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CONTROL STRUCTURE DESIGN OF REACTION SECTION OF HYDRODEALKYLATION PROCESS USING MAXIMUM SCALED GAIN METHOD

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โชติรัตน์ เกียรติพิริยะ : การออกแบบโครงสร้างการควบคุมส่วนปฏิกิริยาของกระบวนการไฮโดรดีอัลคิลเลชันโดยวิธีสเกลเกน (CONTROL STRUCTURE DESIGN OF REACTION SECTION OF HYDRODEALKYLATION PROCESS USING MAXIMUM SCALED GAIN METHOD) อ. ที่ปรึกษา : ผศ. ดร. มนตรี วงศ์ศรี, 206 หน้า.

การออกแบบโครงสร้างการควบคุมกระบวนการที่มีความซับซ้อน เช่น กระบวนการที่มีการนำมวลสาร และพลังงานกลับมาใช้เป็นสารตั้งต้น หรือเพื่อประหยัดพลังงานมีผลทำให้กระบวนการมีความซับซ้อนในการดำเนินการมากขึ้น การออกแบบลูพควบคุมกระบวนการมีผลต่อภาวะการดำเนินการเป็นอย่างยิ่ง

ในงานวิจัยนี้ได้นำเสนอการออกแบบโครงสร้างการควบคุม โดยอาศัยแนวคิด เลือกตัวแปรควบคุมที่ให้มีการสูญเสียน้อยที่สุดเมื่อเกิดการรบกวน (self-optimizing control) ในการเลือกตัวแปรควบคุม และอาศัยวิธีสเกลเกนสูงสุด ในการเลือกตัวแปรควบคุมและจับคู่ตัวแปรควบคุมกับตัวแปรปรับ จากงานวิจัยนี้พบว่าวิธีการออกแบบที่ได้เสนอนี้ เป็นวิธีพื้นฐานที่เข้าใจง่าย และได้ผลดี งานวิจัยนี้ได้ออกแบบโครงสร้างการควบคุมทั้งหมด 3 โครงสร้าง ในการแสดงพฤติกรรมเชิงพลวัตรของการออกแบบโครงสร้างควบคุมแบบแพลนท์ไวด์ในโรงงานไฮโดรดิแอลคิลเลชันส่วนการเกิดปฏิกิริยา โดยสร้างการรบกวนภาระทางด้านเศรษฐกิจ คือ เปลี่ยนอัตราการไหลของทอลูอีน สัดส่วนของมีเทน และอุณหภูมิขาเข้าเครื่องแลกเปลี่ยนความร้อน ซึ่งพบว่าโครงสร้างการควบคุมที่ออกแบบด้วยวิธีนี้ ให้ค่าเวลาความคลาดเคลื่อนแบบสมบูรณ์ การใช้พลังงาน และปริมาณการผลิตผลิตภัณฑ์มีความเบี่ยงเบนน้อยกว่าโครงสร้างการควบคุมอ้างอิง จากนั้นนำโครงสร้างการควบคุมที่ออกแบบได้ทั้ง 3 โครงสร้าง ศึกษาการเปลี่ยนขนาดของเครื่องแลกเปลี่ยนความร้อนที่แตกต่างกัน 3 ขนาด โดยสร้างการรบกวนภาระทางความร้อนของกระแสเย็น กระแสร้อน และเปลี่ยนอัตราการไหลของทอลูอีน พบว่า เครื่องแลกเปลี่ยนความร้อนที่มีขนาดใหญ่ มีการใช้พลังงานในระบบน้อยกว่าเครื่องแลกเปลี่ยนความร้อนที่มีขนาดเล็ก และโครงสร้างการควบคุมมีส่วนช่วยในการควบคุมเครื่องแลกเปลี่ยนความร้อนที่มีขนาดใหญ่ให้สามารถจัดการตัวรบกวนได้โดยไม่ต้องมีเตาเผาขนาดใหญ่

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Design a process control structure for a complex process, such as the process having material or energy recycle, is a complicate task. The design control loop would effect the operation significantly.

This thesis presents a plantwide control design procedure base on basic idea of self-optimizing control to select controlled variables which when kept constant lead to minimum economic loss. The maximum scaled gain is used to selecting and paring controlled variables with manipulated variables. This presented-method is elementary and effective. In the study, three control structures were designed and compared. In order to illustrate the dynamic behaviors of the control structures in reaction section of HDA plant when economic disturbance load occur such as change in toluene flowrates, methane composition in fresh gas feed and disturbance load hot stream were made. All of control structures can operate to achieve the objective and within process constraints. The performance of designed control structures were presented in IAE value and compared with reference structure. The designed structures are faster response than reference structure. The benzene products of designed structures (6.25%) are smaller deviation from steady state than reference structure (6.85%). Thence, the designed structures were studied about variation of heat exchanger duty to cost and dynamic performance of structure. Disturbance load cold stream, disturbance load hot stream and fresh toluene feed flowrates were made for study dynamic response. The large heat exchanger is lower utility cost than the small heat exchanger. The good structure can handle disturbance of large heat exchanger which small furnace duty.

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CHAPTER I

INTRODUCTIONS

1.1 Rationale

Plantwide process control is a strategy for establishing the control structure of an entire chemical plant. Presently, a chemical plant which is composed of many interconnected units can be divided into two sections, reaction and separation section, In a reaction section, the interconnected units are composed of several units such as reactors, heaters, coolers, heat exchangers, furnaces and so on. Furthermore, raw material recycles are integrated in this section. In a separation section, some interconnected units such as separators, extraction, evaporation, and distillation columns are used in the system included heat integration or energy recycle. Because of complicated recycle systems and diverse interconnections of the several units, a production system is complex and burdensome to control. Hence, the appropriate control system is required for the process that has interaction units, energy recycles and mass recycles. Plantwide process control is a proper way to establish this appropriate control system (control structure).

A number of methodologies have been proposed in the chemical engineering literature for the generation of promising plantwide control structures. These methodologies range from optimization base on mathematical programming design methods to heuristic design methods.

The optimization problem may be very large, with hundreds of thousands of equations and hundreds of degree of freedom. The optimization methods are required to solve the optimization problem. These method need to use the correctly mathematical model of the plant. If the mathematical model is not correct, we can not get a good control structure.

The heuristics design procedure has learned from the experience and inventiveness of many practicing control engineers. Sometime users have learned from the former mistakes that other users have made. The heuristics procedure did not describe how arrived at these strategies, and many choices looked mysterious.

The plantwide process control is an open end problem. There is not an exact solution but the solution depends on control objectives, such as maximize profit, minimize cost etc. An economic objective is an interesting trend for chemical plants in many industrials. Larsson and Skogestad (2000), and Sigurd Skogestad (2004) discussed an approach based on economics which presented a systematic procedure for selecting the best set of controlled variables that is the idea of self-optimizing control. The self-optimizing control is when an acceptable loss can be achieved using constant setpoints for the controlled variables, without the need to reoptimize when disturbances occur.

In this paper, a basic idea of self-optimizing control proposed by Sigurd Skogestad and a local analysis base on maximum scaled gain method is used for pre-screening and paring. The local analysis base on maximum scaled gain method is simple but efficacious.

The idea of self-optimizing control and maximum scaled gain method were used to select the best set of controlled variables for design control structure of hydrodealkylation (HDA) process. Hydrodealkylation (HDA) process is widely used because it is a realistically complex chemical process that creates disturbance propagation and the complicated system’s dynamic behavior. Therefore, this research will design plantwide control structures of hydrodealkylation (HDA) process using basic idea of self-optimizing control and maximum scaled gain method to select set of controlled variables and simulate them by using HYSYS simulator in order to study about dynamic behavior and evaluate the performance of the designed structures.

1.2 Objective of the Research

The objectives of this research are:

1. To simulate hydrodealkylation (HDA) of toluene process both steady state and dynamics condition by using HYSYS simulator.

2. To design plantwide control structures of reaction section of hydrodealkylation (HDA) process using self-optimizing control approach.

1.3 Scope of Research

The scope of this research can be listed as follows:

1. The simulator in this research is HYSYS simulator.

2. Description and data of hydrodealkylation (HDA) of toluene process is obtained from Douglas, J. M. (1988), William L. Luyben, Bjorn D. Tyreus, and Michael L. Luyben (1998), and William L. Luyben(2002).

1.4 Contribution of Research

The expected contribution of this research is:

This research provides the good efficacious design control structure by using maximum scaled gain method.

1.5 Procedure Plans

Procedure plans of this research are:

1. Study of plantwide process control theory and the basic idea of self optimizing control.
2. Study of hydrodealkylation (HDA) process and concerned information.
3. Simulations of the hydrodealkylation (HDA) process at steady state and list variables of process.
4. Calculate steady state gain and using the idea of self-optimizing control to select controlled variables.
5. Pairing manipulated variable with control variables of hydrodealkylation (HDA) process
6. Simulation of the hydrodealkylation (HDA) process at dynamic.
7. Collection and summarization of simulation results.

1.6 Research Framework

This thesis has been divided into six chapters.

In Chapter I, the rationale, objectives, scopes, contributions and research planning of this research is introduced in this chapter.

In Chapter II, a review of the previous work on the conceptual design of chemical process and plantwide process control design are given.

In Chapter III, background information of plantwide control, plantwide control design procedure and plantwide energy management are presented.

In Chapter IV describes the description of the hydrodealkylation (HDA) of toluene process that is the case study for this research.

In Chapter V presents a dynamic response of control structure of HDA process when disturbance occurs.

The overall conclusions and recommendations of this thesis are discussed in Chapter VI.

This is followed by:

Appendix A: Cost Estimation

Appendix B: Tuning of Control structures

Appendix C: Parameter Tuning

Appendix D: Maximum Scaled Gain Method

CHAPTER II

LITERATURE REVIEW

The concept of plantwide control structure synthesis is not new to the chemical process industry. Before the details of the present study are given, a brief of the other previous work on the conceptual design of chemical process and plantwide control design are reviewed. This chapter present a review of the previous work in plantwide control that base on heuristic design and base on mathematical design are made first.

2.1 Heuristics- Approach Base

A synthesis/analysis procedure for developing first flowsheets and base case designs has been established by Douglas (1985). The procedure is described in terms of a hierarchy of decision levels, as follows:

1. Batch versus continuous
2. Input-output structure of the flowsheet
3. Recycle structure of the flowsheet
4. Separation system specification, including vapor and liquid recovery system
5. Heat exchanger network (HEN)

Douglas (1985) considered a continuous process for producing benzene by hydrodealkylation of toluene (HDA process) to illustrate the procedure. The complete process is always considered at each decision level, but additional fine structure is added to the flowsheet as he proceeds to the later decision level. Each decision level terminates in an economic analysis. Experience indicates that less than one percent of the ideals for new designs are ever commercialized, and therefore it is highly desirable to discard poor projects quickly. Similarly, the later level decisions are guided by the economic analysis of the early level decisions.

In a series of papers, Fisher et al. (1988a,b,c) presented a study of the interface between design and control including process controllability, process operability and selecting a set of controlled variables. At the preliminary stages of a process design, most plants are uncontrollable. That is normally there are not enough manipulative variables in the flowsheet to be able to satisfy all of the process constraints and to optimize all of the operating variables as disturbances enter the plant. In order to develop a systematic procedure for controllability analysis, Fisher et al. (1988a) used the design decision hierarchy described by Douglas (1985) as the decomposition procedure and considered HDA process as a case study. Where at some levels, that are level 1, 2 and 3, the process is uncontrollable, but controllable at level 4 and level 5. If the available manipulated variables are compared with the constraints and operating variables introduced at each level, the preliminary controllability criterion can often be satisfied.

Beside controllability analysis, Fisher et al. (1988b) also focused on operability analysis. The goal of operability analysis is to ensure that there is an adequate amount of equipment over design so that they could satisfy the process constraints and minimize a combination of the operating costs and over design costs over the entire range of anticipated process disturbances. They also followed the same hierarchical procedure to develop operability analysis. For HDA process, the operability decisions were encountered at each level. Fisher et al. (1988c) proposed steady state control structure for HDA process using an optimum steady state control analysis. They found the values of manipulated variables (that minimize the total operating costs for various values of the disturbances) and used it to define the controlled variables.

