19 (Continued) Dynamic responses of CS1 for the change CO/CO_2 ratio.

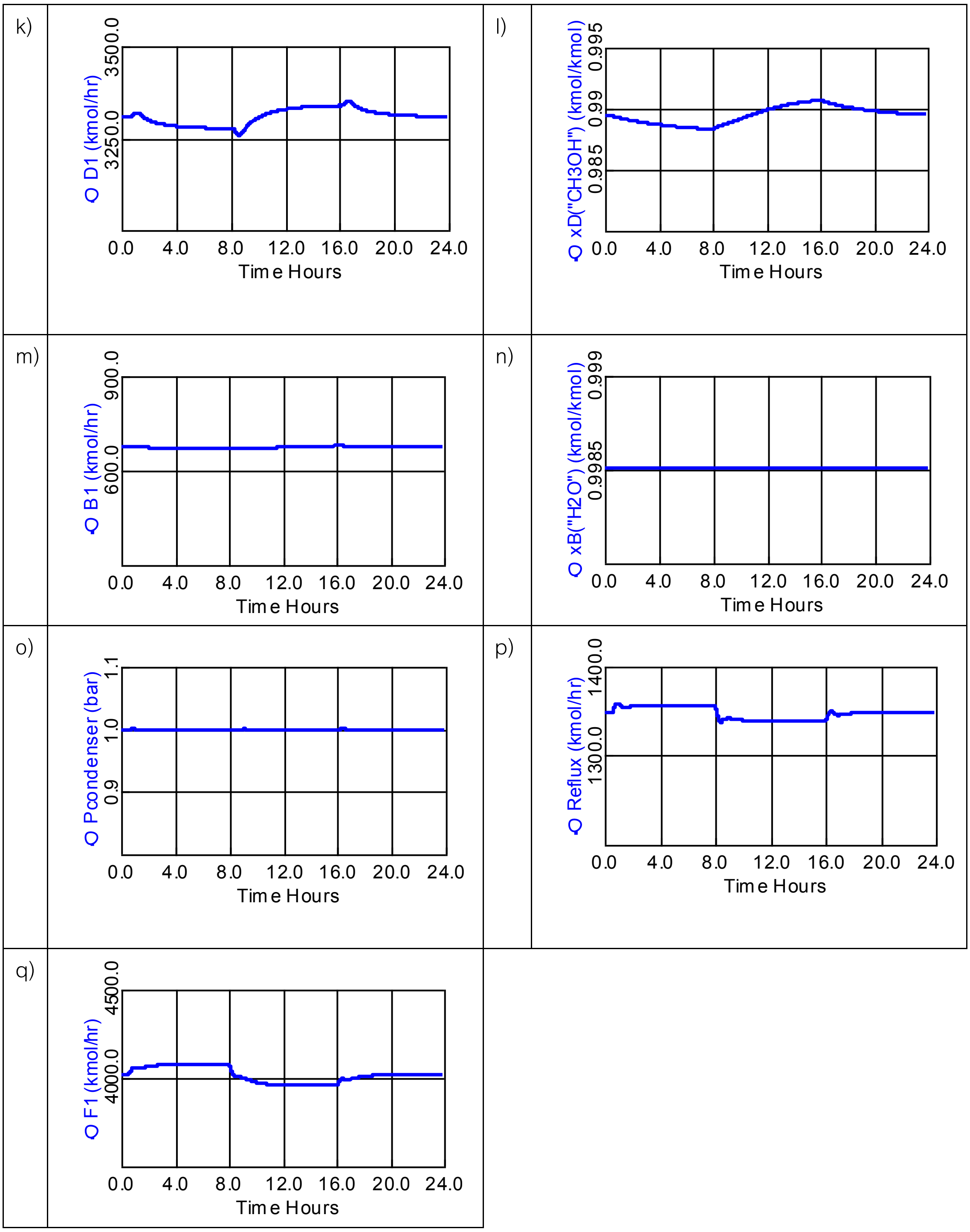


Figure 5.19 (Continued) Dynamic responses of CS1 for the change CO/CO_2 ratio.

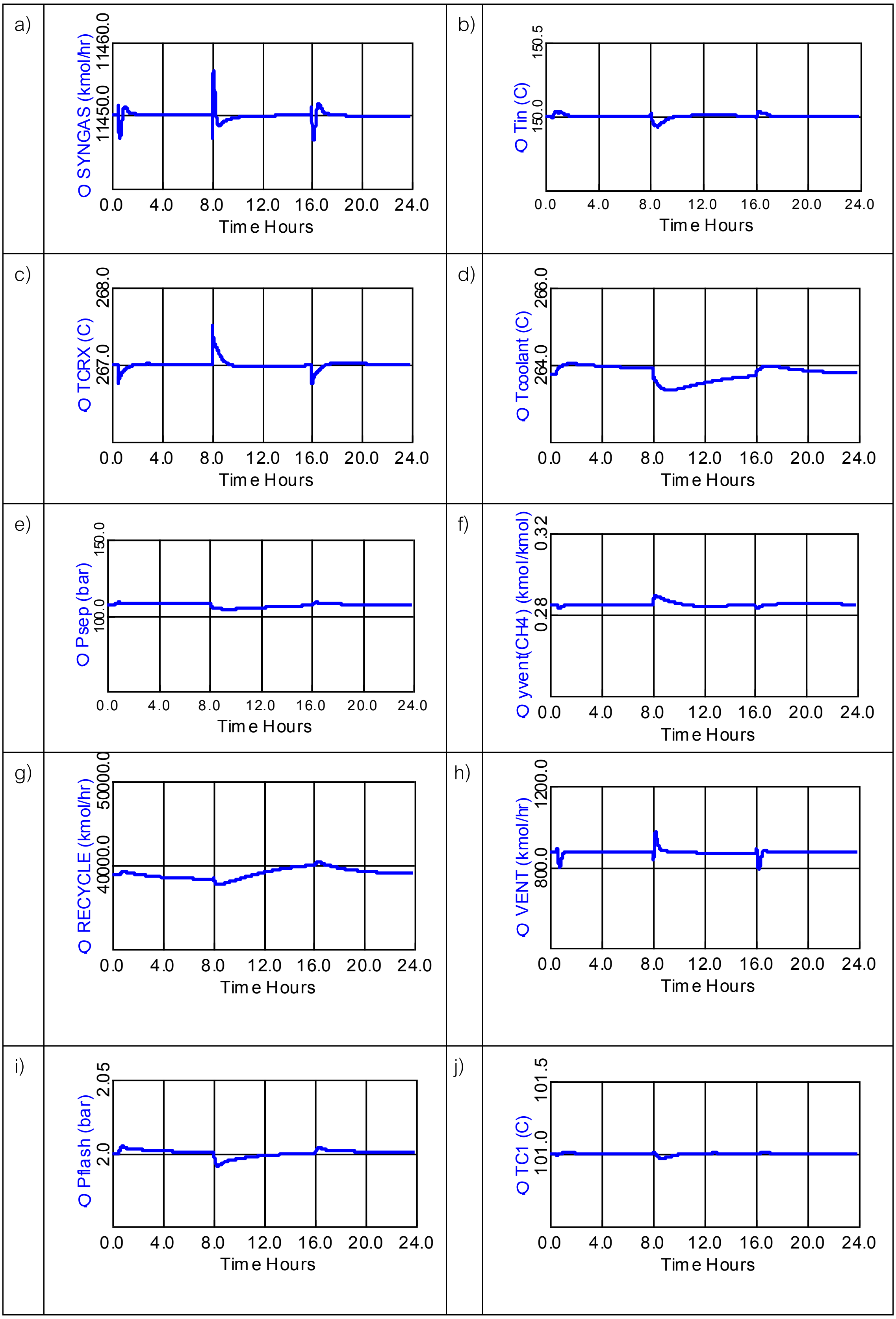


Figure 5.20 Dynamic responses of CS2 for the change CO/CO_2 ratio.

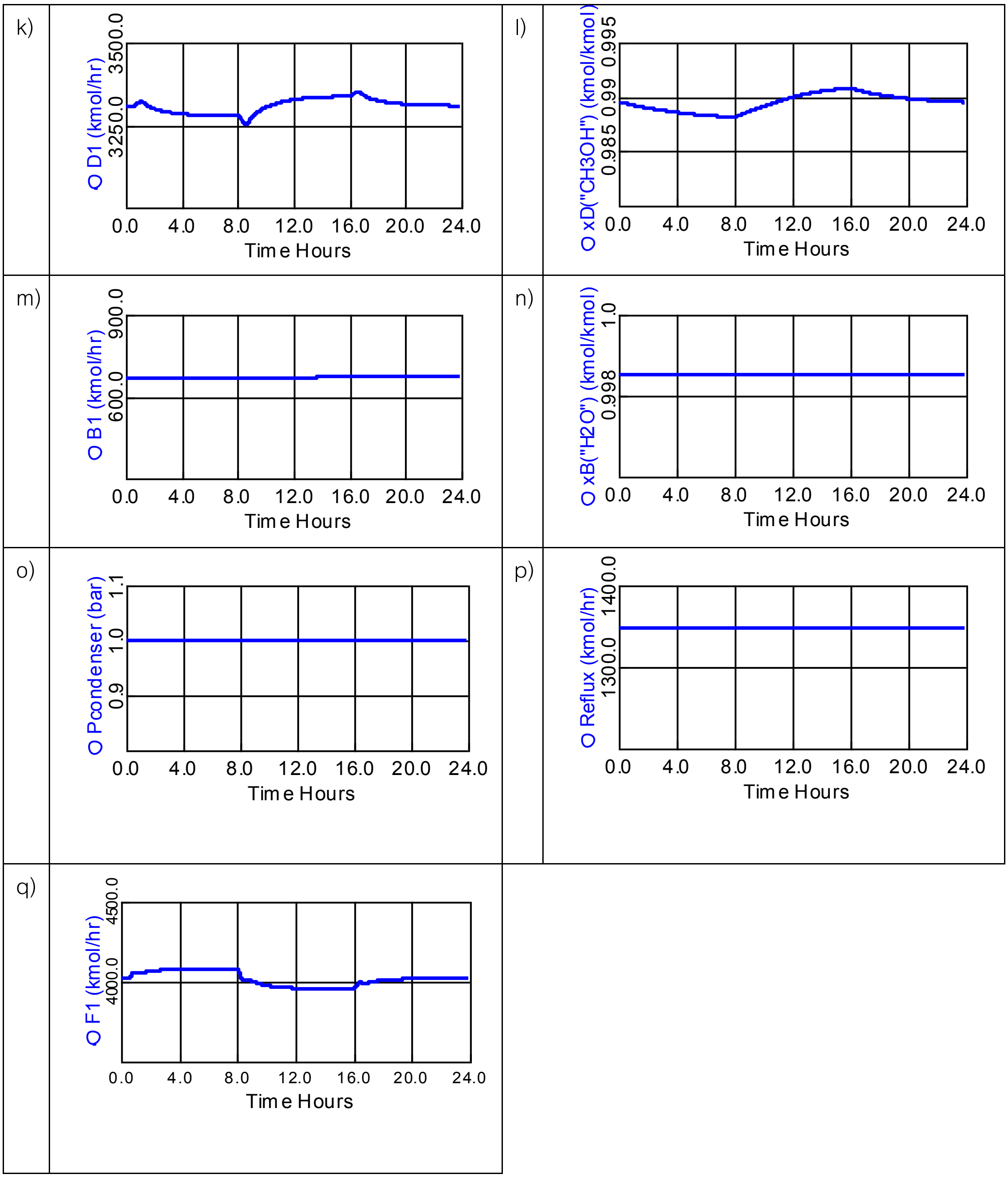


Figure 5.20 (Continued) Dynamic responses of CS2 for the change CO/CO$_2$ ratio.