D. L. Terrill and J. M. Douglas (1988) have studied HDA process from a steady state point of view and determined that the process can be held very close to its optimum for a variety of expected load disturbances by using the following strategy: (1) Fix the flow of recycle gas through the compressor at its maximum value, (2) Hold a constant heat input flowrate in the stabilizer, (3) Eliminate the reflux entirely in the recycle column, (4) Maintain a constant hydrogen-to-aromatic ratio in the reactor inlet by adjusting hydrogen fresh feed, (5) Hold the recycle toluene flowrate constant by adjusting fuel to the furnace, (6) Hold the temperature of the cooling water leaving the partial condenser constant.

Plantwide control involved the systems and strategies required to control an entire chemical plant. Downs and Vogel (1993) described a model of an industrial chemical process for the purpose of developing, studying and evaluating process control technology. It consisted of a reactor/separator/recycle arrangement involving two simultaneous gas-liquid exothermic reactions. This process was well suited for a wide variety of studies including both plant-wide control and multivariable control problems.

In the next year, Price, Lyman and Georgakis' (1994) presented a fundamental characteristic of a well-designed process plant regulatory control system was effective management of the rate of product manufacture and regulation of the inventories within the plant. They proposed guidelines for the development of production rate and inventory controls. The structures resulted satisfy the control objectives and maintained the plantwide characteristics of the problem. The applicability of these guidelines was illustrated using the complex test problem provided by the Tennessee Eastman Company.

Yi and Luyben (1995) presented a method that was aimed at helping to solve this problem by providing a preliminary screening of candidate plant-wide control structures in order to eliminate some poor structures. Only steady-state information was required. Equation-based algebraic equation solvers were used to find the steady-state changes that occur in all manipulated variables for a candidate control structure when load changes occur. Each control structure fixed certain variables: flows, compositions, temperatures, etc. The number of these fixed variables was equal to the number of degrees of freedom of the closed-loop system. If the candidate control structure required large changes in manipulated variables, the control structure was a poor one because valve saturation and/or equipment overloading will occur. The effectiveness of the remaining structures was demonstrated by dynamic simulation. Some control structures were found to have multiple steady states and produce closed-loop instability.

Luyben and Tyreus (1997) constructed nine steps of the proposed procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental and safety constrain;

liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, the Eastman plantwide control process, and the HDA process.

2.2 Mathematical-Approach Base

For plantwide control design based on the idea of self-optimizing control Skogestad and Postlethwaite presented the tasks of control structure design in their publication (Skogestad and Postlethwaite, 1996). The tasks consist of (1) the selection of controlled outputs, (2) the selection of manipulations and measurements, (3) the selection of control configuration, (4) the selection of controller type. The idea of self-optimizing control was used in the first task to select the best set of controlled variables. The self-optimizing control is when an acceptable loss can be achieved using constant setpoints for the controlled variables, without the need to reoptimize when disturbances occur (Skogestad, 2000).

After that Skogestad (2004) interested in control structure design deals with the structural decisions of the control system, including what to control and how to pair the variables to form control loops. He presented a systematic procedure for control structure design for complete chemical plants (plantwide control). It started with carefully defining the operational and economic objectives, and the degrees of freedom available to fulfill them. Other issues, discussed in the paper, include inventory and production rate control, decentralized versus multivariable control, loss in performance by bottom-up design, and a definition of a the ‘‘complexity number’’ for the control system.

Then, the concept of self-optimizing control was considered between steady-state optimization and control (Skogestad 2000).Typical distillation column was controlled for example. Important steps in evaluating self-optimizing control are degrees of freedom analysis, definition of optimal operation (cost and constraints), and evaluation of the loss for the set of disturbances.

The concept of self-optimizing control was applied to the TE process (Larsson and et. al. 2001). The paper described the selection of controlled variables. The systematic procedure for reducing the number of candidate control structures was presented. One step is to eliminate variables that, if they had constant setpoints, would result in large losses or infeasibility when there were disturbances (with the remaining degree of freedom reoptimized). The result (controlled variable set and their setpoints) was confirmed by simulations.

After that, the concept of self-optimizing control was used to select control structure for reactor, separator, and recycle processes (Larsson and et. al. 2003).A suitable controlled variable for the remaining unconstrained degree of freedom was searched for a constant setpoint strategy with an acceptable economic loss. This case need to control two active constraints both minimizing operating costs(case 1) and maximizing production rate(case 2).Both for the case with a given feed rate where the energy costs should be minimized and for the case where the production rate should be maximized. A good controlled variable is the reflux ratio L/F. This applies to single-loop control as well as multivariable model predictive control.

Furthermore, in 2004 (Skogestad 2004), the idea of “self-optimizing control” was explained and illustrated on a large number of examples such as central Bank, cake baking, long distance running, biology, portfolio management, business systems and KPIs and optimal blending of gasoline.

Furthermore Review of various plantwide control based on optimization approaches was presented by Stephanopoulos and Ng (Stephanopoulos and Ng, 2000). They compared analysis of various approaches. The principle of the Optimizing Feedback Control Structures was proposed as the formal medium for the identification of controlled variables. They have proposed that there are three approaches for identifying controlled variables: 1) explicit treatment of uncertaintes, 2) defer treatment of uncertainties for the phase of selecting the manipulated variables, and 3) defer treatment of uncertainties for the phase of tunning the controller. It was shown that the selection of the best sets of input and output variables is governed by classical control-theoretical aspects. Finally, they proposed the hierarchical approach to develop the control structure for the Tennessee Eastman process.

Wang and McAvoy (2001) discussed an optimization-based approach to synthesizing plantwide control architectures. The plantwide controller was synthesized in three stages involving fast and slow safety variables to be controlled, followed by product variables. In each stage a mixed integer linear program was solved to generate candidate architectures. The objective function involved a tradeoff between manipulated variable moves and transient response area.

Narraway and Perkins proposed a systematic method used to select the economically optimal control structure of a process (Narraway and Perkins, 1993). The problem was limited to selecting optimal control structures for steady-state process model. As the problem is combinatorial in nature, the systematic method uses the integer programming techniques for selecting the optimal control structure

CHAPTER III

PLANTWIDE CONTROL FUNDAMENTALS

Plantwide control system design methodology has been widely used to design control systems for complete plants. A chemical plant may have thousands of measurements and control loops. By the term plantwide control it is not meant the tuning and behavior of each of these loops, but rather the control philosophy of the overall plant with emphasis on the structural decisions. So Plantwide Process Control involves the system and strategies required to control an entire chemical plant consisting of many interconnected unit operations.

3.1 Plantwide Control Design Procedures

Plantwide control structure design deals with the structural decisions that must be made before we start the controller design, and involves the following tasks (Foss, 1973); (Skogestad & Postlethwaite, 1996):

1. Selection of manipulated variables ('input')
2. Selection of controlled variables ('output' ;variables with setpoint)
3. Selection of (extra) measurements (for control purposes including stabilization)
4. Selection of control configulation (the structure of the overall controller that interconnects the controlled, manipulated and measured variables)
5. Selection of controller type (control law specification ,e.g. PID, decoupler, LQG, etc.).

There are two main approaches to propose in the chemical engineering literature for the generation of promising plantwide regulatory control structures problem, a mathematically oriented approach (control structure design) and a process oriented approach. Both approaches are reviewed in the paper.

3.1.1 The Mathematically Oriented Approach

In this section we look at the mathematically oriented approach to plantwide control. The mathematically oriented approach is the formulation of the plantwide control problem into the mathematical models (process model). The process model is the set of the equations that describe the behavior of the process. There are some methods that use structural information about the plant as a basis for control structure design. Central concepts are structural state controllability, observability and accessibility. Based on this, sets of inputs and measurements are classified as viable or non-viable. Although the structural methods are interesting, they are not quantitative and usually provide little information other than confirming insights about the structure of the process that most engineers already have.

Furthermore, the mathematically approach are used to prescreening or selecting of the candidate control variables or manipulated variables, such as steady state gain, RGA, singular value, condition number, and etc. The concepts of those mathematically approach to prescreen or select the candidate variables are elucidated in section 3.6.

The control structure design problem is difficult to define mathematically, both because of the size of the problem, and the large cost involved in making a precise problem definition, which would include, for example, a detailed dynamic and steady state model. An alternative to this is to develop heuristic rules based on experience and process understanding. This is what will be referred to as the heuristics oriented approach.

3.1.2 The Process Oriented Approach

In this section we look at the process oriented approach to plantwide control. The process oriented approach has learned from the experience and inventiveness of many practicing control engineers. Sometime users have learned from the former mistakes that other users have made. Some heuristics procedure did not describe how arrived at these strategies, and many choices looked mysterious. The process oriented approach appeals the illuminate comprehension of each process of chemical engineering. A hierarchical strategy is gradually detailed stepwise for the design of alternative flowsheets of the process. The main objectives of this approach are ensuring process operability and enabling appropriate process operation. Operability characterizes the ability of the process to meet safety, environmental, and economical requirements under changing conditions and operational constraints correspond the last approach. The plantwide control design that base on heuristic design procedure was developed for many years of work and research in the fields of process control and process design.

3.2 Basic Concepts of Plantwide Control

3.2.1 Buckley Basic

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

3.2.2 Douglas doctrines

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

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

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

3.2.3 Downs drill

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

3.2.4 Luyben laws

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

1. All recycle loops should be flow controlled. A stream somewhere in all recycle loops should be flow controlled. This is 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 reactants. This law applies to systems with reaction types such as A + B → products. In system with consecutive reactions such as A + B → M + C and M + B →D + C, the fresh feed can be flow controlled into the system, because any imbalance in the ratios of reactants is accommodated by a shift in the amounts of the two products (M and D) that are generated. An excess of A will result in the production of more M and less D. And vice versa, an excess of B results in the production of more D and less M

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

3.2.5 Richardson rule

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

3.2.6 Shinskey schemes

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

3.4.7 Tyreus tuning

Use of P-only controllers for liquid levels, turning of P controller is usually trivial: set the controller gain equal to 1.67. This will have the valve wide open when the level is at 80 percent and the valve shut when the level is at 20 percent. For other control loops, suggest the use of PI controllers. The relay-feedback test is a simple and fast way to obtain the ultimate gain (Ku) and ultimate period (Pu). Then either the Ziegler-Nichols setting or the Tyreus-Luyben (1992) settings can be used:

$K_{ZN} = K_U/2.2$ $\tau_{ZN} = P_U/1.2$

$K_{TL} = K_U/3.2$ $\tau_{TL} = 2.2P_U$

3.3 Self-Optimizing Control

Control structure design for complete chemical plants is also know as plantwide control. In general, the problem is usually solved with the use of existing theoretical tools. For this work present an expanded version of the plantwide design procedure of Larsson and Skogestad (2000). A systematic approach to plantwide control starts by formulating the operational objectives. This is done by defining a cost function J that should be minimized with respect to the optimization degree of freedom, subject to a given set of constraints.

Self-optimizing control is when can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to reoptimize when disturbances occur Skogestad (2000).

Assumptions

1. The overall goal can be quantified in terms of a scalar cost function J

2. For a given disturbance d, there exists an optimal value $u_{opt}(d)$ (and corresponding value $z_{opt}(d)$), which minimizes the cost function J.

3. The reference values r for the controlled outputs z are kept constant, i.e. r is independent of the disturbances d. is

The system behavior is a function of the independent variables u and d, so we may formally write $J = J(u,d)$.For a given disturbance d the optimal value of the cost function is

$$J_{opt}(d) \triangleq J(u_{opt}(d), d) = \min_{u} J(u,d) \qquad (3.1)$$

Define the (economic) loss L as the difference between the actual value of the cost function and the truly optimal value, i.e. $L = J(u,d) - J_{opt}(d)$ where u = f (z, d)

The important variables;

1. u - degrees of freedom (inputs)
2. z - primary (“economic”) controlled variables
3. r - reference value (setpoint) for z
4. y - measurements, process information (often including u)

In the general case, the controlled variables are selected as functions of the measurements, z = H(y). In many case, we select individual measurements as controlled variables. Normally, we select as many controlled variables as the number of available degree of freedom. The controlled variables z are often not important variables in themselves, but are controlled in order to achieve some overall operational objective.