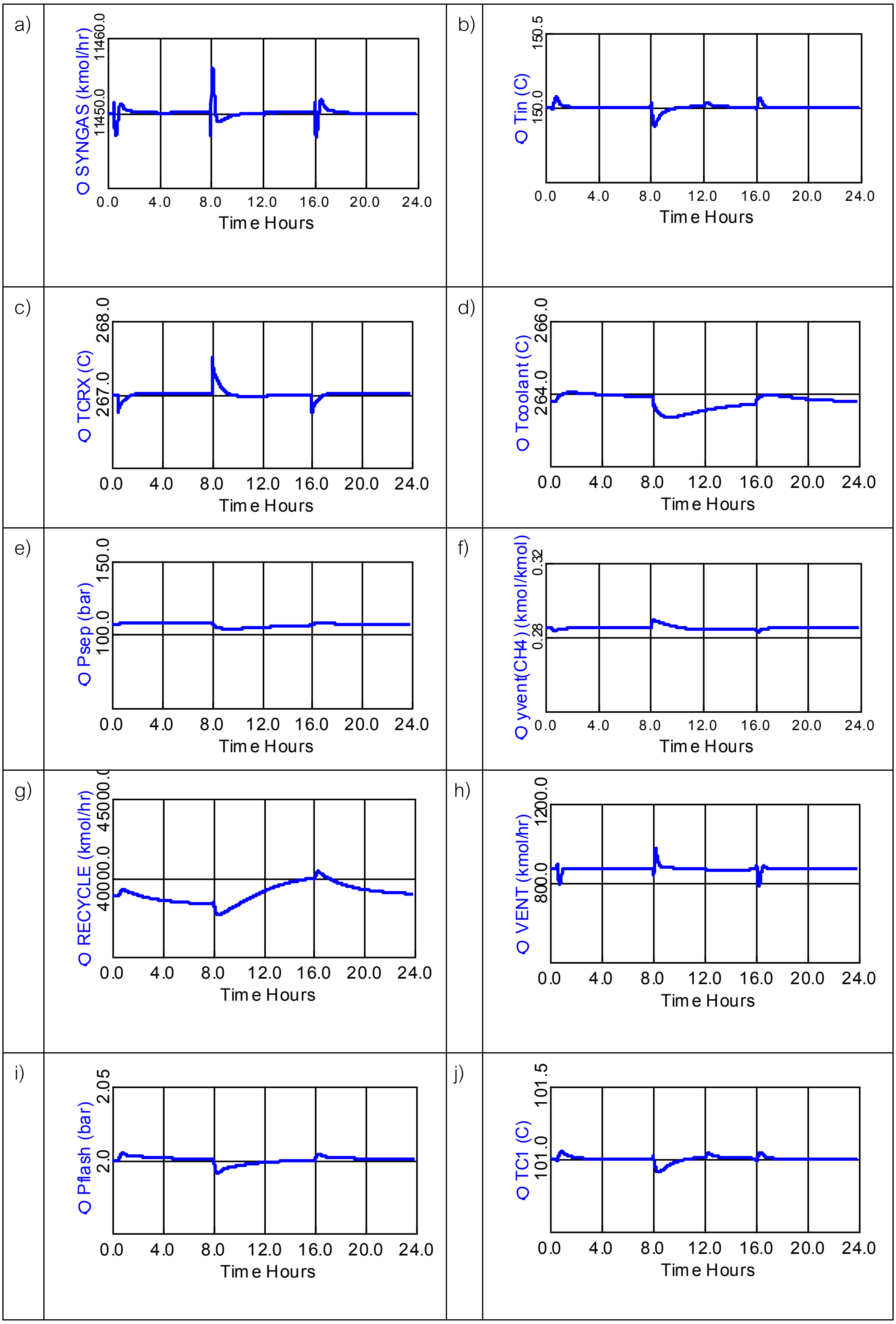


Figure 5.21 Dynamic responses of CS3 for the change CO/CO_2 ratio.

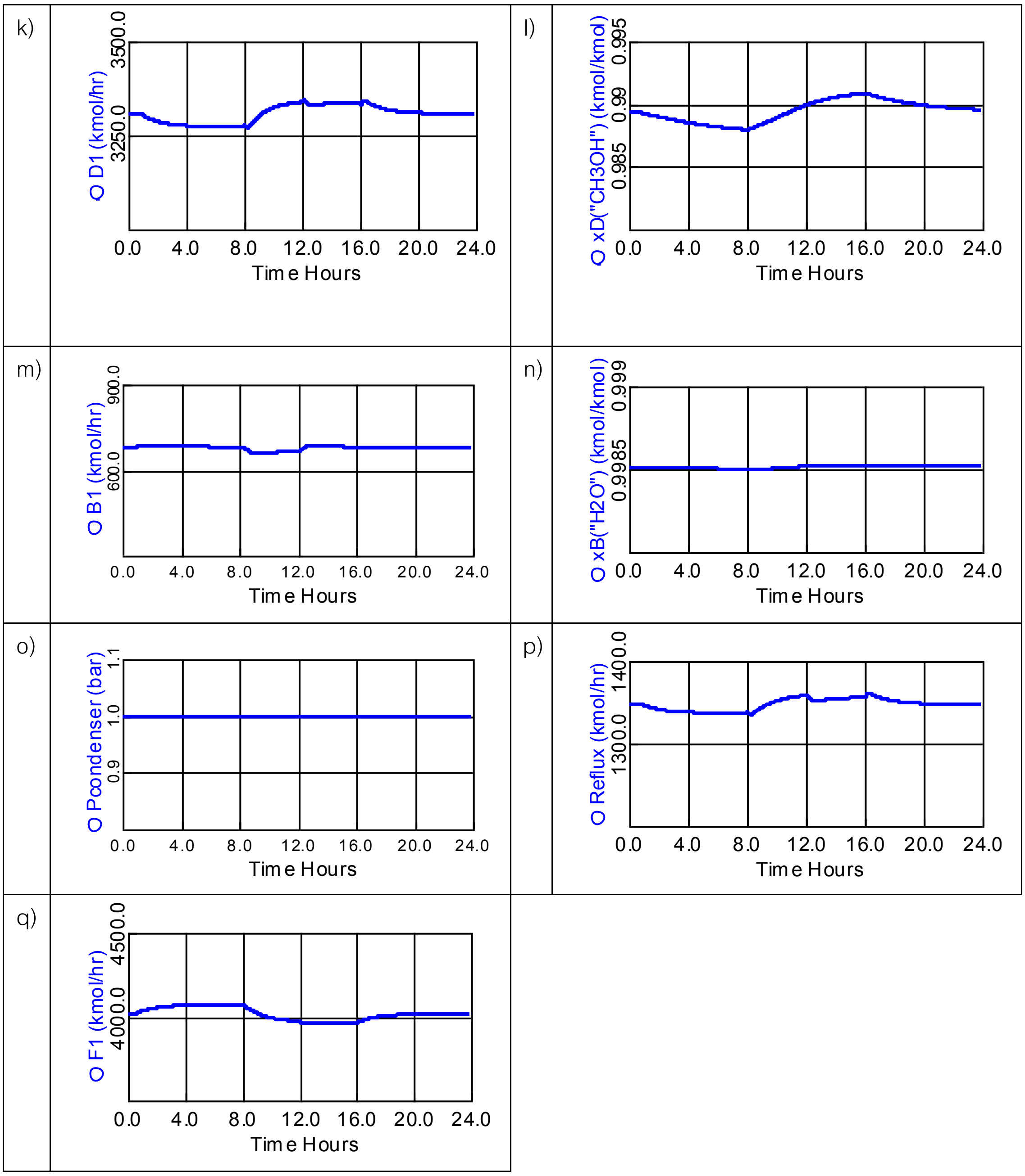


Figure 5.21 (Continued) Dynamic responses of CS3 for the change CO/CO_2 ratio.

5.3.2 Thermal Disturbances

Figure 5.22 shows dynamic response of methanol process for 10% changes in setpoint of the reactor inlet temperature controller. At time equal to 0.5 h, the temperature is increased from 150 to 165 °C and is dropped to 135 °C at time equal to 8 h.

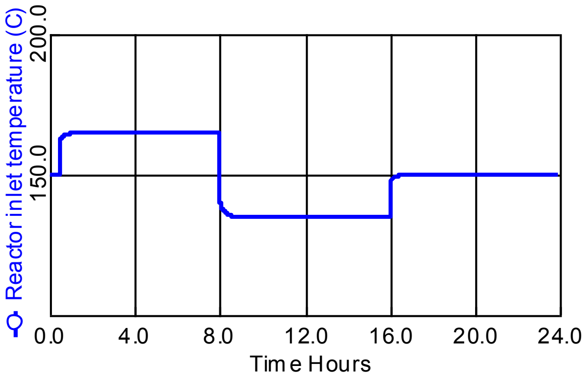


Figure 5.22 Dynamic response of methanol process by step change 10% the reactor inlet temperature.

Figure 5.23 to 5.26 give results of the dynamic responses of all control structures for change thermal disturbances. In all control structures give the same trend result to reject thermal disturbance and return to their setpoint. From all graphs, we can notice that the thermal disturbance in methanol synthesis section does not much effect to pressure condenser and product composition (methanol and water) from column.

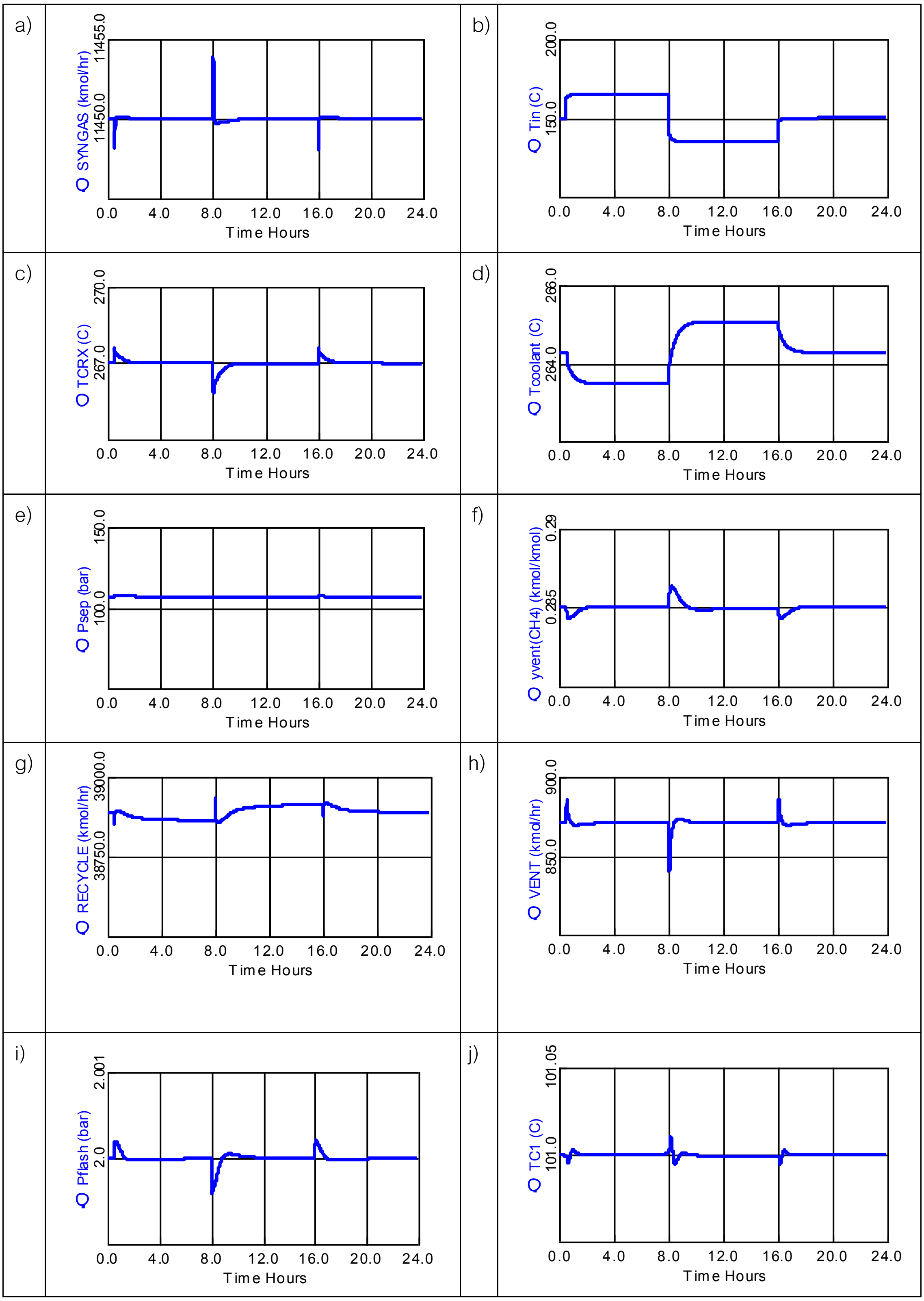


Figure 5.23 Dynamic responses of CS0 for 10% thermal disturbances

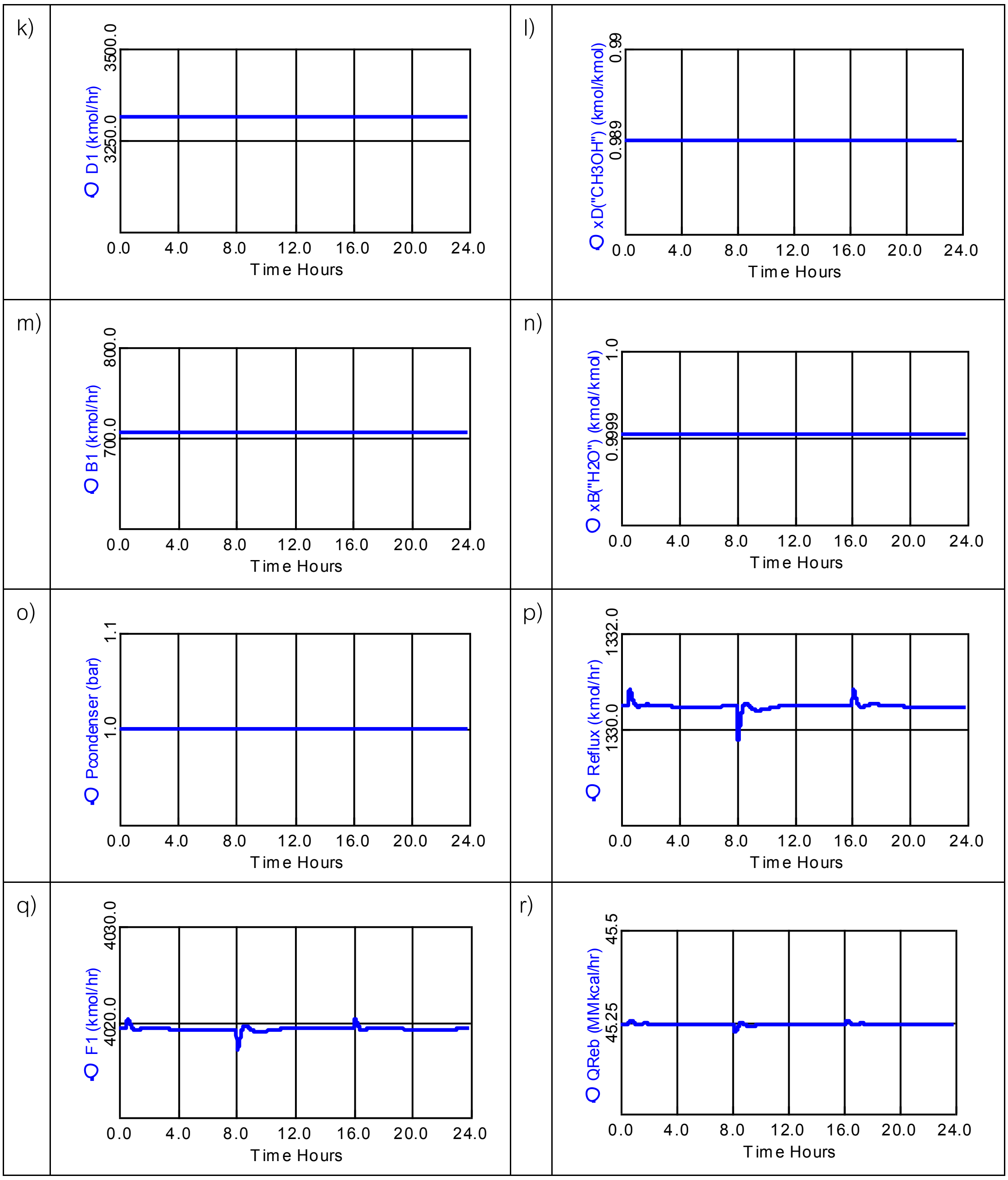


Figure 5.23 (Continued) Dynamic responses of CS0 for 10% thermal disturbances

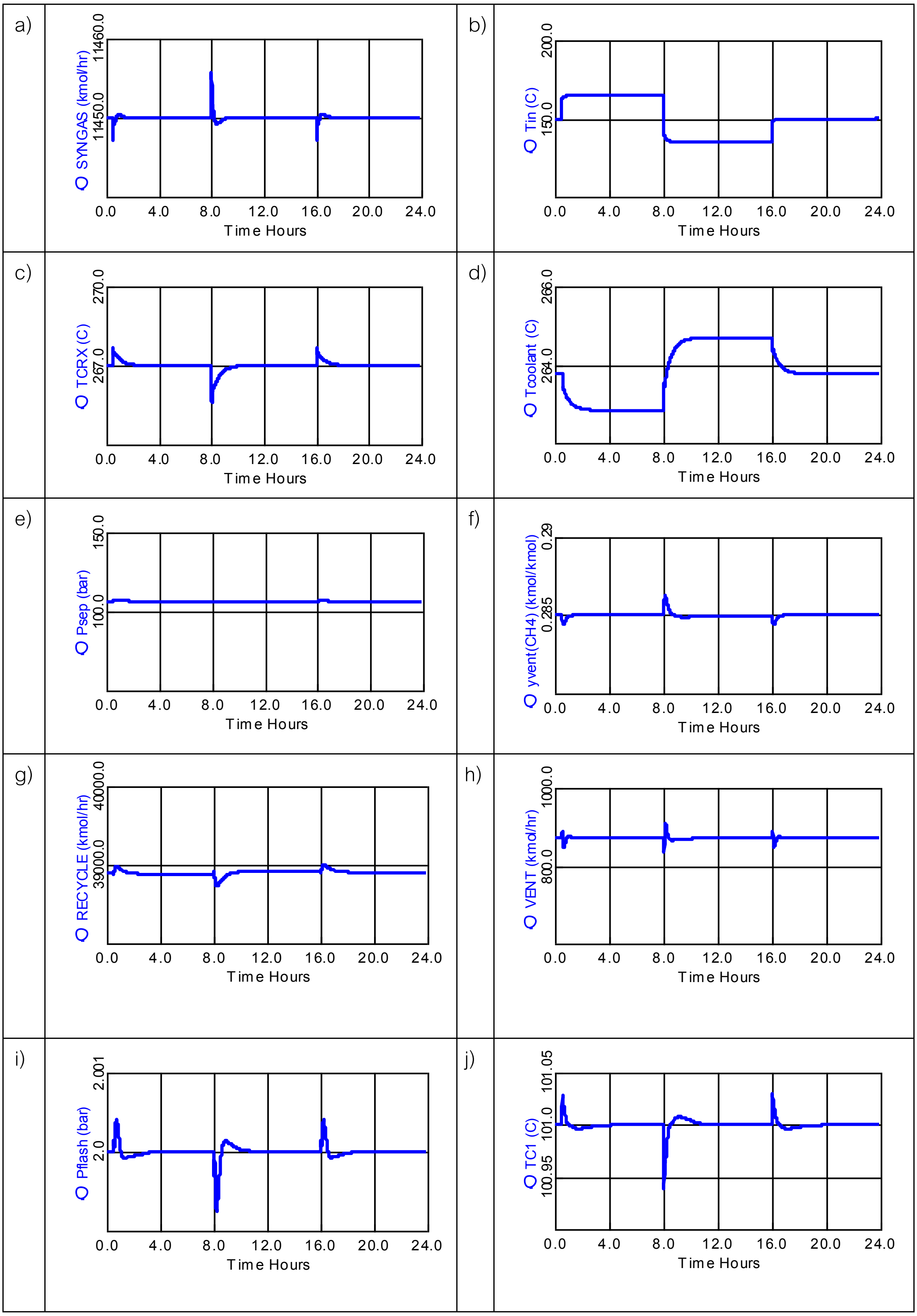


Figure 5.24 Dynamic responses of CS1 for 10% thermal disturbances

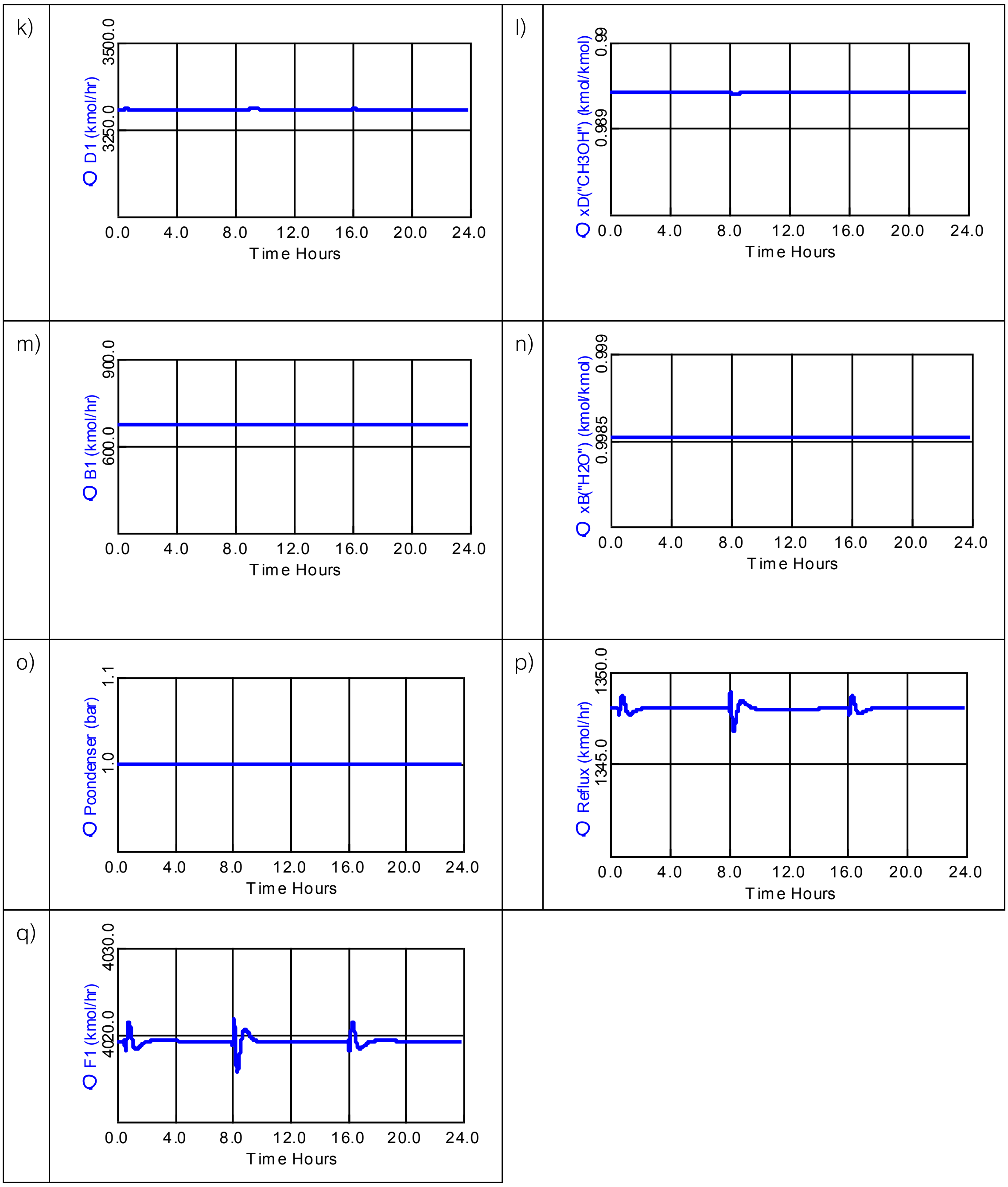


Figure 5.24 (Continued) Dynamic responses of CS1 for 10% thermal disturbances

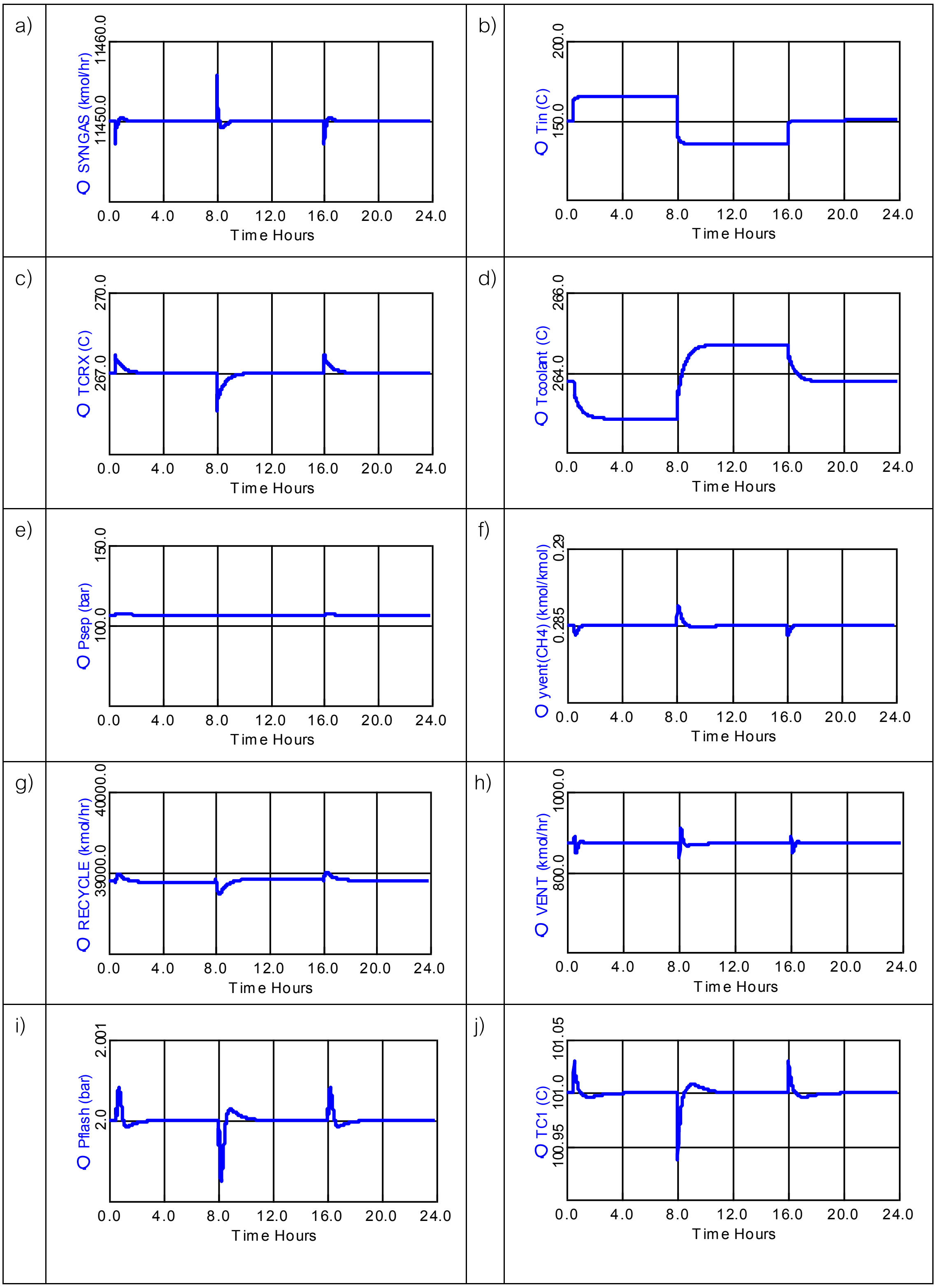


Figure 5.25 Dynamic responses of CS2 for 10% thermal disturbances

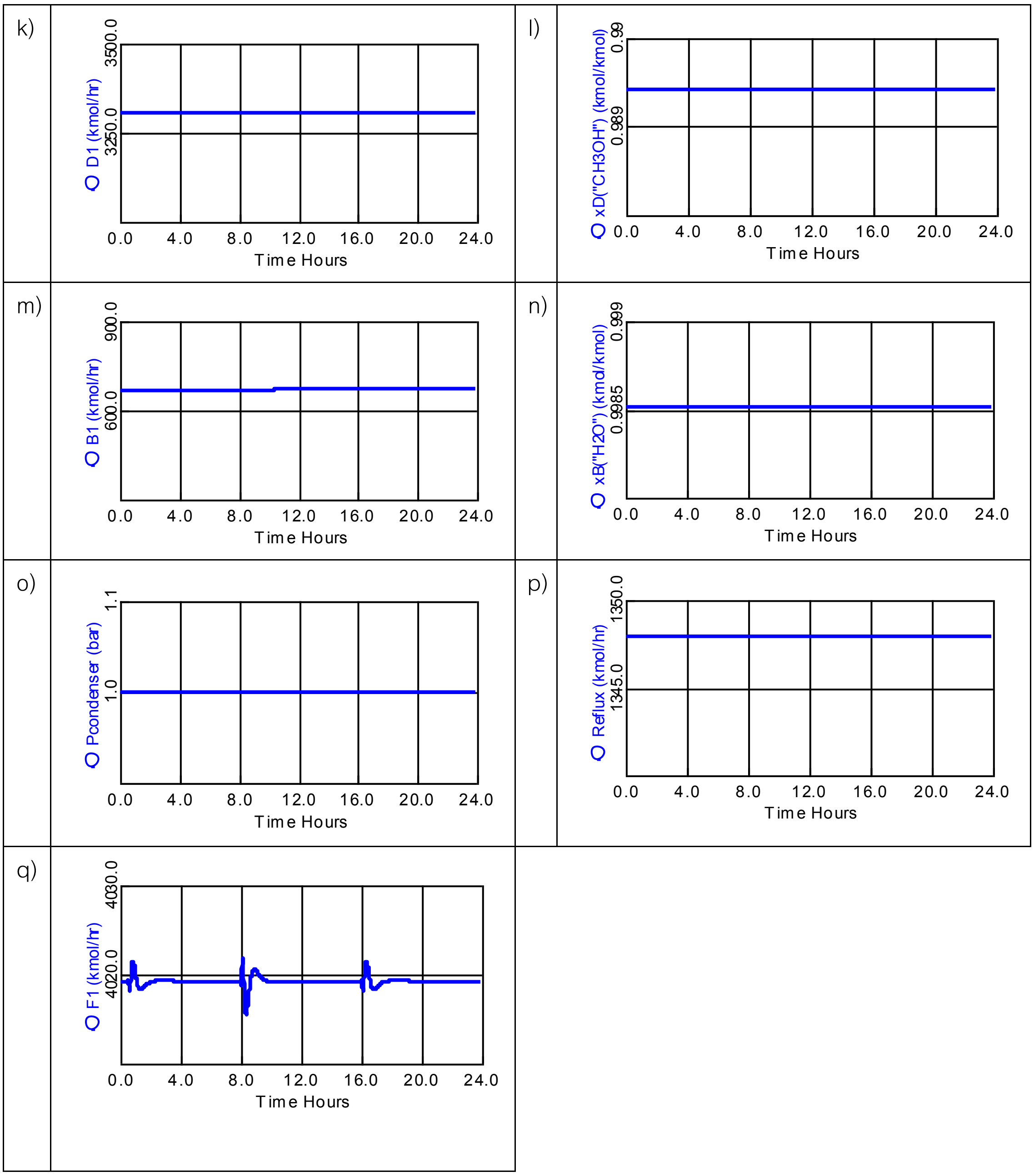


Figure 5.25 (Continued) Dynamic responses of CS2 for 10% thermal disturbances

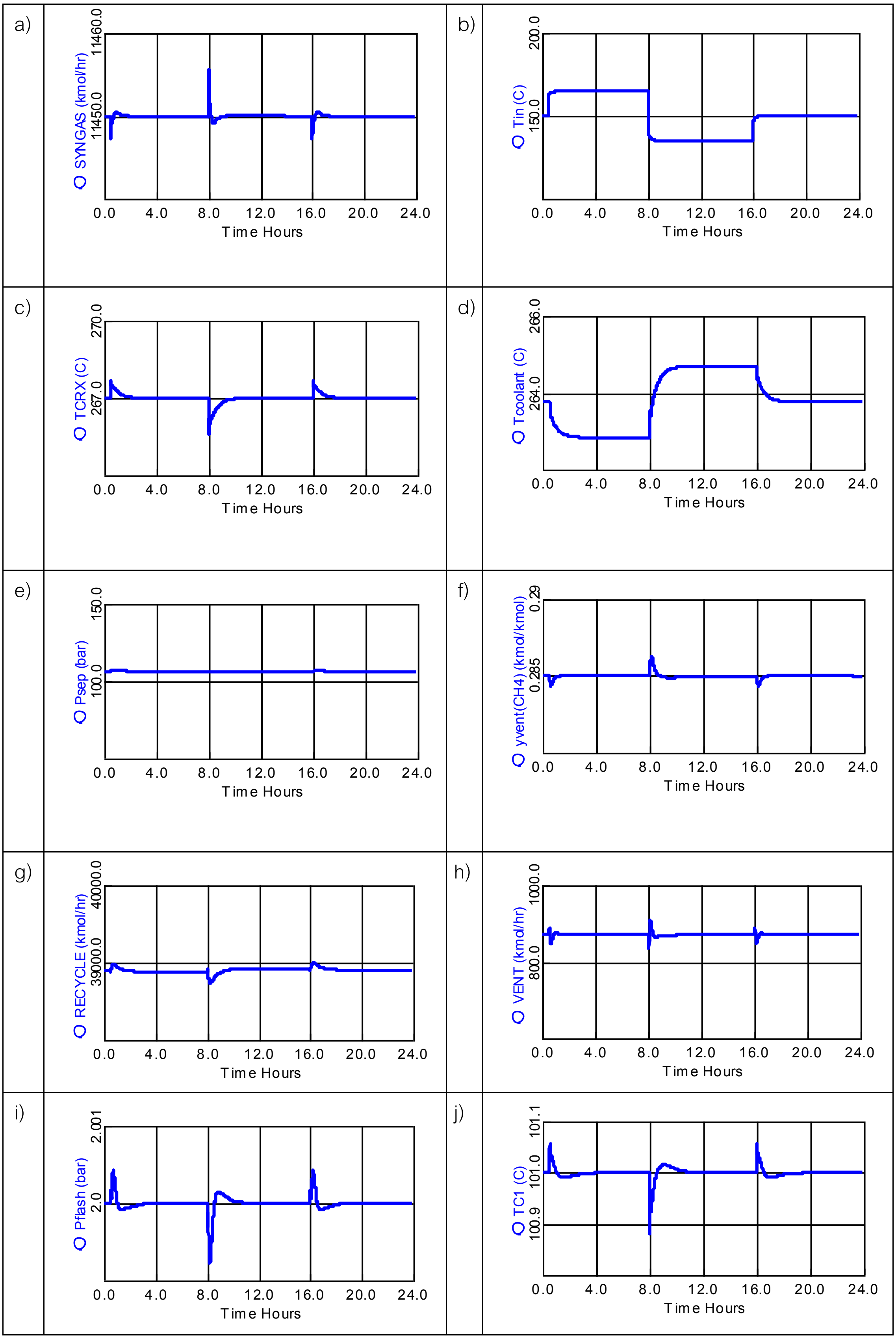


Figure 5.26 Dynamic responses of CS3 for 20% thermal disturbances

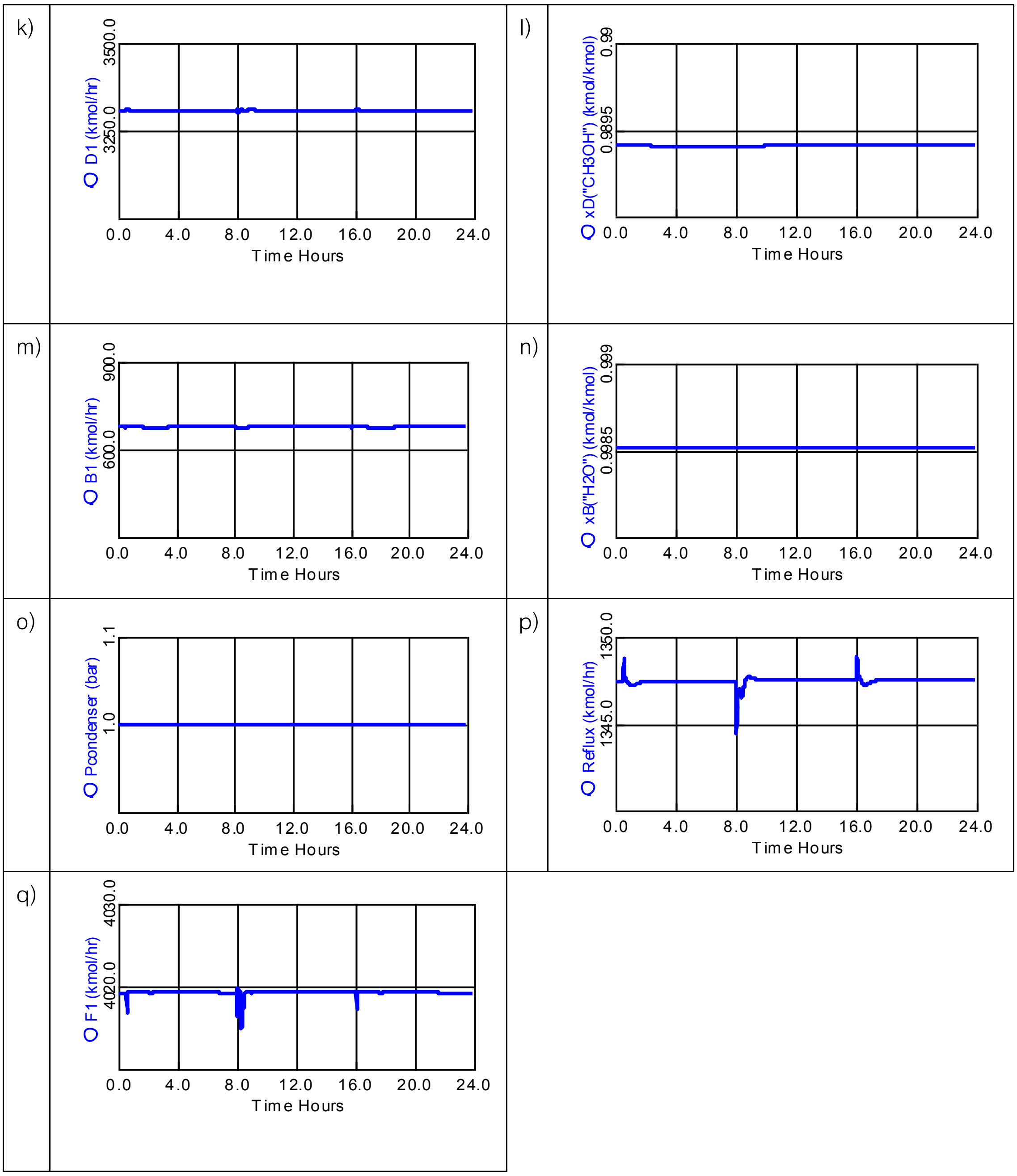


Figure 5.26 (Continued) Dynamic responses of CS3 for 20% thermal disturbances

5.4 Evaluation of the Dynamic Performance

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

$$\text{IAE} = \int |\varepsilon\,(t)|\, dt$$

Note that: $\varepsilon\,(t) = y_{sp}(t) - y(t)$ is the deviation (error) of the response from the desired setpoint.

In this research, IAE method is used to evaluate the dynamic performance of the base case control structure and designed control structures. Temperature, Pressure, and Composition loops are considered to evaluate the IAE results in handle disturbances because they involve in the production rate, product purities, and safety. The loop of temperature consists of the reactor inlet and outlet