The idea of self-optimizing control is further illustrated in Figure 3.1

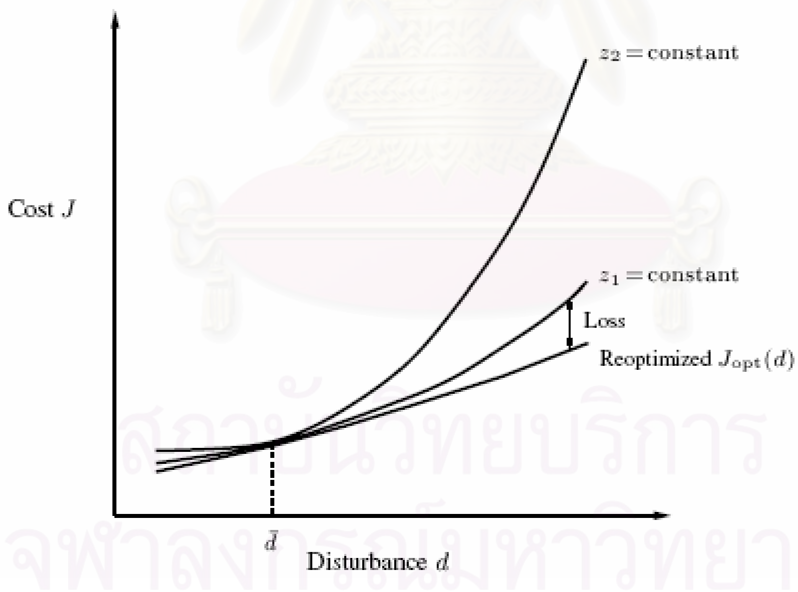


Figure 3.1 Loss imposed by keeping constant setpoint for the controlled variable. In this case z1 is a better “self-optimizing” controlled variable than z2.

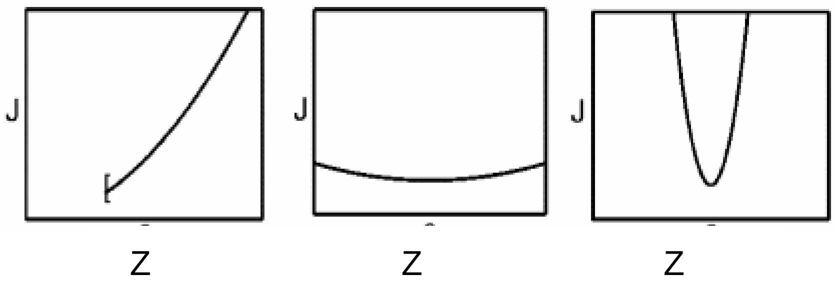
The basic idea of self-optimizing control was formulated about 20 years ago by Morari et al. (1980) who write that ‘‘we want to find a function c of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables.'' To quantify this more precisely, we define the (economic) loss L as the difference between the actual value of the cost function and the truly optimal value,i.e. $L = J(u,d) - J_{opt}(d)$

The main issue here is not to find the optimal setpoints, but rather to find the right variables to keep constant. The idea of self-optimizing control is illustrated in Figure. 3.1. We see that a loss results when we keep a constant setpoint rather than reoptimizing when a disturbance occurs. An additional concern with the constant setpoint strategy is that there is always a difference between the setpoint zs and the actual value z due to implementation errors caused by measurement errors and imperfect control. The implementation error may cause a large additional loss if the optimum surface is 'sharp'. To minimize the effect of the implementation errors, the cost surface as a function of controlled variable z should be as flat as possible. To be more specific, we may, as illustrated in Fig. 3.2 distinguish between three classes of problems when it comes to the actual implementation:

(A) Constrained optimum: implementation easy. In the figure it is shown the case where the minimum value of the cost J is obtained for $z = z_{min}$. In this case there is no loss imposed by keeping a constant $z_s = z_{min}$. In addition, implementation of an 'active' constraint is usually easy; e.g. it is easy to keep a valve closed.

(B) Unconstrained flat optimum: implementation easy. In this case the cost is insensitive to value of the controlled variable z, and implementation is again easy.

(C) Unconstrained sharp optimum: implementation difficult. The more difficult problems for implementation is when the cost (operation) is sensitive to value of the controlled variable z. In this case, we want to find another controlled variable z in which the optimum is flatter.



(A) (B) (C)

Figure 3.2 Implementing the controlled variable: effect of implementation error on cost.

To identify good candidate controlled variables, z, one should look for variables that satisfy all of the following requirements:

1. The optimal value of z should be insensitive to disturbances
2. z should be easy to measure and control (so that the implementation error is acceptable).
3. The value of z should be sensitive to changes in the manipulated variables (the steady-state degrees of freedom). Equivalently, the optimum (J as a function of z) should be flat.
4. For cases with more than one unconstrained degrees of freedom, the selected controlled variables should be independent.

3.4 Step of Plantwide Process Control Design Procedure

To select the controlled variables for self-optimizing control, one may use the stepwise procedure of Skogestad (2000):

3.4.1 Procedure for selecting controlled variables

Step 1 Determine degrees of freedom for optimization
Step 2 Definition of optimal operation (cost and constraints).
Step 3 Identification of important disturbances.
Step 4 Optimization (nominally and with disturbances).
Step 5 Identification of candidate controlled variables.

Step 6 Evaluation of loss for alternative combinations of controlled variables (loss imposed by keeping constant setpoints when there are disturbances or implementation errors).

Step 7 Evaluation and selection (including controllability analysis).

The description of the procedure step by step is shown below.

Step 1 Degrees of freedom Analysis

We start with the number of dynamic or control degrees of freedom, Nm (m here denotes manipulated), which is equal to the number of manipulated variables. The number of manipulated variables Nm is usually easily obtained by process insight as the number of independent variables that can be manipulated by external means (typically, the number of adjustable valves plus other adjustable electrical and mechanical variables). Note that the original manipulated variables are always extensive variables.

Next, we must identify the Nopt optimization degrees of freedom, that is, the degrees of freedom that affect the operational cost J. In most cases, the cost depends on the steady-state only, and Nopt equals the number of steady-state degrees of freedom Nss. The number of steady-state degrees of freedom equals the number of manipulated variables obliterate sum of the number of manipulated variables with no steady-state effect with the number of output variables that need to be controlled, but which have no steady-state effect.

$$N_{ss} = N_m - (N_{0m} + N_{0y})$$

Nom: the number of manipulated (input) variables with no steady-state effect (or more generally, with no effect on the cost). Typically, these are ‘‘extra’’ manipulated variables used to improve the dynamic response, e.g. an extra bypass on a heat exchanger.

Noy : the number of (output) variables that need to be controlled, but which have no steady-state effect (or more generally, no effect on the cost). Typically, these are liquid levels in holdup tanks.

The optimization is generally subject to constraints, and at the optimum many of these are usually ‘‘active’’. The number of ‘‘free’’ (unconstrained) degrees of freedom that are left to optimize the operation is then

$$N_{free} = N_{opt} - N_{active}$$

This is an important number, since it is generally for the unconstrained degrees of freedom that the selection of controlled variables.

Step 2 Definition of optimal operation (cost and constraints)

The operational objectives must be clearly defined before attempting to design a control system. Although this seems obvious, this step is frequently overlooked. Preferably, the operational objectives should be combined into a scalar cost function *J* to be minimized. In many cases, *J* may be simply selected as the operational cost, but there are many other possibilities. Rather than minimizing the cost *J*, it is more natural in this case to maximize the profit P = -*J*, which is the product value minus the feed costs and the operational (energy) costs which are proportional to cooler duty, fuel duty and electric power cost. Other objectives, including safety constraints, should normally be formulated as constraints.

Step 3 Identification of important disturbances.

This step is focus on the load disturbances such as, changes in the feed and in the active constraints, etc. The variables will be important disturbances that have effect to the economic potential. In case, the variables have small effect to the economic potential. We can neglect. The important disturbances of each process are differenced up to particular characteristic of process.

Step 4 Optimization

The purpose of the optimization is to identify the active constraints and recomputed optimal setpoints for controlled variables. In addition to deciding on which unconstrained variables to control (see step 1).

If the active constraints do not change, and we are able to find good self-optimizing controlled variables. There are also situations where the active constraints do change, but where the operators may be able to identify and implement the required changes.

Step 5 Identification of candidate controlled variables.

This step is the main focus of this work. The purpose of this step is to find good candidate controlled variables from all possible candidate controlled variables. The first, from step 1 we know number of unconstrained degree of freedom, and then define all candidate controlled variables of process. From above we can calculate number of possible combinations. There are several possible combinations. It is clearly impossible to evaluate the loss with respect to disturbances and implementation errors for all of these combinations.

The following criteria are proposed to reduce the number of alternatives. Most of them are rather obvious, but nevertheless, we find them useful.

(1) Eliminate variables with no effect on the economics (including variables with no steady-state effect). (The value of these variables can be arbitrarily selected, which reduces the number of degrees of freedom and thus the number of controlled variables to be selected. We must, of course, also eliminate the corresponding variables from further consideration as candidate controlled variables.)

(2) The variables directly associated with equality constraints should be controlled. (Again, this reduces the number of controlled variables to be selected, and we must also eliminate the corresponding variables from further consideration.)

(3) We choose to control the active constraints. (Again, this reduces the number of controlled variables to be selected, and we must also eliminate the corresponding variables from further consideration.)

(4) Eliminate/group closely related variables

(5) Use process insight to eliminate additional variables

(6) Eliminate single variables that, if they had constant setpoints, would yield infeasibility or large losses when there were disturbances or implementation errors (with the remaining degrees of freedom reoptimized).

(7) Eliminate combinations (pairs, triplets, etc.) of variables that yield infeasibility or large loss

(8) Use local analysis to eliminate variables or variable combinations that result in a small minimum singular value of the appropriately scaled gain matrix G

There are many criteria for select controlled variables such as:

Selecting controlled outputs: local analysis

Consider the loss $L = J(u,d) - J_{opt}(d)$, where *d* is a fixed (generally non-zero) disturbance and make the following additional assumptions:

1. The cost function J is smooth, or more precisely twice differentiable.
2. Assume that the optimization problem is unconstrained. If it is optimal to keep some variable at a constraint, then assume that this is implemented ("active constraint control") and consider the remaining unconstrained problem.
3. The dynamics of the problem can be neglected when evaluating the cost; that is, consider steady-state control and optimization.
4. Control as many variables *z* as there are available degrees of freedom.

For a fixed *d* we may then express $J(u,d)$ in terms of a Taylor series expansion in *u* around the optimal point. We get

$$\begin{aligned} J(u,d) \quad &= \quad J_{opt}(d) + \left(\frac{\partial J}{\partial u}\right)_{opt}^{T} (u - u_{opt}(d)) \\ &\quad + \frac{1}{2}(u - u_{opt}(d))^{T} \left(\frac{\partial^2 J}{\partial u^2}\right)_{opt} (u - u_{opt}(d)) + \ldots \end{aligned} \quad (3.2)$$

Assumes that reasonably closes to the optimum, terms of third order and higher is neglected. The second term on the right hand side is zero at the optimal point.

For an unconstrained problem, Equation (3.2) quantifies how a non-optimal input $u - u_{opt}$ affects the cost function. To study how this relates to output selection. we use a linearized model of the plant

$$z = Gu + G_d d \tag{3.3}$$

where G and G_d are the steady-state gain matrix and disturbance model respectively. For a fixed *d*, we have $z - z_{opt} = G(u - u_{opt})$. If *G* is invertible we then get

$$u - u_{opt} = G^{-1}(z - z_{opt}) \tag{3.4}$$

Note that G is a square matrix, since we have assumed that select as many controlled variables as the number of available degrees of freedom. From (3.2) and (3.4) we get

$$L = J - J_{opt} \approx \frac{1}{2}(z - z_{opt})^T G^{-T} J_{uu} G^{-1}(z - z_{opt}) \tag{3.5}$$

where the term $J_{uu} = (\partial^2 J / \partial u^2)_{opt}$ is independent of *z*. Alternatively, we may write

$$L = \frac{1}{2}\|\tilde{z}\|_2^2 \tag{3.6}$$

where $\tilde{z} = J_{uu}^{1/2} G^{-1}(z - z_{opt})$ These expressions for the loss L yield considerable insight. Obviously, we would like to select the controlled outputs z such that $z - z_{opt}$ is zero. However, this is not possible in practice because of (1) varying disturbances e and (2) implementation error associated with control of z. To see this more clearly, we write

$$z - z_{opt} = z - r + r - z_{opt} = e_{opt}(d) + e \tag{3.7}$$

First, an optimization error

$$e_{opt}(d) \triangleq r - z_{opt}(d) \tag{3.8}$$

A control or implementation error

$$e \triangleq z - r \qquad (3.9)$$

In most cases, the errors *e* and $e_{opt}(d)$ can be assumed independent.

From (3.5) and (3.7), conclude that we should select the controlled outputs *z* such that:

1. G^{-1} is small (i.e. G is large); the choice of *z* should be such that the inputs have a large effect on *z*.
2. $e_{opt}(d) = r - z_{opt}(d)$ is small; the choice of *z* should be such that its optimal value $z_{opt}(d)$ depends only weakly on the disturbances (and other changes).
3. $(e = z - r)$ is small; the choice of *z* should be such that it is easy to keep the control or implementation error small.
4. G^{-1} is small, which implies that G should not be close to singular. For cases with two or more controlled variables, the variables should be selected such that they are independent of each other.

By proper scaling of the variables, these four requirements can be combined into the "maximize minimum singular value rule" as discussed next.

Selecting controlled outputs: maximum scaled gain method

1. Scalar case.

In many cases we only have one unconstrained degree of freedom (*z* is a scalar).

Define the "span" or range of *z* as the expected value of $z - z_{opt}$, and introduce the scaled gain from *u* to *z*:

$$G' = G / span(z)$$

Span (*z*) = $z - z_{opt}$ includes both the optimization (setpoint) error and the implementation error. Then, the loss imposed by keeping *z* constant is

$$L = \frac{\alpha}{2}\left(\frac{z - z_{opt}}{G}\right)^2 = \frac{\alpha}{2}\frac{1}{|G'|^2} \qquad (3.10)$$

Where $\alpha = |J_{uu}|$, the Hessian of the cost function is independent of the choice for z. From (3.10), see that the “scaled gain” $G' = G/$ span should be maximized to minimize the loss. Note that the loss decreases with the square of the scaled gain.

2. Multivariable case

The general case u and z are vectors. Let each output z_i be scaled such that the expected magnitude of $z_i - z_{i_{opt}}$ (“span”) is of order 1, or more precisely, mainly for mathematical convenience, such that the combined error measured by the 2-norm is less than 1, $\|z - z_{opt}\|_2 \le 1$. From (3.7) that the “span” includes the sum of the optimal variation $(e_{opt} = r - z_{opt})$ and the implementation error $(e = z - r)$. Assume that:

(A1) The variations in $z_i - z_{i_{opt}}$ are uncorrelated, or more precisely, the “worst-case” combination of output deviations $z_i - z_{i_{opt}}$, with $\|z - z_{opt}\|_2 \le 1$, can occur in practice.

(A2) The inputs are scaled such that the effect of a given deviation $u_j - u_{j_{opt}}$ on the cost function *J* is similar for each input such that $J_{uu} = (\partial^2 J / \partial u^2)_{opt}$ is close to a constant times a unitary matrix, i.e. $J_{uu} = \alpha \cdot U$, where $\alpha = \bar{\sigma}(J_{uu})$.

From (3.6), $L = \frac{1}{2}\|\tilde{z}\|_2^2$, where $\tilde{z} = J_{uu}^{1/2} G^{-1}(z - z_{opt})$, and from the worst-case $\|\tilde{z}\|_2$ for $\|z - z_{opt}\|_2 = 1$ is $\|\tilde{z}\|_2 = \bar{\sigma}(J_{uu}^{1/2} G^{-1})$. Then, the resulting worst-case loss is

$$\max_{\|z - z_{opt}\|_2 \le 1} L = \frac{1}{2}\bar{\sigma}^2\left(\alpha^{1/2} G^{-1}\right) = \frac{\alpha}{2}\frac{1}{\underline{\sigma}^2(G)} \qquad (3.11)$$

Since the constant α is independent of the choice of *z*, to minimize the loss *L*, we should select controlled variables that maximize $\underline{\sigma}(G)$.

Step 6 Evaluation of loss for alternative combinations of controlled variables

This step evaluates loss of alternative combinations of controlled variables. This is done by computing the loss imposed by keeping constant setpoints when there are disturbances or implementation error. The computations were performed on the cost model for important disturbance defined at step3. The selection of controlled variables by the local methods may not be able to assure the control structure. So that the selecting controlled outputs by direct evaluation of cost is introduced below.

Selecting controlled outputs: direct evaluation of cost

The local methods presented above are very useful. However, in many practical examples nonlinear effects are important. In particular, the local methods may not be able to detect feasibility problems. In such cases, we may need to use a “brute force” direct evaluation of the loss and feasibility for alternative sets of controlled variables. This is done by solving the nonlinear equations, and evaluating the cost function *J* for various selected disturbances *d* and control errors *e*, assuming $z = r + e$ where *r* is kept constant (Skogestad, 2000). Here *r* is usually selected as the optimal value for the nominal disturbance, but this may not be the best choice and its value may also be found by optimization (“optimal back-off”) (Govatsmark, 2003). The set of controlled outputs with smallest worst-case or average value of *J* is then preferred. This approach may be time consuming because the solution of the nonlinear equations must be repeated for each candidate set of controlled outputs.

Step 7 Evaluation and selection

This step is final evaluation and selection. The analysis up to now has been base purely on steady-state economics, and we have said nothing about implementation of the proposed controlled variables. Obviously, this is also and important consideration, as on choice of controlled variables might result in a system that is easy to control, whereas another might result in serious control problems. Here, we first identify candidate set of controlled variables with acceptable steady-state economics. We then check the controllability of the best alternative. If it is acceptable, then we have found a viable solution. If it is not acceptable, then we check the remaining candidates. If none of these turns out to be controllable, then we must relax our requirements on the steady-state economics and consider more candidates. A procedure for controllability analysis is given by Skogestad & Postlethwaite (1996). In other words, use the simulation approach to evaluate the controllability. In simulation approach, we propose a particular control structure, tune the controllers, and show with simulations that control is acceptable. If we can find a particular tuning with acceptable control, then we can conclude that the plant is controllable, at least for the disturbance and uncertainty scenario considered. However, the simulation approach generally suffers from the problem that it depends on the particular tunings and disturbances used in the simulations, and this can make it difficult to draw definite conclusions.

The procedure of select controlled variables for self-optimizing control by used the stepwise procedure of Skogestad is descriptively finished. The main focus of this work is to find good candidate controlled variables by using simple and effective method that scaled gain of process. We summarize many criteria about gain of process from several authors to analyses and bring to confirm the selection of controlled variables. The many criteria are shown below.

3.5 The Mathematically Systematic Tool for Prescreen and Selection

This section describe about the principal tool for deciding what variables to control. A good understanding of the process leads in most cases to a logical choice of what need to be controlled. Considerations of economics, safety, constraints, availability and reliability of sensors, etc. must be factored into this decision. In most cases these choices are fairly obvious. However, sometimes the selection of appropriate controlled variable is not so easy. In cases, the process has several measurements or has problem about difficult and expensive to measure variables. The best selection of the best control variables to use requires a considerable amount of knowledge about the process, its operation, and its performance besides, the applied the mathematics to select controlled variables and to analyses interaction of variables are the other helpfulness method. The mathematical method can used to screen variables, check stability, controllability and interaction of process. Those method are described in this section relate to the scaled gain of process only. The computation of the steady-state gains for multivariable processes is elucidated below

3.5.1 Steady-state Gains.

The availability of accurate steady-state gains for a multivariable process facilitates significantly the control system design procedure. The steady-state gains provide the zero frequency characteristics of the system. This piece of information enables the initial screening and selection of proper manipulated and/ or controlled variables, variable pairing, and initial evaluation of candidate control structures (Grosdidier et al., 1985: Yu and Luyben, 1986; Shinskey, 1988).

The steady-state gains can be determined by using either plant tests (although it has been shown (Luyben, 1987a) that the results might be seriously different from those of a linearized model of the process) or some kind of a rating program (Buckley et al., 1985). A third and more complex alternative is to get the steady-state gains through a transfer function identification procedure, if dynamic plant data or data from a dynamic model of the process are available.

The usual method to determine the gains is an open loop type of test. A specific control structure is assumed. A small perturbation is introduced in one of the manipulated variables. All the remaining manipulated variables are held constant. The rating program is converged. All measurement variables changes are recorded. The steady-state gain between the *i* controlled variable and the *j* manipulated variable is calculated as

$$g_{ij} = \Delta x_{ij} / \Delta m_j \quad i = 1, 2, ..., n;\ j = 1, 2, ..., m \tag{3.12}$$

where g , is the *ij* element of the gain matrix and Δx_{ij} is the change in the *i* controlled variable because of the Δm_j change in the *j* manipulated variable.

According to this procedure, *m* tests need to be performed for every candidate control structure where m is the number of manipulated variables. For controlled variable selection, this procedure is ideal because it provides gains for all controlled variables.

Furthermore, the method for calculates steady-state gains is presented by Papastathopoulou (1990).They present a new method for the derivation of steady-state gains for a multivariable process is presented. It is based on small perturbations in the controlled variables instead of changes in the manipulated variables, as is the case in the traditional method. This method is a closed loop type of test. It involves calculation of the inverse of the steady-state process gain matrix. A small change in one of the controlled variables is introduced into the system. All the remaining controlled variables are kept constant. Notice that in the traditional method the perturbation is in one of the manipulated variables.

The size of the perturbation must be small enough to assure that the process response will be linear. Positive and negative perturbations in the controlled variables are suggested. If for both kinds of changes the process gains are approximately equal, the perturbation is small enough to keep the process in the linear region. The linear process gains also satisfy the consistency relations suggested by Haggblom and Waller (1988).

The method for calculates steady-state gains was several technique. To select of method for calculate the process gains depend the discrimination of the user and the appropriation of each process.

The problem of the effect of scaling on the steady-state gains process is handled by expressing the gains of all the plant transfer functions in dimensionless form. The gains with engineering units are divided by transmitter spans and multiplied by valve gains. The method for scaling on the steady-state gains are elucidated below.

3.5.1.1 Scaling

Scaling is very important in practical applications as it makes model analysis and controller design (weight selection) much simpler. It requires the engineer to make a judgment at the start of the design process about the required performance of the system. To do this, decisions are made on the expected magnitudes of disturbance and reference changes, on the allowed magnitude of each input signal, and on the allowed deviation of each input.

Let the unscaled (or originally scaled) linear model of the process in deviation variable be

$$\hat{y} = \hat{G}\hat{u} + \hat{G}_d\hat{d}; \quad \hat{e} = \hat{y} - \hat{r} \tag{3.13}$$

Where a hat (^) is used to show that the variables are in their unscaled units. A useful approach for scaling is to make the variables less than 1 in magnitude. This is done by dividing each variable by its maximum expected or allowed change. For disturbances and manipulated inputs, we used the scaled variables

$$d = \hat{d}/\hat{d}_{\max}, \quad u = \hat{u}/\hat{u}_{\max} \tag{3.14}$$

where:

- $\hat{d}_{\max}$ – largest expected change in disturbance
- $\hat{u}_{\max}$ – largest allowed input change

The maximum deviation from a nominal value should be chosen by thinking of the maximum value one can expect, or allow, as function of time. The variables $\hat{y}, \hat{e}$ and $\hat{r}$ are in the same units, so the same scaling factor should be applied to each. Two alternatives are possible:

- $\hat{e}_{\max}$ – largest allowed control error
- $\hat{r}_{\max}$ – largest expected change in reference value

Since a major objective of control is to minimize the control error, we here usually choose to scaled with respect to the minimum control error:

$$y = \hat{y}/\hat{e}_{\max}, \quad r = \hat{r}/\hat{e}_{\max}, \quad e = \hat{e}/\hat{e}_{\max} \tag{3.15}$$

To formalize the scaling procedure, we introduce the scaling factors

$$D_e = \hat{e}_{\max}, \; D_u = \hat{u}_{\max}, \; D_d = \hat{d}_{\max}, \; D_r = \hat{r}_{\max} \tag{3.16}$$

For multi-input multi-output (MIMO) systems, each variable in the vectors $\hat{d}, \hat{r}, \hat{u}$ and $\hat{e}$ may have a different maximum value, in which case D_e, D_u, D_d and D_r become diagonal scaling matrices. This ensures, for example, that all errors (output) are of about equal importance in term of their magnitude.