temperature (TCin and TCRX), the separator temperature (TCsep), and the tray temperature in the methanol column (TC1). For pressure loop, we considered the pressure in condenser column (PC1) and flash tank (PCflash). Moreover, methane composition in the recycle stream, and product purities (methanol and water) concern with composition loop. Table 5.6 to Table 5.8 shows the summation of IAE value result in each loop for handle all disturbances. The least of IAE value is clearly in temperature loop of the designed control structure II (CS2).

Table 5.6 The IAE Result of the temperature loop for handle all disturbances

Controller	Integral Absolute Error (IAE)			
	CS0	CS1	CS2	CS3
TCin	0.1293	0.1576	0.1495	0.1527
TCRX	0.1407	0.1539	0.1566	0.1604
TCsep	0.1118	0.0712	0.0746	0.1035
TC1	0.1126	0.0565	0.0376	0.0695
SUM	0.4945	0.4392	0.4183	0.4861

Table 5.7 The IAE Result of the pressure loop for handle all disturbances

Controller	Integral Absolute Error (IAE)			
	CS0	CS1	CS2	CS3
PCflash	0.0062	0.0061	0.0062	0.0053
PC1	0.0012	0.0012	0.0010	0.0072
SUM	0.0074	0.0073	0.0071	0.0125

Table 5.8 The IAE Result of the composition loop for handle all disturbances

Controller	Integral Absolute Error (IAE)			
	CS0	CS1	CS2	CS3
CCvent	0.0468	0.0385	0.0383	0.0408
x_{CH3OH}	0.0244	0.0244	0.0268	0.0275
x_{H2O}	0.0001	0.0001	0.0001	0.0009
SUM	0.0714	0.0630	0.0653	0.0693

For all disturbances testing, Figure 5.27 shows the result of integral absolute error of all control structures for handle disturbances (includes all loops). Control structure II (CS2) can be handle disturbances the best.

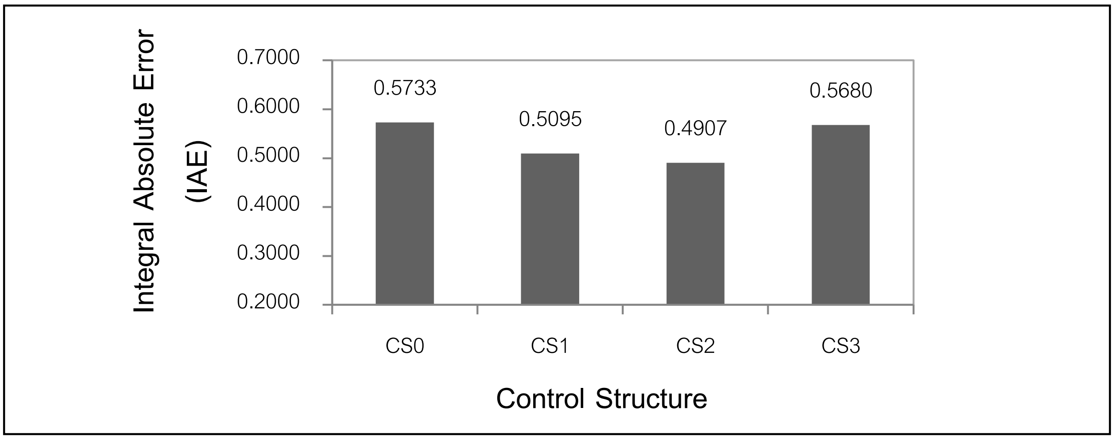


Figure 5.27 The IAE summation for handle disturbances to the change in all disturbances testing

For energy use, the summation value of all energy use is used to evaluate the dynamic performance of all control structures (the most minimize energy use) From Table 5.9 to 5.12 show the summation value of all energy.

Table 5.9 The summation value of all energy use for the change in synthesis gas flow

Energy	CS0	CS1	CS2	CS3
Wk1	3.92E+05	3.56E+05	3.96E+05	3.56E+05
Wk2	9.47E+05	8.99E+05	9.96E+05	8.91E+05
Wk3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Wk4	7.20E+01	7.26E+01	8.00E+01	6.94E+01
Wkflash	1.99E+05	1.87E+05	2.08E+05	1.91E+05
Qcond	3.73E+06	3.31E+06	2.70E+06	1.54E+06
H-101	4.65E+05	4.45E+05	4.94E+05	4.45E+05
H-102	4.58E+05	0.00E+00	0.00E+00	0.00E+00
H-103	6.42E+06	3.40E+06	4.02E+06	3.91E+06
Qreb	4.16E+06	0.00E+00	0.00E+00	0.00E+00
Qreact	4.65E+06	4.53E+06	4.52E+06	4.54E+06
SUM	2.14E+07	1.31E+07	1.33E+07	1.19E+07

Table 5.10 The summation value of all energy use for the change methane composition

Energy	CS0	CS1	CS2	CS3
Wk1	6.83E+04	4.52E+04	4.53E+04	4.53E+04
Wk2	2.66E+06	1.56E+06	1.56E+06	1.56E+06
Wk3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Wk4	3.12E+02	1.84E+02	1.84E+02	1.83E+02
Wkflash	8.51E+05	5.31E+05	5.32E+05	5.29E+05
Qcond	3.25E+06	1.85E+06	1.17E+06	1.79E+06
H-101	5.73E+04	3.96E+04	3.96E+04	3.97E+04
H-102	4.02E+06	0.00E+00	0.00E+00	0.00E+00
H-103	1.85E+07	5.64E+06	5.83E+06	6.04E+06
Qreb	3.73E+06	0.00E+00	0.00E+00	0.00E+00
Qreact	3.34E+06	3.33E+06	3.35E+06	3.50E+06
SUM	3.65E+07	1.30E+07	1.25E+07	1.35E+07

Table 5.11 The summation value of all energy use for the change CO/CO_2 ratio

Energy	CS0	CS1	CS2	CS3
Wk1	1.29E+04	1.80E+04	1.80E+04	1.83E+04
Wk2	2.54E+05	2.55E+05	2.54E+05	2.54E+05
Wk3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Wk4	3.87E+01	3.80E+01	3.82E+01	3.79E+01
Wkflash	4.79E+05	4.72E+05	4.72E+05	4.73E+05
Qcond	6.53E+04	1.24E+05	2.30E+05	4.01E+05

Table 5.11(Continued) The summation value of all energy use for the change CO/CO_2 ratio

Energy	**CS0**	**CS1**	**CS2**	**CS3**
H-101	8.65E+03	1.27E+04	1.27E+04	1.29E+04
H-102	3.99E+05	0.00E+00	0.00E+00	0.00E+00
H-103	1.54E+06	1.57E+06	1.60E+06	1.65E+06
Qreb	3.75E+04	0.00E+00	0.00E+00	0.00E+00
Qreact	3.04E+06	3.21E+06	3.21E+06	3.22E+06
SUM	5.83E+06	5.66E+06	5.80E+06	6.03E+06

Table 5.12 The summation value of all energy use for the change reactor inlet temperature

Energy	**CS0**	**CS1**	**CS2**	**CS3**
Wk1	6.86E+02	1.84E+03	1.84E+03	2.82E+03
Wk2	1.93E+04	2.13E+04	2.13E+04	2.13E+04
Wk3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Wk4	2.45E+00	2.71E+00	2.71E+00	2.70E+00
Wkflash	2.79E+03	2.77E+03	2.77E+03	2.77E+03
Qcond	1.89E+03	2.90E+03	2.50E+03	4.45E+03
H-101	5.81E+02	1.81E+03	1.81E+03	1.87E+03
H-102	1.33E+07	0.00E+00	0.00E+00	0.00E+00
H-103	6.12E+04	3.09E+04	3.09E+04	3.08E+04
Qreb	1.99E+03	0.00E+00	0.00E+00	0.00E+00
Qreact	1.39E+07	1.32E+07	1.36E+07	1.37E+07
SUM	2.74E+07	1.33E+07	1.37E+07	1.38E+07

From Figure 5.28, the summation values of energy consumption for all handling disturbances entering the process are similar in the designed control structure with resilient heat exchanger network (CS1, CS2, and CS3). They are less than the base case control structure (CS0).

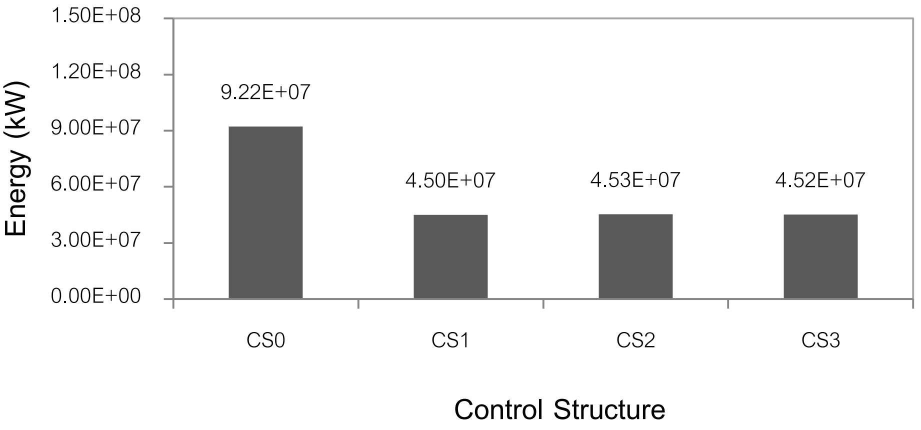


Figure 5.28 The summation value of all energy use in all disturbances testing

For all disturbances testing, Figure 5.29 shows the results of the Integral Absolute Error (IAE) for product variation. Control structure I (CS1) is the best control structure to maintain product quality when disturbances occur because of the reflux to feed ratio control.

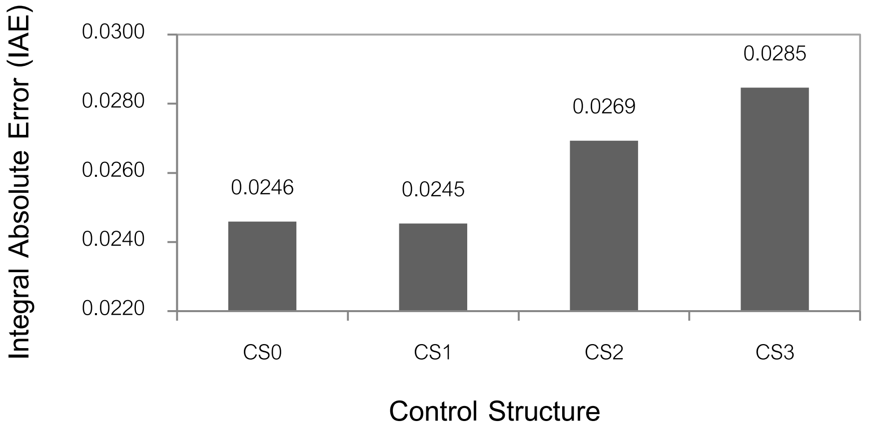


Figure 5.29 The IAE summation of product variation in all disturbances testing

5.5 Cost Estimation

In order to estimate the cost, we consider both capital investment and utility costs of the methanol process. The costs associated with supplying a given utility have been presented in Table 5.13 from Turton et al, 2009.

Table 5.13 Utility Costs

Utility	Description	Cost ($/GJ)
Steam from Boilers	Process steam: latent heat only	
	a. Low pressure (5 barg, 160°C) from HP steam	7.78
	b. Medium pressure (10 barg, 184°C) from HP steam	8.22
	c. High pressure (41 barg, 254°C) from reactor	6.00
Cooling Tower Water	Processes cooling water	0.354
Electrical	Electric Distribution	16.8

In this process, total capital investment is estimated from economic basis (Luyben, 2010). It includes the cost of compressors, the inter-stage cooler, heat exchangers, the preheater, the reactor, cooler/condenser, the separator, the flash tank, column reboiler and the distillation column vessel. The total capital investment of the base case control structure is about $27,056,904 and all designed control structures with resilient heat exchanger networks (CS1 to CS3) are about $26,735,530.

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The costs of utilities are directly impacted by the cost of fuel which is the high pressure steam in the reactor ($6.00 per GJ). The compressors use electricity. The cooling water is used in coolers and the condenser. The reactor preheater and column reboiler use the medium pressure steam and the low pressure steam, respectively. Based on the methanol process is operated for 24 hours per day and 340 days per year. The utility cost of base case control structure is about $24,805,740 and all designed control structures with resilient heat exchanger networks are about $11,585,701. Total annual cost involves in total capital investment, utility costs, and payback period. For this process, the period of time to recover the initial investment is three years.

$$\text{Total annual cost (TAC)} = \frac{\text{Total capital investment}}{\text{payback period}} + \text{Utility costs}$$

Therefore, total annual cost (TAC) of base case control structure and designed control structures is $34,176,209 and $20,497,545, respectively.

In the face of disturbances, utility costs of each control structure have been presented in Figure 5.30. The utility costs of all designed control structures with resilient heat exchanger networks (CS1 to CS3) can be reduce utility costs and less than the base case control structure (CS0).

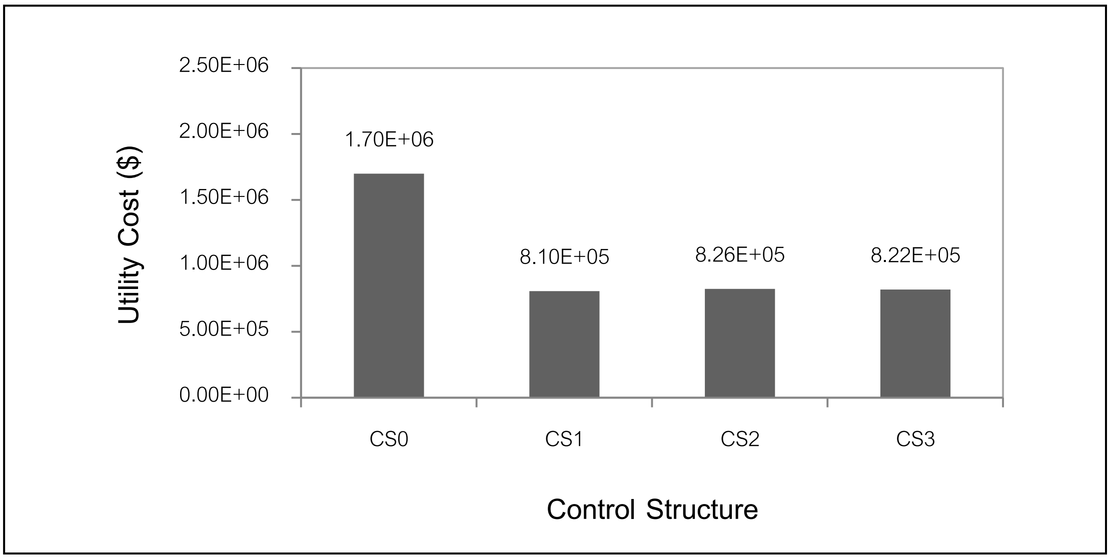

Figure 5.30 Utility costs of all control structures in all disturbances testing.

CHAPTER VI

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

In this research has discussed control structures designed for methanol process, using Wongsri's procedure (2009). The appropriate set of controlled variables is selected by the "Fixture point theorem". The proposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple, and straightforward.

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

For the material disturbances: change flow rate, methane composition and carbon monoxide to carbon dioxide composition ratio in the synthesis gas feed stream. Designed control structure II (CS2) can handle disturbances the best, designed control structure II (CS2) is the most minimize energy use, and designed control structure I (CS1) is the least of product variation.