The corresponding scaled variables to use for control purposes are then

$$d = D_d^{-1}\hat{d},\ u = D_u^{-1}\hat{u},\ y = D_e^{-1}\hat{y},\ e = D_e^{-1}\hat{e},\ r = D_e^{-1}\hat{r} \tag{3.17}$$

On substituting (3.17) into (3.13) we get

$$D_e y = \hat{G} D_u u + \hat{G}_d D_d d; \quad D_e e = D_e y - D_e r$$

And introduction of the scaled transfer functions

$$G = D_e^{-1}\hat{G} D_u, \quad G_d = D_e^{-1}\hat{G}_d D_d \tag{3.18}$$

Yields the following model in terms of scaled variables:

$$y = Gu + G_d d; \quad e = y - r \tag{3.19}$$

Here u and d should be less than 1 in magnitude, and it is useful in some cases to introduce a scaled reference $\tilde{r}$, which is less than 1 in magnitude. This is done by dividing the reference by the maximum expected reference change

$$\tilde{r} = \hat{r} / \hat{r}_{\max} = D_r^{-1}\hat{r} \tag{3.20}$$

We then have that

$$r = R\tilde{r} \quad \text{where} \quad R \triangleq D_e^{-1} D_r = \hat{r}_{\max} / \hat{e}_{\max} \tag{3.21}$$

Here R is the largest expected change in reference relative to the allowed control error (typically, $R \geq 1$). The block diagram for the system in term of scaled variables may then be written as shown in figure 3.3, for which the following control objective is relevant:

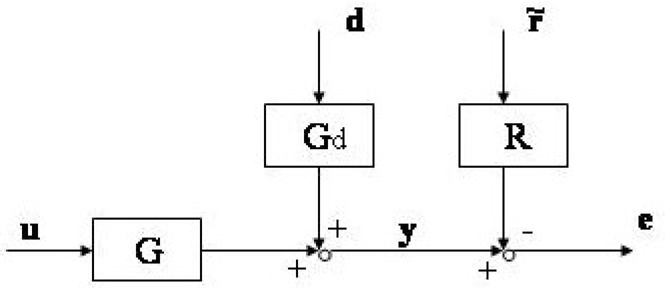


Figure 3.3. Model in terms of scaled variables

We summarize many criteria about gain of process from several authors. The some of criteria that relates with scaled gain of process are descriptively finished.

3.5.2 Singular Value Analysis

In this section, a powerful analytical technique, singular value analysis (SVA) is discussed below, which can be used to solve the following important control problems:

1. Selection of controlled and manipulated variables.
2. Evaluating of the robustness of a proposed control strategy.
3. Determination of the best multiloop control configuration.

Singular value analysis and its extensions, including singular value decomposition (SVD), also have many uses in numerical analysis and the design of multivariable control system. Let ***K*** is the process gain. The singular values are nonnegative numbers that are defined as the positive square root of the eigenvalues of ***KTK***. The first r singular values are positive numbers where r is the rank of matrix ***KTK***. The remaining *n -r* singular values are zero. Usually the nonzero singular values are ordered with σ1 denoting the largest and σr denoting the smallest.

3.5.3 The Morari Resiliency Index (MRI)

Some processes are easier to control than others. Some choices of manipulated and controlled variables produce systems that are easier to control than others. This inherent property of ease of controllability is called resiliency. Morari (Chemical Eng. Science, 1983) developed a very useful measure of this property. The Morari resiliency index (MRI) gives an indication of the inherent controllability of a process. It depends on the controlled and manipulated variables, but it does not depend on the paring of these variables or on the tuning of the controllers. Thus it is a useful tool for comparing alternative processes and alternative choices of manipulated variables.

The MRI is the minimum singular value of the process openloop transfer function matrix. It the latter case, only the steady-state gain is needed. σr denoting the smallest singular value.

$$\mathrm{MRI} = \sigma r \tag{3.22}$$

The larger value of the MRI, the more controllable or resilient the process. Without going into an elaborate mathematical proof, we can intuitively understand why a big MRI is good. The larger the minimum singular value of a matrix, the farther it is from being singular and easier it is to find its inverse.

One important aspect of the MRI calculations should be emphasized at this point. The singular value depends on the scaling use in the steady state gains of the transfer functions. It different engineering units are used for the gains; different singular values will be calculated. The practical solution to the problem is to always use dimensionless gains in the transfer functions. The method compute dimensionless gains are described below in section 3.4.

3.5.4 Relative Gain Array

The quantity λ_{11} is known as the *relative gain* between output $y1$ and input $m1$; it provides a measure of the extent of the influence of process interactions when $m1$ is used to control $y1$. Even though we introduced this quantity in reference to a 2 x 2 system, it can be generalized to any other multivariable system of arbitrary dimension.

Let us define λ_{ij} the relative gain between output variable yi and input variable mj, as the ratio of two steady-state gains:

$$\lambda_{ij} = \frac{\left(\dfrac{\partial y_i}{\partial m_j}\right)_{\text{all loops open}}}{\left(\dfrac{\partial y_i}{\partial m_j}\right)_{\text{all loops closed except for the } m_j \text{ loop}}} \tag{3.23}$$

$$= \left(\frac{\text{open - loop gain}}{\text{closed - loop gain}}\right) \text{ for loop } i \text{ under the control of } mj$$

When the relative gain is calculated for all the input/output combinations of a multivariable system and the results are presented in an array of the form shown below:

$$\Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix} \tag{3.24}$$

The result is what is known as the *relative gain array* (RGA) or the *Bristol array*. The RGA was first introduced by Bristol (1996) and has become the most widely used measure of interaction. The RGA has the advantage of being easy to calculate and only requires steady state gain information.

The elements in the RGA can be numbers that vary from very large negative value to vary large positive values. The closer the number is to 1, the less difference closing the other loop makes on the loop being considered. Therefore there should be less interaction, so the proponents of the RGA claim that variables should be paired so that they have RGA elements near1. Numbers around 0.5 indicate interaction. Numbers that are very large indicate interaction. Numbers that are negative indicate that the sign of the controller may have to be different when other loops are on automatic.

As pointed out earlier, the problem with pairing on the basis of avoiding interaction is that interaction is not necessarily a bad thing. Therefore, the use of the RGA to decide how to pair variables is not and effective tool for process control applications. Likewise the use of the RGA to decide what control structure (choice of manipulated and controlled variables) is best is not effective. What is important is the ability of the control system to keep the process at setpoint in the face of load disturbances. Thus, load rejection is the most important criterion on which to make the decision of what variables to pair, and what controller structure is best.

The RGA is useful for avoiding poor pairings. If the diagonal element in the RGA is negative, the system may show integral instability: the same situation that we discussed in the use of the Niederlinski index. Very large values of the RGA indicate that the system can be quite sensitive to changes in the parameter values.

3.6 Plantwide Energy Management

Energy conservation has always been important in process design. Thus, it is common practice to install feed-effluent heat exchangers (FEHEs) around rectors and distillation columns. In any process flowsheet, a number of steams must be heated, and other streams must be cooled. For example, in HDA process, the toluene fresh feed, the makeup hydrogen, the recycle toluene, and the recycle gas stream must be heated up to the reaction temperature 621.1 C. And, the reactor effluent stream must also be cooled to the cooling water temperature to accomplish a phase split. Therefore, the energy integration is required to reduce the utility cost and also to improve thermodynamic efficiency of the process.

3.6.1 Heat Exchanger Dynamics

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

For the purpose of plantwide control studies it is not necessary to have such detailed descriptions of the exchanger dynamics, since these units rarely dominate the process response. Instead, it is often possible to construct useful models by letting two sets of well-stirred tanks in series exchange heat. This simplifies the solution procedure.

3.6.2 Heat pathways

The most of energy required for heating certain streams within the process is matched by similar amount required for cooling other streams. Heat recover from cooling a stream could be recycled back into the process and used to heat another stream. This is the purpose of heat integration and heat exchanger networks (HENs).

From a plantwide perspective we can now discern three different “heat pathways” in the process. See Figure 3.4 for an illustration. The first pathway dissipates to the environment heat generated by exothermic reaction and by degradation of mechanical work (e.g. compression, pressure drop, and friction). This pathway is from inside the process and flow out. It is of course possible to convert some of the heat to work as it is removed from high temperature in the process.

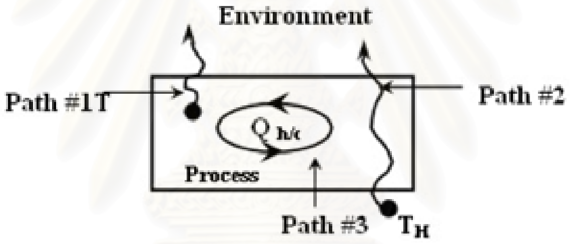


Figure 3.4 Heat pathways

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

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

3.6.3 Heat recovery

We can make great improvements in the plant’s thermal efficiency by recycling much of the energy needed for heating and cooling process streams. There is of course a capital expense associated with improved efficiency but it can usually be justified when the energy savings are accounted for during the lifetime of the project. Of more interest to us in the current context is how heat integration affects the dynamics and control of a plant and how we can manage energy in plants with a high degree of heat recovery.

3.7 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 provided we can independently manipulate the two inlet flowrates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom for temperature control. We can restore one of these degrees of freedom fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Figure 3.5a. It is possible to combine the P/P exchanger with a utility exchanger as in Figure 3.5b.

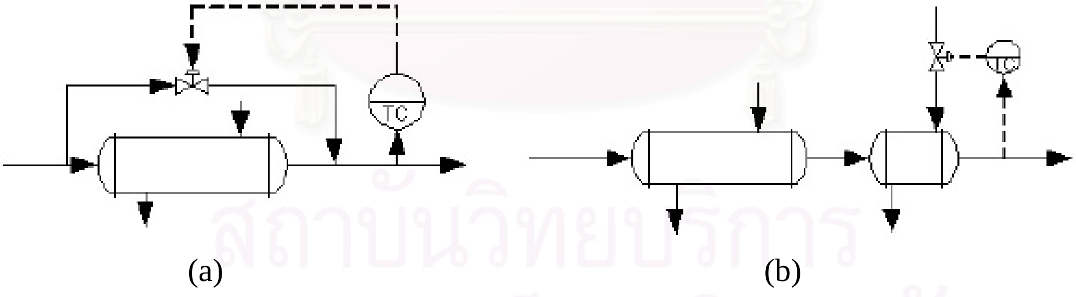


Figure 3.5: Control of P/P heat exchangers (a) use of bypass; (b) use of auxiliary utility exchanger.

3.7.1 Use of auxiliary utility exchangers

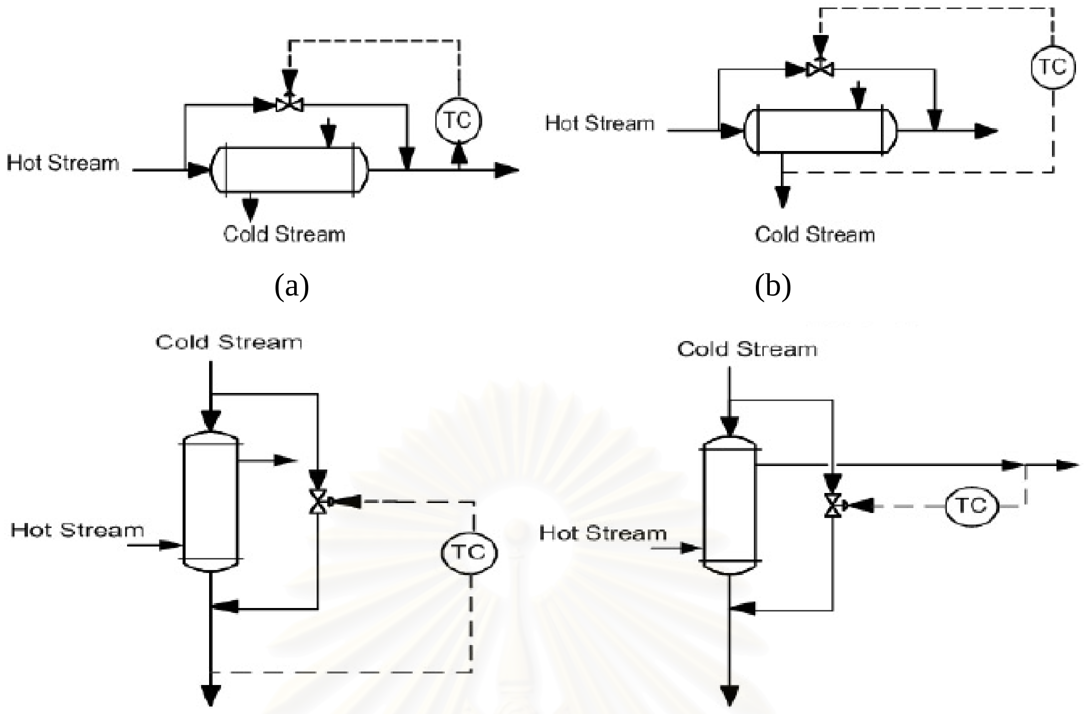
When the P/P exchanger is combined with a utility exchanger, we also have a few design decisions to make. We must first establish the relative sizes between the recovery and the utility exchangers. From a design standpoint we would like to make the recovery exchanger large and the utility exchanger small. This gives us the most heat recovery, and it is also the least expensive alternative from an investment standpoint. However, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control standpoint.

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

Consider a distillation column that uses a large amount of high-pressure stream in its thermo siphon reboiler. To reduce operating costs we would like to heat-integrate this column with the reactor. A practical way of doing this is to generate stream in a waste heat boiler connected to the reactor as suggested. We can then use some or all of this steam to help reboil the column by condensing the stream in the tubes of a stab-in reboiler. However, the total heat from the reactor may not be enough to reboil the column, so the remaining heat must come from the thermo siphon reboiler that now serves as an auxiliary reboiler. The column tray temperature controller would manipulate the stream to the thermo siphon reboiler.

3.7.2 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 3.6 shows the most common alternatives. We may ask which option is the best. It depends on how we define “best”. As with many other examples, it boils down to a trade-off between design and control. Design considerations 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 considerations 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 we control. 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 heat exchanger.



(a) (b)

(c) (d)

Figure 3.6: 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 cold stream.

CHAPTER IV
HYDRODEALKYLATION PROCESS

4.1 Process Description

The hydrodealkylation (HDA) process was proposed by Douglas (1988). The HDA process contains nine basic unit operations: reactor, furnace, vapor-liquid separator, recycle compressor, two heat exchangers, and three distillation columns. Two raw materials, hydrogen, and toluene, are converted into the benzene product, with methane and diphenyl produced as by-products. The two vapor-phase reactions are

Toluene + H2 → benzene + CH4

2BenZene ↔ diphenyl + H2

The kinetic rate expressions are functions of the partial pressure (in psia) of toluene pT, hydrogen pH, benzene pB, and diphenyl pD, with an Arrhenius temperature dependence. Zimmerman and York (1964) provide the following rate expression:

r1 = 3.6858 * 106exp(-25616/T) pT pH1/2

r2 = 5.987 * 104exp(-25616/T) pB2 – 2.553 * 105exp(-25616/T) pD pH

Where r1 and r2 have units of lb*mol/(min*ft3) and T is the absolute temperature in Kelvin. The heats of reaction given by Douglas (1988) are –21500 Btu/lb*mol of toluene for r1 and 0 Btu/lb*mol for r2.

The effluent from the adiabatic reactor is quenched with liquid from the separator. This quenched stream is the hot-side feed to the process-to-process heat exchanger, where the cold stream is the reactor feed stream prior to the furnace. The reactor effluent is then cooled with cooling water and the vapor (hydrogen, methane) and liquid (benzene, toluene, diphenyl) are separated. The vapor stream from the separator is split and the remainder is sent to the compressor for recycle back to the reactor.

The liquid stream from the separator (after part is taken for the quench) is fed to the stabilizer column, which has a partial condenser component. The bottoms stream from the stabilizer is fed to the product column, where the distillate is the benzene product from the process and the bottoms is toluene and diphenyl fed to the recycle column. The distillate from the recycle column is toluene that is recycled back to the reactor and the bottom is the diphenyl byproduct.

Makeup toluene liquid and hydrogen gas are added to both the gas and toluene recycle streams. This combined stream is the cold-side feed to the process-to-process heat exchanger. The cold-side exit stream is then heated further up to the required reactor inlet temperature in the furnace, where heat is supplied via combustion of fuel.

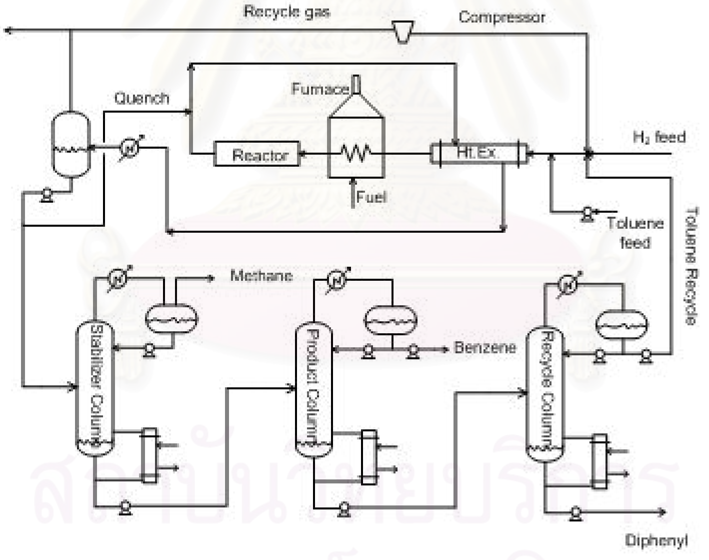


Figure 4.1 Hydrodealkylation (HDA) of toluene process

Component physical property data for the HDA process were obtain from William L. Luyben, Bjorn D. Tyreus, Michael L. Luyben (1999)

Equipment data and specifications

Table 4.1 Column specifications

	Stabilizer column	Product column	Recycle column
Number of theoretical trays	6	27	7
Feed tray	3	15	5
Diameter (ft)	1	5.7	2.5
Reboiler volume (ft3)	250	293	36
Condenser volume (ft3)	7.5	316	46
Reflux ratio	1.57	3	0.32

Table 4.2 Equipment data and specifications of HDA process

Unit	specification	Unit	specification
Reactor	Diameter (ft) 9.53 Length (ft) 57 Number of tubes 1	Heater	Tube volume (ft3) 60
Exchanger (E1)	Shell volume (ft3) 500 Tube volume (ft3) 500	Exchanger	Shell volume (ft3) 100 Tube volume (ft3) 100
Exchanger	Shell volume (ft3) 500	Cooler	Tube volume (ft3) 300
	Tube volume (ft3) 500	Separator	Volume (ft3) 80
Exchanger	Shell volume (ft3) 500	Furnace	Tube volume (ft3) 300
	Tube volume (ft3) 500	Aux	Tube volume (ft3) 30

4.2 Steady-State Modeling

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet stream data taken from Skogestad and Atonio (2006). The equipment design information was taken from Douglas (1988); Luyben et al. (1998). Table 4.1-4.2 presents the data and specifications for the equipment employed other than the three columns. For our simulation, Peng-Robinson model is selected for physical property calculations because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions. The reaction kinetics of both reactions are modeled with standard Arrhenius kinetic expressions available in HYSYS.PLANT, and the kinetic data are taken from Luyben et al. (1998). Since there are four material recycles, four RECYCLE operations are inserted in the streams, Hot-In, Gas-Recycle, Quench, and Stabilizer-Feed . Proper initial values should be chosen for these streams, otherwise the iterative calculations might converge to another steady-state due to the non-linearity and unstable characteristics of the process.

When columns are modeled in steady-state, besides the specification of inlet streams, pressure profiles, numbers of trays and feed tray, two specifications need to be given for columns with both reboiler and condenser. These could be the duties, reflux rate, draw stream rates, composition fractions, etc. We chose reflux ratio and overhead benzene mole fraction for the stabilizer column. For the remaining two columns, bottom and overhead composition mole fractions are specified to meet the required purity of products. The detailed design data and specifications for the columns are summarized in Table 4.1-4.2. This table also includes details of trays, which are required for dynamic modeling. The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on Glitsch design parameters for valve trays. Though the tray diameter and spacing, and weir length and height are not required in steady-state modeling, they are required for dynamic simulation. The flowsheet of HDA process indicates that this process could be separated into two parts: the reaction part containing reactor, separator, FEHE, compressor, cooler and gas recycle, etc. and the separation part that includes the three distillation columns. This work considers only reaction part. Figure 4.2 show the reaction section of HDA process.

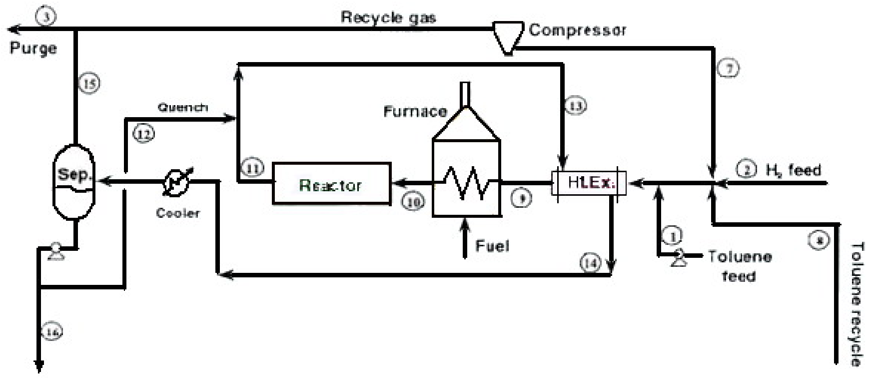


Figure 4.2 Reaction section of Hydrodealkylation (HDA) of toluene process

Figure 4.3 show the simulated HDA process at steady-state by HYSYS.PLANT. Results from steady-state simulation are found to be consistent with those in Skogestad and Antonio (2006). However, there are also some differences: for example, pressure of recycle gas flow is larger than those in Skogestad and Antonio (2006). The possible reasons for these differences may be because increasing pressure of gas recycles flow affect to pressure inside process to be consistent with earlier study. Besides pressure of toluene recycle flow is smaller than those in the earlier study because decreasing pressure of toluene recycle flow affect to pressure inside process. The other variables are rather consistent with those in Skogestad and Antonio(2006).