For the thermal disturbances, all designed control structures (CS1 to CS3) are similar for the IAE values and the summation of energy consumption. The product quality can be held at the specified values.

For all disturbances testing, designed control structure II (CS2) is the least of the IAE value and the most minimize energy use. However, the product variation of CS2 is more than the designed control structure I (CS1) while both of control structures (CS1 and CS2) is nearly the IAE value and the summation of energy consumption. Therefore, the best designed control structure is CS1 for the handle disturbances entering the process, minimize energy use, and maintain product quality.

The best control configurations depend on the direction of controlled variable with manipulated variable. Therefore this research establishes that the Wongsri's procedure, which combines heuristics, analytical method and dynamic simulation, a useful design procedure that leads to a good-performance plantwide control system.

6.2 Recommendation

Study and design the control structure of other process in plantwide control via design procedure of Wongsri. The reactor pressure should be controlled when the high pressure methanol synthesis is required.

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APPENDICES

APPENDIX A

PROCESS STREAM DATA AND EQUIPMENT SIZING

Table A.1 Data stream of methanol process

Name	SYNGAS	1	2	K2OUT
Vapor Fraction	1.0000	1.0000	1.0000	1.0000
Temperature (°C)	49.6700	95.6400	38.0000	83.3400
Pressure (bar)	51.2000	75.0500	74.5500	110.0000
Molar Flow (kmol/h)	11450	11450	11450	11450
Mass Flow (kgl/h)	129245.90	129245.90	129245.90	129245.90
Comp Mole Frac (H_2)	0.6746	0.6746	0.6746	0.6746
Comp Mole Frac (Water)	0.0023	0.0023	0.0023	0.0023
Comp Mole Frac (CO)	0.2297	0.2297	0.2297	0.2297
Comp Mole Frac (CO_2)	0.0686	0.0686	0.0686	0.0686
Comp Mole Frac (Methanol)	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0217	0.0217	0.0217	0.0217
Comp Mole Frac (N_2)	0.0030	0.0030	0.0030	0.0030

Table A.1 (Continued) Data stream of methanol process

Name	R1	R2	R3	TOTAL	COUT	R1IN	R1OUT	HIN	HOUT
Vapor Fraction	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Temperature (°C)	41.38	498.86	542.94	52.91	144.53	150.00	266.61	266.61	174.53
Pressure (bar)	110.00	110.00	110.00	110.00	109.41	109.31	107.54	107.54	106.95
Molar Flow (kmol/h)	38767.31	224.823	0.669	50442.8	50442.8	50442.65	43882.67	43882.67	43882.67
Mass Flow (kg/h)	449131.9	7765.225	24.283	586167.4	586167.4	586163	586163	586163	586163
CompMole Frac (H_2)	0.551	0.044	0.018	0.577	0.577	0.577	0.498	0.498	0.498
CompMole Frac (Water)	595 ppm	0.016	123 ppm	0.001	0.001	0.001	0.017	0.017	0.017
CompMole Frac (CO)	0.039	0.006	514 ppm	0.082	0.082	0.082	0.035	0.035	0.035
CompMole Frac (CO_2)	0.08	0.612	0.421	0.080	0.080	0.080	0.077	0.077	0.077
CompMole Frac (Methanol)	0.005	0.114	0.545	0.004	0.004	0.004	0.080	0.080	0.080
CompMole Frac (Methane)	0.285	0.203	0.014	0.225	0.225	0.225	0.258	0.258	0.258
CompMole Frac (N_2)	0.040	0.005	539 ppm	0.031	0.031	0.031	0.036	0.036	0.036

Table A.1 (Continued) Data stream of methanol process

Name	3	4	GAS	RECYCLE	VENT	6	LIQ	5	VFLASH
Vapor Fraction	0.903	0.903304	1.000	1.000	1.000	1.000	0.000	0.053	1.000
Temperature (°C)	38.00	38.000	38.000	38.000	38.000	37.600	38.000	36.25	36.25
Pressure (bar)	106.48	106.460	106.460	106.460	106.460	101.460	106.460	2.000	2.000
Molar Flow (kmol/h)	43882.67	43882.67	39639.38	38767.31	872.066	872.066	4243.266	4243.266	224.823
Mass Flow (kg/h)	586163	586163	459233.7	449131.9	10103.14	10103.14	126928.8	126928.8	7765.225
Comp Mole Frac (H_2)	0.498	0.498	0.551	0.551	0.551	0.551	0.002	0.002	0.044
Comp Mole Frac (Water)	0.017	0.017	595 ppm	595 ppm	595 ppm	595 ppm	0.168	0.168	0.016
Comp Mole Frac (CO)	0.035	0.035	0.039	0.039	0.039	0.039	302 ppm	302 ppm	0.006
Comp Mole Frac (CO_2)	0.077	0.077	0.080	0.080	0.080	0.080	0.040	0.040	0.612
Comp Mole Frac (Methanol)	0.080	0.08	0.005	0.005	0.005	0.005	0.778	0.778	0.114
Comp Mole Frac (Methane)	0.258	0.258	0.285	0.285	0.285	0.285	0.011	0.011	0.203
Comp Mole Frac (N_2)	0.036	0.036	0.040	0.040	0.040	0.040	283 ppm	283 ppm	0.005

Table A.1 (Continued) Data stream of methanol process

Name	LFLASH	7	F1	D1	V1	B1
Vapor Fraction	0.000	0.000	0.003	0.000	1.000	0.000
Temperature (°C)	36.25	36.400	36.220	50.000	50.000	109.83
Pressure (bar)	2.000	7.000	1.260	1.000	1.000	1.410
Molar Flow (kmol/h)	4018.443	4018.443	4018.443	3310.848	0.669	706.926
Mass Flow (kg/h)	119163.5	119163.5	119163.5	106402.8	24.283	12736.46
Comp Mole Frac (H_2)	3 ppm	3 ppm	3 ppm	0.000	0.018	0.000
Comp Mole Frac (Water)	0.177	0.177	0.177	0.001	123 ppm	1.000
Comp Mole Frac (CO)	824 ppb	824 ppb	824 ppb	897 ppb	514 ppm	0.000
Comp Mole Frac (CO_2)	0.008	0.008	0.008	0.009	0.421	0.000
Comp Mole Frac (Methanol)	0.815	0.815	0.815	0.989	0.545	1000 ppm
Comp Mole Frac (Methane)	165 ppm	165 ppm	165 ppm	198 ppm	0.014	0.000
Comp Mole Frac (N_2)	689 ppb	689 ppb	689 ppb	727 ppb	539 ppm	0.000

Table A.2 Data stream of methanol process with resilient heat exchanger

Name	SYNGAS	1	2	K2OUT	R1	R2	R3
Temperature (°C)	49.6000	95.6000	38.0000	83.3000	41.4000	498.8000	543.0000
Pressure (bar)	51.2000	75.0500	74.5500	110.0000	110.0000	110.0000	110.0000
Vapor Frac	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Mole Flow kmol/hr	11450.0000	11450.0000	11450.0000	11450.0000	38680.6910	224.7050	0.6610
Mass Flow kg/hr	129245.9460	129245.9460	129245.9460	129245.9460	448216.0820	7757.6440	23.9860
Comp Mole Frac (H_2)	0.6750	0.6750	0.6750	0.6750	0.5500	0.0440	0.0190
Comp Mole Frac (Water)	0.0020	0.0020	0.0020	0.0020	597 PPM	0.0160	122 PPM
Comp Mole Frac (CO)	0.2300	0.2300	0.2300	0.2300	0.0390	0.0060	512 PPM
Comp Mole Frac (CO_2)	0.0690	0.0690	0.0690	0.0690	0.0800	0.6120	0.4210
Comp Mole Frac (Methanol)	0.0000	0.0000	0.0000	0.0000	0.0050	0.1140	0.5450
Comp Mole Frac (CH4)	0.0220	0.0220	0.0220	0.0220	0.2850	0.2040	0.0140
Comp Mole Frac (N_2)	0.0030	0.0030	0.0030	0.0030	0.0400	0.0050	542 PPM

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

Name	TOTAL	C1OUT	H1IN	H1OUT	ROUT	HIN
Temperature (°C)	52.9000	150.0000	266.6000	163.8000	266.6000	266.6000
Pressure (bar)	110.0000	109.8000	107.9300	107.7300	108.0300	107.9300
Vapor Frac	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Mole Flow kmol/hr	50356.0570	50356.0570	41605.1590	41605.1590	43794.9000	43794.9000
Mass Flow kg/hr	585243.6600	585243.6600	555982.1670	555982.1670	585243.6600	585243.6600
Comp Mole Frac (H_2)	0.5760	0.5760	0.4970	0.4970	0.4970	0.4970
Comp Mole Frac (Water)	0.0010	0.0010	0.0170	0.0170	0.0170	0.0170
Comp Mole Frac (CO)	0.0820	0.0820	0.0350	0.0350	0.0350	0.0350
Comp Mole Frac (CO_2)	0.0800	0.0800	0.0760	0.0760	0.0760	0.0760
Comp Mole Frac (Methanol)	0.0040	0.0040	0.0800	0.0800	0.0800	0.0800
Comp Mole Frac (CH4)	0.2250	0.2250	0.2590	0.2590	0.2590	0.2590
Comp Mole Frac (N_2)	0.0320	0.0320	0.0360	0.0360	0.0360	0.0360

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

Name	BP	BP1	H1	BP2IN	BP2	H2IN
Temperature (°C)	266.6000	266.6000	169.0000	169.0000	168.9000	169.0000
Pressure (bar)	107.9300	107.7300	107.7300	107.7300	106.9500	107.7300
Vapor Frac	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Mole Flow kmol/hr	2189.7450	2189.7450	43794.9040	4379.4900	4379.4900	39415.4140
Mass Flow kg/hr	29262.1830	29262.1830	585244.3490	58524.4350	58524.4350	526719.9170
Comp Mole Frac (H_2)	0.4970	0.4970	0.4970	0.4970	0.4970	0.4970
Comp Mole Frac (Water)	0.0170	0.0170	0.0170	0.0170	0.0170	0.0170
Comp Mole Frac (CO)	0.0350	0.0350	0.0350	0.0350	0.0350	0.0350
Comp Mole Frac (CO_2)	0.0760	0.0760	0.0760	0.0760	0.0760	0.0760
Comp Mole Frac (Methanol)	0.0800	0.0800	0.0800	0.0800	0.0800	0.0800
Comp Mole Frac (CH4)	0.2590	0.2590	0.2590	0.2590	0.2590	0.2590
Comp Mole Frac (N_2)	0.0360	0.0360	0.0360	0.0360	0.0360	0.0360

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

Name	H2OUT	C2IN	B1	10	11	VT	BOIL
Temperature (°C)	144.0000	109.6000	109.8000	110.4000	110.6000	109.8000	109.8000
Pressure (bar)	106.9500	2.7000	1.4100	16.4100	3.0000	1.4100	1.4000
Vapor Frac	1.0000	0.0490	0.0000	0.0000	0.0000	1.0000	1.0000
Mole Flow kmol/hr	39415.4140	5441.8140	708.2020	708.2020	708.2020	4733.6110	4733.5250
Mass Flow kg/hr	526719.9170	102287.4390	12773.2060	12773.2060	12773.2060	89514.2320	89512.9290
Comp Mole Frac (H_2)	0.4970	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Water)	0.0170	0.9440	0.9990	0.9990	0.9990	0.9360	0.9360
Comp Mole Frac (CO)	0.0350	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CO_2)	0.0760	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methanol)	0.0800	0.0560	0.0010	0.0010	0.0010	0.0640	0.0640
Comp Mole Frac (CH4)	0.2590	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (N_2)	0.0360	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

Name	H2	HX4OUT	FSEP	GAS	RCY	VENT	6
Temperature (°C)	146.5000	38.0000	38.0000	38.0000	38.0000	38.0000	37.5967
Pressure (bar)	106.9500	106.4800	106.4600	106.4600	106.4600	106.4600	101.4600
Vapor Frac	1.0000	0.9030	0.9030	1.0000	1.0000	1.0000	1.0000
Mole Flow kmol/hr	43794.9040	43794.9040	43794.9040	39550.8070	38680.6910	870.1180	870.1178
Mass Flow kg/hr	585244.3490	585244.3490	585244.3490	458298.2400	448216.0820	10082.5610	10082.5612
Comp Mole Frac (H_2)	0.4970	0.4970	0.4970	0.5500	0.5500	0.5500	0.5504
Comp Mole Frac (Water)	0.0170	0.0170	0.0170	597 PPM	597 PPM	597 PPM	0.0006
Comp Mole Frac (CO)	0.0350	0.0350	0.0350	0.0390	0.0390	0.0390	0.0385
Comp Mole Frac (CO_2)	0.0760	0.0760	0.0760	0.0800	0.0800	0.0800	0.0803
Comp Mole Frac (Methanol)	0.0800	0.0800	0.0800	0.0050	0.0050	0.0050	0.0048
Comp Mole Frac (CH4)	0.2590	0.2590	0.2590	0.2850	0.2850	0.2850	0.2852
Comp Mole Frac (N_2)	0.0360	0.0360	0.0360	0.0400	0.0400	0.0400	0.0401

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

Name	LIQ	5	VFLASH	LFLASH	LF1	F1
Temperature (°C)	38.000	36.300	36.300	36.300	36.400	36.200
Pressure (bar)	106.460	2.000	2.000	2.000	7.000	1.260
Vapor Frac	0.000	0.053	1.000	0.000	0.000	0.003
Mole Flow kmol/hr	4244.081	4244.081	224.705	4019.376	4019.376	4019.376
Mass Flow kg/hr	126945.600	126945.600	7757.644	119187.954	119187.954	119187.954
Comp Mole Frac (H_2)	0.002	0.002	0.0440	3 PPM	3 PPM	3 PPM
Comp Mole Frac (Water)	0.1680	0.168	0.0160	0.1770	0.1770	0.1770
Comp Mole Frac (CO)	0.0000	0.000	0.0060	821 PPB	821 PPB	821 PPB
Comp Mole Frac (CO_2)	0.0400	0.04	0.6120	0.0080	0.0080	0.0080
Comp Mole Frac (Methanol)	0.7780	0.778	0.1140	0.8150	0.8150	0.8150
Comp Mole Frac (CH4)	0.0110	0.011	0.2040	166 PPM	166 PPM	166 PPM
Comp Mole Frac (N_2)	0.0000	0.000	0.0050	691 PPB	691 PPB	691 PPB

Table A.2 (Continued) Data stream of methanol process with resilient heat exchanger

D1	L1	8	9	M
50.0000	106.1000	113.8940	80.0000	80.0766
1.0000	1.4000	3.2000	16.0000	13.0000
0.0000	0.0000	0.0372	0.0000	0.0000
3310.4270	5441.8140	5441.8136	3310.4270	3310.4267
106389.458	102287.439	102287.439	106389.458	106389.4
trace	0.0000	0.0000	0.0000	0.0000
990 PPM	0.9440	0.9443	990 PPM	0.0010
894 PPB	0.0000	0.0000	894 PPB	0.0000
0.0090	0.0000	0.0000	0.0090	0.0094
0.9890	0.0560	0.0557	0.9890	0.9894
198 PPM	0.0000	0.0000	198 PPM	0.0002
731 PPB	0.0000	0.0000	731 PPB	0.0000

Table A.3. Equipment data of methanol process

Unit		
C1	Column ID (m)	5.405
	Reflux Drum (m^3)	42.41
	Base (m^3)	24.52
Reactor	Diameter (m)	0.03675
	Length (m)	12.20
Separator	Diameter (m)	6.50
	Length (m)	13.00
Flash Tank	Diameter (m)	2.80
	Length (m)	5.60
FEHE1	UA (kJ/sec-K)	413.321
	Heat duty (MW)	47.01
FEHE2	UA (kJ/sec-K)	231.77
	Heat duty (MW)	10.58

APPENDIX B

TUNING OF CONTROL STRUCTURES

B.1 Tuning Controllers

P and PIs controllers are the types of controllers that notice throughout in this research.

Flow Controllers

The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be turned with a small integral. Sometime flow measurements signal are noisy because of turbulent flow. A controller gain should be kept modest. A value of τ_I = 0.3 minutes and controller gain of K_c = 0.5 are often used. Derivative action should not be used.

Level Controllers

Proportional control should be used for level controllers. A recommended controller gain is 2 for the flow smoothing. There will be steady state offset (the level will not be returned to its setpoint value). However, maintaining a liquid level at a certain value is often not necessary when the liquid capacity is simply being used as surge volume.

Pressure Controllers

Most pressure controllers can be easily tuned. The integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Typical pressure controller tuning constants are K_c = 2 and τ_I = 10 minutes but it has smaller integral times in very fast loops (compressor controls).

Temperature Controllers

The dynamic responses of temperature are slow. Typically the controller gain, Kc, should be set between 2 and 10, the integral time, τ_I, should be set between 2 and 10 minutes. Temperature loop needs dynamic lags and/or deadtimes. The existence of lags in the control loop is smaller than process time constant but they have an important impact on performance.

B.2 Relay-Feed back Testing

A quick and simple method for identifying the dynamic parameters needs for designing a feedback controller. The relay feedback testing is a tool for tuning. The results of the test are the ultimate gain and the ultimate frequency. This information is usually sufficient to permit us to calculate some reasonable controller tuning constants.

The method consists of inserting an on-off relay in the feedback loop. The height of relay h must be specified and it is 5 to 10% of the controller output range. The maximum amplitude of the PV signal is used to calculate the ultimate gain K_u from the equation:

$$K_u = \frac{4h}{a\pi}$$

The period of the output PV curve is the ultimate period P_u. From these two parameters, controller tuning constants can be calculated for PI or PID controllers, using a types of tuning methods, e.g.,Ziegler-Nichols, Tyreus-Luyben, etc.

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

1. Specified relay height.
2. The run time for test is short.
3. The test is closed loop, so the process is not deviated from the setpoint.
4. The information obtained is very accurate in the frequency range that is important for the design of a feedback controller (the ultimate frequency).
5. The impact of load changes that occur during the test can be detected by a change to asymmetric in the manipulated variable.

Knowing the ultimate gain K_u and ultimate period P_u leads to calculate controller parameters. This research used the Tyreus-Luyben tuning method. These tuning constants are frequently too aggressive for chemical engineering. This method provides more conservative setting with increased robustness. The TL equations for a PI controller are:

$$K_c = \frac{Ku}{3.2}$$

$$\tau_I = 2.2\, Pu$$

Relay feedback testing can be done in Aspen Dynamics. It simply click the Tuning button on controller faceplate, select autotuning, specified relay height and select the close loop. Then click the start testing button. The loop will start to oscillate. After several cycles, the tuning is stopped. We click the calculated parameters, a PI controller are suggested following by the selected tuning method.

B.3 Inclusion of Lag

These are typically temperature and composition controllers. These loops have significant dynamic lags/or deadtimes. Realistic dynamic simulations require that we explicitly include lags/or deadtimes in all the important lops. Usually this means controllers that affect product quality (temperature or composition) or process constraint (safety and environmental).

In this plant, a 3-minute deadtime is assumed in product composition measurement.

Table B.1 Typical measurement lags

		Number	Time constant (minutes)	Type
Temperature	Liquid	2	0.5	Deadtime
	Gas	3	1	Deadtime
Composition	Chromatograph	1	3 to 10	Deadtime

Table B.2 Same parameters tuning of methanol process in all control structures

Controller	Controlled Variable	Manipulated Variable	Control Action	Kc	τ_I
FCfeed	Synthesis gas flowrate	Compressor work (K1)	Reverse	0.5	0.3
PCk2	Compressor outlet pressure	Compressor work (K2)	Direct	2	10
TChx1	Inter stage cooling temperature	Heat removal in H-101	Reverse	0.115	13.2
TCin	Reactor inlet temperature	Valve VBP1	Direct	52.19	54.12
TCRX	Reactor outlet temperature	Coolant temperature	Reverse	0.456	9.2
TCsep	Separator temperature	Heat removal in H-103	Reverse	0.911	13.2
PCsep	Separator pressure	Valve WENT	Direct	2	10
PCflash	Flash tank pressure	Compressor work (Kflash)	Reverse	2	10
FCk4	Vapor flowrate from column	Compressor work (K4)	Reverse	0.5	0.3
PC1	Condenser pressure	Condenser duty	Reverse	2	10
TC1	Tray temperature column	Valve VBP2	Reverse	11.01	376.20
LCflash	Flash tank level	Valve VFLASH	Direct	2	-
LCsep	Separator level	Valve VL	Direct	2	-
CCvent	Methane Composition	Valve WENT	Direct	23.16	55.44

Table B.3 Different parameters tuning of methanol process in all control structures

Controller	Controlled Variable	Manipulated Variable	Control Action	Kc	τ_I
CS3	Reflux flow rate	Valve V9	Direct	4	-
VPC					
CS1, CS2	Reflux drum level	Valve V9	Direct	2	-
LC1					
CS1, CS3	Reflux to feed ratio	Reflux flow rate	-	-	-
R/F					

APPENDIX C

FIXTURE POINT THEOREM DATA

Table C.1 List of Manipulated variables for methanol process

Manipulated Variable	Description
K1	Work compressor
K2	Work compressor
K3	Work Compressor
K4	Work compressor
KFLASH	Work compressor
H-101	Heat duty
H-102	Heat duty
V1	Reactor outlet valve
REACT1	Coolant temperature
H-103	Heat duty
VL	Separator liquid outlet valve
VVENT	Vent valve
VSEP	Inlet separator valve
VFLASH	Flash tank liquid outlet valve
V9	Column distillate valve
V8	Column bottom valve
Qcond	Column condenser duty
Qreb	Column reboiler duty
Reflux	Reflux flow rate
Tcool	Reactor coolant temperature

Table C.2 IAE Results of vessel unit

Unit	Variables	K1	H-101	K2	H-102	Tcool	V1	H-103	VL	WENT	KFLASH
SEP	Level	0.06353	0.01485	0.07590	0.00006	0.21388	0.00015	0.00425	0.00000	0.00000	0.00000
	Pressure	0.13139	0.02434	0.15700	0.00012	0.46774	0.00028	0.13903	0.00000	0.00000	0.00000
	Temperature	0.03754	0.00304	0.04413	0.00000	0.05619	0.00000	0.21454	0.09860	0.00000	0.00005
FLASH	Level	0.01272	0.00380	0.07590	0.00003	0.04585	0.00008	0.01504	0.00000	0.00000	0.00000
	Pressure	0.02033	0.00205	0.02409	0.00002	0.06970	0.00004	0.07672	0.00000	0.00000	0.00000
C1-Condenser	Level	0.07427	0.00513	0.08686	0.00003	0.03025	0.00010	0.52143	0.09572	0.00506	0.05195
	Pressure	0.01548	0.00132	0.01830	0.00000	0.03200	0.00001	0.06681	0.00823	0.00096	0.00562
C1-Reboiler	Level	0.06237	0.00353	0.07278	0.00006	0.05273	0.00017	0.46156	0.23753	0.00193	0.14541

Table C.2 (Continued) IAE Result of vessel unit

Unit	Variables	VFLASH	V9	V8	Qcod	Qreb	K4	Reflux	K3	VSEP	SUM IAE
SEP	Level	0.00000	0.00000	0.00084	0.00000	0.00000	0.00000	0.00001	0.01218	0.00016	0.38582
	Pressure	0.00000	0.00000	0.00007	0.00000	0.00000	0.00000	0.00003	0.00708	0.00023	0.92730
	Temperature	0.00000	0.00000	0.00006	0.00000	0.00000	0.00000	0.00000	0.06032	0.00058	0.51508
FLASH	Level	0.00000	0.00000	0.00148	0.00000	0.00000	0.00000	0.00257	0.01272	0.00018	0.17035
	Pressure	0.00000	0.00000	0.00021	0.00000	0.00000	0.00000	0.00001	0.00708	0.00023	0.20048
C1-Condenser	Level	0.12563	0.00002	0.20506	0.30470	0.29722	0.00110	0.31082	0.15580	0.00144	2.27257
	Pressure	0.01148	0.00003	0.00053	0.11881	0.13249	0.00023	0.00181	0.02219	0.00020	0.43651
C1-Reboiler	Level	0.61120	0.06601	0.00030	0.27870	0.69420	0.00013	0.34750	0.14576	0.00150	3.18338

Table C.3 IAE Result of Tray Temperature Deviation for C1 Column

Tray	K1	H-101	K2	H-102	Tcool	V1	H-103
1	0.03692	0.00290	0.04324	0.00002	0.03890	0.00001	0.23702
2	0.02781	0.00243	0.03271	0.00002	0.05506	0.00002	0.13774
3	0.02777	0.00242	0.03267	0.00002	0.05494	0.00002	0.13646
4	0.02776	0.00241	0.03266	0.00002	0.05465	0.00002	0.13544
5	0.02777	0.00241	0.03269	0.00002	0.05438	0.00002	0.13461
6	0.02781	0.00240	0.03274	0.00002	0.05413	0.00002	0.13397
7	0.02786	0.00240	0.03280	0.00002	0.05389	0.00002	0.13350
8	0.02790	0.00239	0.03285	0.00002	0.05362	0.00002	0.13318
9	0.02791	0.00239	0.03287	0.00002	0.05333	0.00002	0.13296
10	0.02789	0.00238	0.03285	0.00002	0.05298	0.00002	0.13279
11	0.02781	0.00237	0.03276	0.00002	0.05257	0.00001	0.13259
12	0.02767	0.00235	0.03258	0.00002	0.05208	0.00002	0.13229
13	0.02745	0.00233	0.03232	0.00002	0.05151	0.00002	0.13180
14	0.02715	0.00230	0.03198	0.00002	0.05088	0.00002	0.13107
15	0.02680	0.00227	0.03156	0.00002	0.05018	0.00001	0.13003
16	0.02639	0.00224	0.03108	0.00002	0.04945	0.00001	0.12864
17	0.02594	0.00220	0.03056	0.00002	0.04869	0.00001	0.12691
18	0.02548	0.00216	0.03002	0.00002	0.04792	0.00001	0.12486
19	0.02501	0.00212	0.02948	0.00002	0.04716	0.00001	0.12253
20	0.02455	0.00208	0.02895	0.00002	0.04643	0.00001	0.11999
21	0.02411	0.00204	0.02844	0.00002	0.04572	0.00001	0.11731