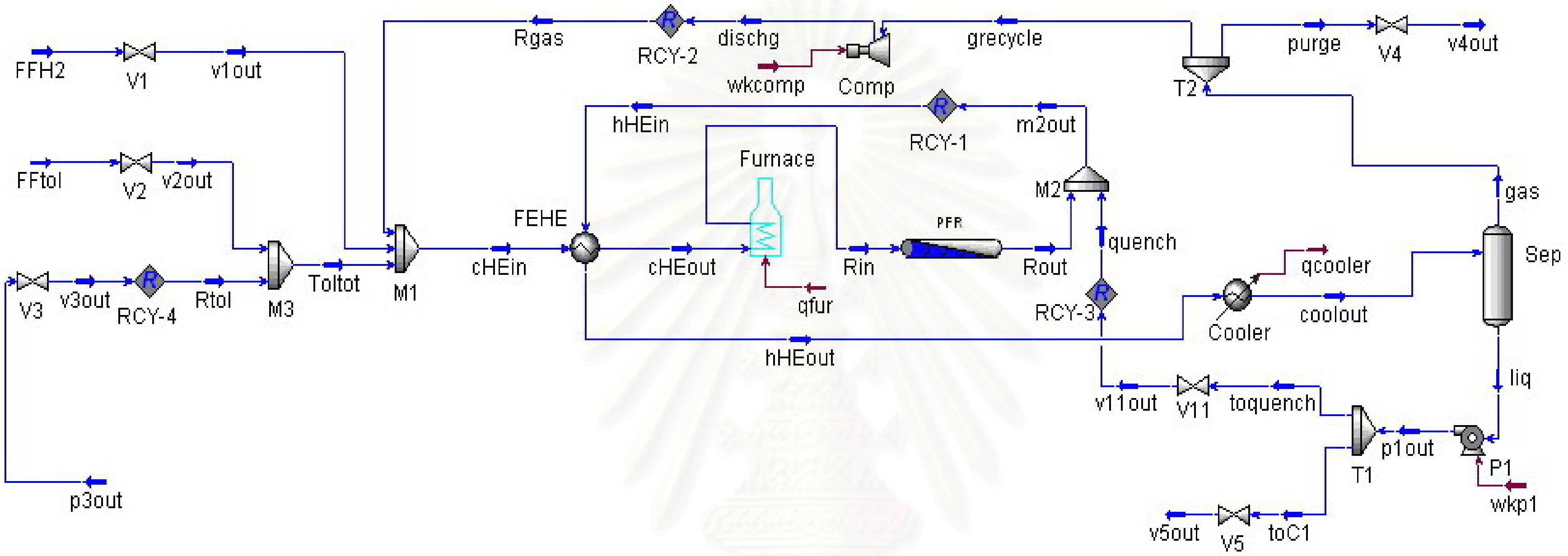


Figure 4.3 Flowsheet of simulation Reaction section of Hydrodealkylation (HDA) of toluene process by HYSYS.PLANT

4.3 Dynamic Modeling

In this section consist of: the way to switch from steady-state to dynamic mode and procedure to use transfer function block replaced separation section that includes the three distillation columns. This transfer function is adopted to represent the dynamics of columns in our reduced dynamic model. Those procedures are explained below.

In the integrated steady state and dynamic simulation environment provided by HYSYS.PLANT, the dynamic model shares the same physical property packages and flowsheet topology as the steady-state model. Thus it is easy to switch from steady-state to dynamic mode. All flowsheet information from the steady-state simulation case transfers easily to the dynamic simulation environment. On the other hand, the dynamic model uses a different set of conservation equations that account for changes occurring over time. Besides the normal material and energy balances, an advanced method is provided to calculate the pressure and flow profiles. In this method (HYSYS.PLANT, 1998), volume balances and resistance equations are set-up, and the required number of pressure-flow (P-F) specifications is given by the user. These equations are solved simultaneously to find unknown pressure or flow rates. Before the transition from steady-state to dynamic mode, the flowsheet should be set up so that a definite pressure drop exists across the plant and, if necessary, valves and pumps should be added to the flowsheet. P-F specifications should be selected properly for the P-F solver to converge. Besides the proper sizing of the equipment, removal of redundant logical operations, and addition of controllers to increase the realism and stability of the model should also be considered as outlined below. Valves and pumps are added to the reflux streams in the column sub-flowsheet. For a more rigorous dynamic modeling of columns, condenser part of the column should be changed to a cooler followed by an accumulator. In our case, linear valve type is chosen and the valves are all sized with a 50% valve opening for nominal steady-state flow rates. The valve parameters are sized with the sizing function in HYSYS.PLANT. All the vessels including the separator, condensers and reboilers are initiated with 50% liquid level.

The HDA process is an open loop unstable system, and is caused by heat integration (i.e. recycle of energy) via feed-effluent heat exchanger (FEHE). This phenomenon is referred as external instability by Luyben (1998).Also, multiple steady-states exists for this process, and is described by Luyben et al. (1998). From dynamic simulation, we find that closing the reactor inlet temperature with furnace duty loop, the system becomes stable. Further, there are seven levels in the whole plant that need to be controlled due to their integrating characteristics. Initially, all these loops are implemented with the control scheme suggested by Luyben et al. (1998). Since these controllers are set for stability, a proportional (P) only controller is adopted. The model is now ready for switching from steady-state to dynamic mode. Before activating the Integrator to run the dynamic simulation, one P-F specification is given for each flowsheet boundary stream and the strip charts are set up to monitor the response of process variables of interest. After initiating the run, the responses eventually settle, after some initial transients, at the operating values obtained from steady-state simulation. Since dynamic modeling is a complex procedure, it is very important to perform model validation carefully.

To study the plant-wide control problem, transient responses from open loop tests on the process are often required. However, we faced some difficulties to obtain these from the model developed in HYSYS.PLANT. To get proper transient responses, it is required to close the condenser levels in columns. Thus, the model is only suitable for studying the plant-wide control problem after these level loops are closed. For more general design including level loops, this model is not appropriate (Qiu, Rangaiah, Krishnaswamy; 2003). Though one modification of column modeling is tried, it worked for the stabilizer column but did not work for the other two columns. Due to this difficulty, a reduced dynamic model in which the three columns are modeled by a simple transfer function between Tol-Recycle and Stabilizer-Feed streams will be used in our plant-wide control design. This is justified by the following analysis.

The flowsheet of HDA process indicates that this process could be separated into two parts: the reaction part containing reactor, separator, FEHE and gas recycle, etc. and the separation part that includes the three distillation columns. The separation part affects the reaction part only by the nearly pure toluene recycle stream. The reduced model effectively assumes that the distillation part is under good control and a simple transfer function can model the dynamics of toluene recycle stream. It is meaningful to study plant-wide control based on this reduced model because

1. Distillation columns serve only as separating units, and hence the difficulties for plant-wide control such as manipulation of product rates and handling recycle streams and heat integration are not often present in the separation part.
2. The control loops of distillation columns are usually built within the unit operation, and the control of distillation columns has been widely studied. The transfer function in the reduced model relates the toluene molar flow rate in the Stabilizer-Feed stream and the flow rate of Tol-Recycle stream. Very little toluene leaves the distillation system in methane, benzene and diphenyl product streams. Almost all of the toluene entering this part recycles back to the reaction part, and purity of Tol-Recycle stream is high (99.94%). Hence, it is satisfactory to model the dynamics of toluene recycle stream as a transfer function block. This approximation, however, will not provide results on the effect of disturbances and control strategies on benzene product purity, recycle composition and toluene inventory.

The transfer function could be identified through an open loop test. A step change in toluene molar flow of Stabilizer-Feed stream is effected to obtain the response of Tol-Recycle flow rate. First order plus dead time transfer function is used to model this response. We found the transfer function parameters by minimizing the integral of squared error (ISE) between the predicted responses of the transfer functions model and the dynamic response from the HYSYS.PLANT. The resulting model (with gain =1, time constant =19.54 min and dead time=33.13 min) is found to represent the simulation results quite well (Qiu, Rangaiah, Krishnaswamy; 2003). This transfer function is adopted to represent the dynamics of columns in our reduced dynamic model. Note that a dead time much larger than the time constant is introduced by this toluene recycle stream. It could be expected that the difficulty in plant-wide control will increase with this large dead time. The robust compensator for recycle effect suggested by Scali and Ferrari (1997, 1999), Taiwo and Krebs (1996) may be adopted to improve control of the process with such a large dead time.

4.4 Plantwide Control Design Procedures

This section describes the self-optimizing control procedure used to select the best set of controlled variables and a local analysis based on maximum scaled gain method is used for screening and pairing controlled variables with appropriate manipulated variables applied to the HDA process model in HYSYS PLANT.

Step1. Degree of freedom analysis

The reaction section of hydrodealkylation (HDA) process considered 8 manipulated variables and 64 candidate measurement variables. The manipulated variables and measurement variables are list in Table 4.4-4.5. The 8 manipulated variables are 8dynamic degree of freedom. However, at steady state there is only 7 degree of freedom because there is 1 liquid level at separator that needs to be controlled which has no effect on the economics (including variables with no steady-state effect). This is confirmed by the alternative steady-state degree of freedom analysis in Table 4.3. (Antonio A.,Marius G.,Sigurd S.,2006)

Table 4.3 Typical number of steady-state degree of freedom for some process units

Process unit	DOF
1.Each external feed stream	1(feedrate)
2.Splitter	n-1split fractions(n is the number of exit streams)
3.Mixer	0
4.Compressor, Turbine, and Pump	1(work)
5.Adiabatic flash tank	0*
6.Liquid phase reactor	1(holdup)
7.Gas phase reactor	0*
8.Heat exchanger	1(duty or net area)
9.Columns (e.g. distillation)	0* + number of side streams

*Add 1 degree of freedom for each extra pressure that is set (need an extra valve, compressor, or pump), e.g. in flash tank, gas phase reactor, or column.

There is 7 degree of freedoms and 64 candidate controlled variables, there are $\binom{64}{7} = \frac{64!}{57!7!} = 6.212 \cdot 10^8$ possible combinations of control structure, without including the alternative ways of controlling liquid level. It is clearly impossible to evaluate the loss with respect to disturbances and implementation errors for all of these combinations. So that, Reduction the number of alternatives is explained in the next step below.

Table 4.4 Steady-state degree of freedom for HDA process

	Manipulated variable	8
U1	Fresh feed Toluene	Steady state
U2	Fresh feed hydrogen	Steady state
U3	Furnace fuel valve	Steady state
U4	Cooler cooling water valve	Steady state
U5	Compressor power	Steady state
U6	Purge flow	Steady state
U7	Quench Flow	Steady state
U8	stabilizer feed flow	(level control)
Level with no steady-state effect		1
steady-state degree of freedom for optimization		7

Table 4.5 Candidate controlled variables for the HDA process

	Controlled variables	Unit
Y1	Fresh toluene feed rate	lbmole/hr
Y2	Fresh gas feed flow rate	lbmole/hr
Y3	Total toluene flow rate to the reaction section	lbmole/hr
Y4	Mixer outlet temperature	°F
Y5	Mixer outlet pressure	psi
Y6	Mixer outlet flow rate	lbmole/hr
Y7	Mixer outlet hydrogen mole fraction	-
Y8	Mixer outlet methane mole fraction	-

Y9	Mixer outlet benzene mole fraction	-
Y10	Mixer outlet toluene mole fraction	-
Y11	Mixer outlet diphenyl mole fraction	-
Y12	FEHE hot side outlet temperature	° F
Y13	FEHE hot side outlet pressure	psi
Y14	Furnace inlet temperature	° F
Y15	Furnace inlet pressure	psi
Y16	Furnace outlet temperature	° F
Y17	Furnace heat duty	Btu/hr
Y18	Hydrogen to aromatic ratio in reactor inlet	-
Y19	Reactor inlet temperature	° F
Y20	Reactor inlet pressure	psi
Y21	Reactor outlet temperature	° F
Y22	Reactor outlet pressure	psi
Y23	Reactor outlet hydrogen mole fraction	-
Y24	Reactor outlet methane mole fraction	-
Y25	Reactor outlet benzene mole fraction	-
Y26	Reactor outlet toluene mole fraction	-
Y27	Reactor outlet diphenyl mole fraction	-
Y28	Toluene conversion at reactor outlet	%
Y29	Benzene conversion at reactor outlet	%
Y30	Hydrogen mole fraction in the reactor outlet	-
Y31	Separator temperature	° F
Y32	Separator pressure	psi
Y33	Separator vapor outlet flow rate	lbmole/hr
Y34	Separator liquid outlet flow rate	lbmole/hr
Y35	Separator overhead vapor hydrogen mole fraction	-
Y36	Separator overhead vapor methane mole fraction	-
Y37	Separator overhead vapor benzene mole fraction	-
Y38	Separator overhead vapor toluene mole fraction	-
Y39	Separator overhead vapor diphenyl mole fraction	-
Y40	Separator liquid outlet hydrogen mole fraction	-
Y41	Separator liquid outlet methane mole fraction	-

Y42	Separator liquid outlet benzene mole fraction	-
Y43	Separator liquid outlet toluene mole fraction	-
Y44	Separator liquid outlet diphenyl mole fraction	-
Y45	Quencher outlet temperature	°F
Y46	Quencher outlet flow rate	lbmole/hr
Y47	Flow of cooling stream to quencher	lbmole/hr
Y48	Quencher outlet hydrogen mole fraction	-
Y49	Quencher outlet methane mole fraction	-
Y50	Quencher outlet benzene mole fraction	-
Y51	Quencher outlet toluene mole fraction	-
Y52	Quencher outlet diphenyl mole fraction	-
Y53	Recycle gas flow rate	lbmole/hr
Y54	Gas recycle hydrogen mole fraction	-
Y55	Gas recycle methane mole fraction	-
Y56	Gas recycle benzene mole fraction	-
Y57	Gas recycle toluene mole fraction	-
Y58	Gas recycle diphenyl mole fraction	-
Y59	Compressor inlet temperature	°F
Y60	Compressor outlet temperature	°F
Y61	Compressor outlet pressure	psi
Y62	Compressor power	hp
Y63	Purge flow rate	lbmole/hr
Y64	Cooler heat duty	Btu/hr

Step2. Definition of optimal operation (cost and constraints)

Rather than minimizing the cost J, it is more natural in this case to maximize the profit P = -J, which is the product value minus the feed costs and the operational (energy) costs which are proportional to cooler duty, fuel duty and electric power cost. The HDA process produces benzene from toluene and hydrogen. Two raw materials, toluene and hydrogen, are converted into the benzene product, with diphenyl and methane produced as by products. So that, product is benzene, by products; diphenyl, methane and purge gas, are sold as fuel. The operational cost are cost of fuel to the furnace, cost of cooling water to cooler and cost of power of compressor. The economic potential of HDA process is elucidated below.