Table C.3 (Continued) IAE Result of Tray Temperature Deviation for C1 Column

Tray	VL	VVENT	KFLASH	VFLASH	V9	V8	Qcod
1	0.01839	0.00241	0.00730	0.03880	0.00007	0.00011	0.46917
2	0.01403	0.00174	0.00981	0.02168	0.00002	0.00093	0.26541
3	0.01395	0.00174	0.00970	0.02166	0.00002	0.00092	0.26093
4	0.01368	0.00174	0.00947	0.02171	0.00002	0.00091	0.25674
5	0.01339	0.00174	0.00923	0.02180	0.00002	0.00090	0.25291
6	0.01310	0.00175	0.00898	0.02193	0.00002	0.00088	0.24940
7	0.01280	0.00176	0.00870	0.02208	0.00002	0.00087	0.24620
8	0.01250	0.00178	0.00842	0.02225	0.00002	0.00086	0.24327
9	0.01220	0.00179	0.00812	0.02241	0.00002	0.00085	0.24055
10	0.01192	0.00180	0.00781	0.02254	0.00002	0.00084	0.23797
11	0.01165	0.00180	0.00750	0.02261	0.00002	0.00083	0.23546
12	0.01141	0.00180	0.00720	0.02262	0.00002	0.00082	0.23292
13	0.01121	0.00180	0.00692	0.02254	0.00002	0.00081	0.23026
14	0.01104	0.00179	0.00666	0.02236	0.00002	0.00080	0.22742
15	0.01090	0.00177	0.00642	0.02208	0.00002	0.00079	0.22432
16	0.01080	0.00175	0.00620	0.02172	0.00002	0.00078	0.22092
17	0.01073	0.00172	0.00601	0.02128	0.00002	0.00077	0.21723
18	0.01068	0.00169	0.00585	0.02079	0.00002	0.00077	0.21324
19	0.01065	0.00166	0.00570	0.02027	0.00002	0.00076	0.20902
20	0.01063	0.00163	0.00558	0.01974	0.00002	0.00075	0.20462
21	0.01061	0.00159	0.00546	0.01921	0.00002	0.00074	0.20013

Table C.3 (Continued) IAE Result of Tray Temperature Deviation for C1 Column

Tray	Qreb	K4	Reflux	K3	VSEP	SUM IAE
1	0.29077	0.00005	0.00892	0.06313	0.00062	1.25877
2	0.25013	0.00039	0.00431	0.03985	0.00038	0.86445
3	0.27793	0.00038	0.00503	0.03998	0.00038	0.88689
4	0.29694	0.00038	0.00598	0.04024	0.00038	0.90114
5	0.30805	0.00037	0.00709	0.04058	0.00038	0.90835
6	0.31347	0.00037	0.00836	0.04097	0.00038	0.91070
7	0.31516	0.00037	0.00977	0.04141	0.00038	0.91001
8	0.31449	0.00036	0.01130	0.04185	0.00038	0.90746
9	0.31233	0.00036	0.01288	0.04227	0.00038	0.90365
10	0.30921	0.00036	0.01445	0.04262	0.00039	0.89883
11	0.30546	0.00035	0.01594	0.04287	0.00039	0.89300
12	0.30131	0.00035	0.01725	0.04299	0.00038	0.88608
13	0.29694	0.00034	0.01829	0.04298	0.00038	0.87795
14	0.29249	0.00034	0.01899	0.04284	0.00038	0.86852
15	0.28806	0.00034	0.01929	0.04258	0.00037	0.85781
16	0.28377	0.00033	0.01915	0.04222	0.00037	0.84587
17	0.27969	0.00033	0.01859	0.04181	0.00036	0.83287
18	0.27588	0.00032	0.01763	0.04137	0.00035	0.81906
19	0.27237	0.00032	0.01632	0.04092	0.00035	0.80469
20	0.26917	0.00032	0.01475	0.04050	0.00034	0.79006
21	0.26629	0.00031	0.01300	0.04012	0.00033	0.77546

Table C.3 (Continued) IAE Result of Tray Temperature Deviation for C1 Column

Tray	K1	H-101	K2	H-102	Tcool	V1	H-103
22	0.02369	0.00200	0.02796	0.00002	0.04505	0.00001	0.11456
23	0.02330	0.00197	0.02752	0.00002	0.04441	0.00001	0.11182
24	0.02294	0.00193	0.02711	0.00002	0.04381	0.00001	0.10914
25	0.02261	0.00190	0.02673	0.00002	0.04325	0.00001	0.10657
26	0.02231	0.00188	0.02639	0.00001	0.04272	0.00001	0.10414
27	0.02204	0.00185	0.02608	0.00001	0.04222	0.00001	0.10186
28	0.02318	0.00186	0.02775	0.00001	0.04209	0.00001	0.10113
29	0.02711	0.00191	0.03328	0.00001	0.04080	0.00001	0.10157
30	0.03900	0.00209	0.04941	0.00001	0.03731	0.00001	0.10520
31	0.06838	0.00264	0.08644	0.00007	0.02717	0.00005	0.11858
32	0.11675	0.00408	0.14103	0.00023	0.00266	0.00016	0.15832
33	0.15076	0.00660	0.17320	0.00048	0.05452	0.00033	0.24890
34	0.13150	0.00754	0.14673	0.00058	0.10728	0.00040	0.38087
35	0.08330	0.00558	0.09237	0.00040	0.09872	0.00027	0.48584
36	0.04819	0.00346	0.05407	0.00019	0.04336	0.00013	0.52439
37	0.03151	0.00248	0.03605	0.00006	0.01318	0.00004	0.51383
38	0.02480	0.00206	0.02883	0.00002	0.02732	0.00001	0.47453
39	0.02221	0.00190	0.02603	0.00001	0.03702	0.00001	0.40989
40	0.02117	0.00183	0.02490	0.00001	0.04054	0.00001	0.31775
41	0.02069	0.00180	0.02438	0.00001	0.04164	0.00001	0.21701
42	0.02042	0.00177	0.02407	0.00002	0.04185	0.00001	0.14360

Table C.3 (Continued) IAE Result of Tray Temperature Deviation for C1 Column

Tray	VL	VVENT	KFLASH	VFLASH	V9	V8	Qcod
22	0.01060	0.00156	0.00535	0.01871	0.00002	0.00073	0.19561
23	0.01058	0.00153	0.00524	0.01822	0.00002	0.00072	0.19115
24	0.01056	0.00150	0.00513	0.01777	0.00002	0.00072	0.18681
25	0.01053	0.00148	0.00502	0.01736	0.00001	0.00071	0.18263
26	0.01049	0.00145	0.00491	0.01698	0.00001	0.00070	0.17866
27	0.01045	0.00143	0.00480	0.01663	0.00001	0.00069	0.17490
28	0.01040	0.00143	0.00768	0.01690	0.00002	0.00069	0.17339
29	0.00892	0.00145	0.02545	0.01834	0.00003	0.00069	0.17237
30	0.00428	0.00153	0.07420	0.02335	0.00005	0.00068	0.17316
31	0.01024	0.00179	0.16010	0.03948	0.00013	0.00067	0.17953
32	0.05045	0.00249	0.24858	0.08581	0.00034	0.00064	0.20251
33	0.13987	0.00390	0.27184	0.19126	0.00065	0.00060	0.26584
34	0.26294	0.00448	0.20185	0.34789	0.00079	0.00062	0.36650
35	0.34227	0.00338	0.10353	0.47921	0.00055	0.00060	0.44652
36	0.33670	0.00215	0.03931	0.53660	0.00028	0.00065	0.46611
37	0.27121	0.00163	0.01008	0.53532	0.00012	0.00067	0.43587
38	0.18127	0.00141	0.00156	0.49524	0.00005	0.00068	0.37767
39	0.09739	0.00133	0.00578	0.41647	0.00002	0.00069	0.30614
40	0.04170	0.00130	0.00727	0.29678	0.00002	0.00068	0.23919
41	0.01558	0.00129	0.00777	0.16842	0.00001	0.00067	0.19425
42	0.00783	0.00127	0.00791	0.07874	0.00001	0.00067	0.17175

Table C.3 (Continued) IAE Result of Tray Temperature Deviation for C1 Column

Tray	Qreb	K4	Reflux	K3	VSEP	SUM IAE
22	0.26372	0.00031	0.01115	0.03980	0.00032	0.76116
23	0.26143	0.00031	0.00929	0.03954	0.00032	0.74739
24	0.25941	0.00031	0.00747	0.03934	0.00031	0.73431
25	0.25763	0.00030	0.00575	0.03922	0.00031	0.72204
26	0.25606	0.00030	0.00416	0.03915	0.00030	0.71064
27	0.25468	0.00029	0.00272	0.03915	0.00030	0.70015
28	0.38025	0.00030	0.00322	0.05595	0.00031	0.84658
29	0.53517	0.00029	0.00497	0.09573	0.00035	1.06844
30	0.65423	0.00031	0.01093	0.16337	0.00048	1.33958
31	0.71066	0.00036	0.03000	0.24349	0.00086	1.68066
32	0.70344	0.00047	0.08291	0.30397	0.00184	2.10668
33	0.61770	0.00064	0.19273	0.30317	0.00334	2.62632
34	0.46306	0.00072	0.33170	0.22759	0.00391	2.98695
35	0.31576	0.00058	0.41898	0.13384	0.00281	3.01451
36	0.22876	0.00043	0.42500	0.07397	0.00149	2.78523
37	0.18975	0.00035	0.37518	0.04664	0.00076	2.46475
38	0.17400	0.00031	0.29386	0.03580	0.00046	2.11988
39	0.16755	0.00030	0.19687	0.03165	0.00034	1.72161
40	0.16457	0.00029	0.10705	0.03001	0.00029	1.29536
41	0.16285	0.00029	0.04708	0.02927	0.00028	0.93330
42	0.16160	0.00028	0.01742	0.02886	0.00027	0.70835

Table C.4 IAE Result of Methanol Reactor

Reactor	Variables	K1	H-101	K2	H-102	Tcool	V1	H-103	VL	WENT	KFLASH
Inlet Stream	Temperature	0.02160	0.00644	0.02427	0.00582	0.15526	0.00000	0.10992	0.00182	0.00286	0.00002
Outlet Stream	Temperature	0.00399	0.00030	0.00469	0.00030	0.26778	0.00000	0.00645	0.00096	0.00026	0.00000

Table C.4 (Continued) IAE Result of Methanol Reactor

Reactor	Variables	VFLASH	V9	V8	Qcod	Qreb	K4	Reflux	K3	VSEP	SUM IAE
Inlet Stream	Temperature	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01181	0.00010	0.33992
Outlet Stream	Temperature	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00039	6.0E-06	0.28482

Table C.5 IAE Result of Compressor Unit

Multi-stage compressor		K1	H-101	K2	H-102	Tcool	V1	H-103	VL	WENT	KFLASH
K1-Inlet stream	Flow rate	0.38231	0.08698	0.43328	0.00048	0.48356	0.000	0.13224	0.09210	0.00675	0.00075
K1-Outlet stream	Pressure	0.26882	0.02689	0.13194	0.00017	0.15370	0.000	0.04082	0.02849	0.00201	0.00022
K2-Inlet stream	Temperature	0.05044	0.05858	0.00408	0.00000	0.00473	0.000	0.00126	0.00088	0.00006	0.00001

Table C.5 (Continued) IAE Result of Compressor Unit

Multi-stage compressor		VFLASH	V9	V8	Qcod	Qreb	K4	Reflux	K3	VSEP	SUM IAE
K1-Inlet stream	Flow rate	0.00000	0.00000	0.00060	0.00000	0.00000	0.0000	0.00006	0.03330	0.00005	1.65250
K1-Outlet stream	Pressure	0.00000	0.00000	0.00019	0.00000	0.00000	0.0000	0.00003	0.01038	0.01038	0.67405
K2-Inlet stream	Temperature	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.00000	0.00032	6.07332	0.12038

Table C.6 IAE Result of Recycle Stream

Stream	Variables	K1	H-101	K2	H-102	Tcool	V1	H-103	VL	WENT	KFLASH
V1	Flow rate	1.83E-05	1.40E-06	2.15E-05	1.16E-08	3.28E-05	1.57E-09	9.78E-05	0.00000	0.00000	0.00000
Recycle	Composition										
	MeOH	0.00836	0.00060	0.00987	0.00000	0.00995	0.00000	0.04063	0.00060	0.00055	0.00045
	CH4	0.10246	0.01670	0.12125	0.00029	0.90703	0.00073	0.15391	0.02003	0.04852	0.00188
	CO	0.00587	0.00015	0.00682	0.00010	0.39965	0.00027	0.03257	0.01340	0.00509	0.00531
	CO2	0.01759	0.00101	0.02061	0.00004	0.14003	0.00012	0.10224	0.03707	0.00793	0.01839
	H2	0.08275	0.01718	0.09827	0.00019	0.49175	0.00047	0.02745	0.02307	0.04279	0.02554
	H2O	0.00106	0.00007	0.00125	0.00000	0.00124	0.00000	0.00518	0.00007	0.00007	0.00007
	N2	0.01316	0.00206	0.01556	0.00004	0.13349	0.00011	0.02079	0.00767	0.00666	0.00022

Table C.6 (Continued) IAE Result of Recycle Stream

Stream	Variables	VFLASH	V9	V8	Qcod	Qreb	K4	Reflux	K3	VSEP	SUM IAE
V1	Flow rate	0.00000	0.00000	0.00019	0.00000	0.00000	0.00000	2.29E-06	0.00000	0.00000	0.00039
Recycle	Composition										
	MeOH	0.00000	0.00000	0.00000	0.00002	0.00001	0.00000	0.00000	0.01468	0.00013	0.08587
	CH4	0.00042	0.00073	0.00073	0.00032	0.00152	0.00074	0.00001	0.03797	0.00023	1.41549
	CO	0.00059	0.00027	0.00026	0.00036	0.00006	0.00023	0.00001	0.00210	0.00004	0.47314
	CO2	0.00122	0.00012	0.00012	0.00037	0.00069	0.00002	0.00003	0.00768	0.00010	0.35536
	H2	0.00200	0.00046	0.00046	0.00026	0.00219	0.00060	0.00006	0.07004	0.00055	0.88608
	H2O	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00191	0.00002	0.01094
	N2	0.00016	0.00011	0.00011	0.00019	0.00003	0.00011	0.00000	0.00616	0.00004	0.20668

VITA

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