The following profit is maximized (Douglas's EP)

$$(-J) = (\text{product+byproduct}) - (\text{raw material}) - (\text{operational cost})$$

$$(-J) = (p_{ben}D_{ben} + \sum_{i=1}^{nc} p_{f,i}F_{f,i}) - (p_{tol}F_{tol} + p_{gas}F_{gas} + p_{fuel}Q_{fuel} + p_{cw}Q_{cw} + p_{pow}W_{pow})$$

Where

p_{ben} = the prices of product benzene

p_{tol} = the prices of fresh toluene feed

p_{gas} = the prices of fresh gas feed

p_{fuel} = the prices of fuel to the furnace

p_{cw} = the prices of cooling water

p_{pow} = the prices of power to the compressor, and steam

$p_{f,i}$ = the prices associated to $F_{f,i}, i = 1,.,nc$

D_{ben} = the flows of product benzene

F_{tol} = the flows of fresh toluene feed

F_{gas} = the flows of fresh gas (hydrogen) feed

Q_{fuel} = the flows of fuel to the furnace

Q_{cw} = the flows of cooling water

W_{pow} = power to the compressor and pump

$F_{f,i}, i = 1,.,nc$ = the flow though the purge and diphenyl by product (nc is the number of component in the system)

The economic data for HDA process from Douglas (1988). The economic data are shown in Table 4.6.

Table 4.6 Economic data for the HDA process

	Cost/price($/lbmole)
Raw material	
Hydrogen feed (95% hydrogen; 5% methane)	1.14
Toluene feed (100% toluene)	6.04
Product	
Benzene product (99.97% benzene)	9.04
Fuel value	
Hydrogen	0.492
Methane	1.532
Benzene	5.64
Toluene	6.72
Diphenyl	5.38
Utility	Cost($/Btu)
power	0.042($/bhp)
Cooling (water)	$23.42 \cdot 10^{-8}$
Fuel	$4.0 \cdot 10^{-6}$

Constraint during operation

1. Production rate: Dben $\geq$ 265 lbmol/h.
2. Hydrogen excess in reactor inlet: FH2 / (Fben + Ftol + Fdiph) $\geq$ 5.
3. Bound on toluene feed rate: Ftol $\leq$ 300 lbmol/h.
4. Reactor pressure: Preactor $\leq$ 500 psia.
5. Reactor outlet temperature: Treactor $\leq$ 1300 °F.
6. Quench outlet temperature: Tquencher $\leq$ 1150 °F.
7. Product purity: xDben $\geq$ 0.9997.
8. Separator inlet temperature: 95 °F $\leq$ Tflash $\leq$ 105 °F.
9. Reactor inlet temperature: Treactor $\geq$ 1150 °F.

The HDA process has several control objectives and constraints are given in Douglas (1988).These include: achieving a specified production rate of essentially pure benzene: achieving ratio of hydrogen to aromatics greater than 5:1 in the reactor feed;

quenching reactor effluent to a temperature of 1150°F to prevent coking; the reactor outlet temperature constraint prevents hydrocracking; and the constraints reactor inlet temperature and reactor pressure gets a reasonable reaction rate.

Step3. Identification of important disturbances

The control system should be able to handle several disturbances such as setpoint changes for the base case and load disturbances. In this work interested important disturbance that have effect on economic potential. The consideration disturbances listed in Table 4.7.They include changes in the fresh feed toluene, in the fresh gas feed methane mole fraction and in the active constraints. Those disturbances have effect on economic of this system. Nominal value and magnitude of disturbance variables are shown in Table4.7

Table4.7 Nominal variables and magnitude of disturbance variables have effect on economic potential.

	Disturbance Variables	Type	Nominal	Magnitude
D1.	Fresh feed Toluene flow rate	Step	300lbmole/hr	-15
D2.	Fresh feed Toluene flow rate	Step	300lbmole/hr	+15
D3.	Fresh gas feed rate methane mole fraction	Step	0.03	+0.05
D4.	Hydrogen aromatic ratio in reactor inlet	Step	5	+0.5
D5.	Reactor-inlet pressure	Step	500psia	+20
D6.	Quench outlet temperature	step	1150 ° F	+20

Step 4 Optimization

The purpose of the optimization in this step is to identify the active constraints and recomputed optimal setpoints for controlled variables. In addition to deciding on which unconstrained variables to control (see step1). Data of the optimization of the HDA process in this step attain from Antonio A.,Marius G.,Sigurd S.,2006. They solve the optimization problem using the above cost function, and they provide a good explanation of what happens at the optimum. At the optimum, they separated optimization into two parts: optimization of the distillation columns and optimization of reactor and recycle. In section of optimization of the distillation columns, there are

6 steady state degrees of freedom and there is only one active constraint (benzene mole fraction in benzene column distillate, xDben $\geq$ 0.9997). For the remaining distillation products, the optimal conditions were obtained by a trade off between maximizing the recovery of valuable component and minimizing energy. The resulting of optimal variables for the five remaining degree of freedom are benzene mole fraction in stabilizer distillate, methane mole fraction in stabilizer bottoms, benzene mole fraction in benzene column bottom, diphenyl mole fraction in toluene column distillate, and toluene mole fraction in toluene column bottoms. So that, these six specifications for the distillation columns consumes six steady-state degrees of freedom. This is other imperative result that why we do not consider separation section in this work. In section of optimization of the reaction section, there are 7 steady state degrees of freedom, there are five active constraints, and they need to be controlled to achieve optimal operation. As expected, the benzene purity at the outlet of the process is kept at its bound for economic reasons. Moreover, fresh feed toluene is maintained at its maximum flow rate to maximize the profit. The separator inlet temperature is kept at its lower bound in order to maximize the recycle of hydrogen and to avoid the accumulation of methane in the process. Five active constraints and their bound are shown in Table4.8

Table4.8 Five active constraints and their bounds

	Active constraint	Bound
Y1.	Fresh feed Toluene flow rate	Upper
Y18.	Hydrogen aromatic ratio in reactor inlet	Lower
Y20.	Reactor-inlet pressure	Upper
Y31.	Separator Temperature	Lower
Y45.	Quench outlet temperature	Upper

All the 5 active constraints should be controlled to achieve optimal operation (Maarleveld and Rijnsdorp, 1970). Consequently, the remaining number of unconstrained degree of freedom is 2(7-5 = 2). This reduces the number of possible sets of controlled variables to $\binom{64}{2} = \frac{64!}{62!2!} = 2016$, where the number 64 is found by considering flow, temperature, pressure and composition of every stream in reaction section.

Step 5 Identification of candidate controlled variables

We are now at step 5: Identification of candidate controlled variables. This step is the main focus of this work.

Let us initially make the assumption that we will satisfy specifications or use active constraint control. We then have seven degree of freedom, and we want to control five active constraints at constant setpoint that were obtained from optimization step. First, the reactor temperature must be controlled to stabilize the reactor operation. As mentioned, the input with the most direct effect on the reactor temperature is the furnace heat duty. We chose to control the reactor inlet temperature because the furnace heat duty has a direct effect on the reactor temperature. We can also see from maximum scaled gain between the furnace heat duty and the reactor temperature. And then, active constraints should be controlled by some manipulated variable in system. So that, the maximum scaled gain between five active constraints and seven manipulated variables were scrutinized. The maximum scaled gain between six controlled variables that are reactor temperature and five active constraints and seven manipulated variables were shown in Table 4.9.

Table 4.9 The maximum scaled gain between six controlled variables and seven manipulated variables.

	Y1	Y18	Y19	Y20	Y31	Y45
U1	0.0112	-0.0441	0.0000	0.0010	0.0312	0.0010
U2	-0.0054	0.0412	0.0000	0.0014	-0.0147	-0.0005
U3	-0.0347	-0.0876	0.0208	0.0080	0.2365	0.0137
U4	0.0083	0.0307	0.0000	-0.0033	-0.1375	0.0006
U5	-0.0064	0.0043	0.0000	0.0000	0.0308	0.0001
U6	0.0100	-0.0134	0.0000	-0.0021	0.0067	0.0008
U7	-0.0018	-0.0060	0.0000	0.0007	0.0256	-0.0017

The maximum scaled gain show the furnace heat duty (U3) has a direct effect on the reactor temperature (Y19), the fresh feed toluene (U1) has effect on the fresh feed toluene flow rate (Y1), and the fresh gas feed (U2) has effect on the hydrogen aromatic ratio in reactor inlet (Y18), the purge flow (U6) has effect on the reactor pressure (Y20), the cooler heat duty (U4) has effect on the separator temperature (Y31), the quench flow (U7) has effect on the quench outlet temperature (Y45) respectively. The compressor power has slightly effect on six controlled variables. Then, Remained two manipulated variable were compressor power and setpoint of the reactor temperature controller, and we want to select two controlled variables that are to be controlled at constant setpoints. We can choose from 59 candidate variables exempted five active constraints. Even in the simplest case, there are many possible combinations among 1,711. There are too many possible combinations to evaluate the loss with respect to disturbances for all of these combinations.

The following criteria are proposed to reduce the number of alternatives. Most of them are rather obvious, but nevertheless, we find them useful.

1. Eliminate variables with no effect on the economic. The valve of these variables can be arbitrarily selected, which reduces the number of degrees of freedom and thus the number of controlled variables to be selected. In this work, there is one variable with no steady state effect, namely, separator level. Of course, we need to measure and control the separator level to obtain stable operation. Really, the separator level has direct effect on the stabilizer feed flow.
2. The variable directly associated with equality constraints should be controlled. In this paper, reaction section have only inequality constraints, does not have equality constraint.
3. We choose to control the active constraints. As mentioned, there are five active constraints, and this reduces the number of controlled variables to be selected. Again, the directly related variables should be eliminated from further consideration. We know that five active constraints are related to manipulated variables which were obtained from maximum scaled gain. This eliminates these five manipulated variables and also directly related measurement (fresh gas feed is the measurement directly related to fresh gas flow rate (measurement variable), etc) from further consideration. Five of the constraints are related to output (reactor pressure, reactor temperature, etc), which eliminates other measurements.
4. Eliminate/group closely related variables. The controlled variables should be independent (requirement 3).

The remaining manipulated variables are measured, that is, there is a one-to-one correlation with a measurement (purge flow rate is a one-to-one correlation with purge flow, eliminate purge flow rate). We should eliminate that measurement. Some streams have the same composition and small differences. Some of the same composition streams were eradicated for reduces number of candidate variables. Such as the gas, gas recycle and purge streams have the same composition, it follows that there are only small differences between controlling the gas and the gas recycle compositions. We therefore eliminate gas recycle composition. The main idea is to keep one variable in each group of related variables.

The basic criteria help to reduce the number of candidate measurements. The number of measurements is really very large, 64, but in this work not all of them can be regarded for a possible use due to operational limitations or impediments, f.e. some composition measurements are rather difficult and very costly. This pre-screening can substantially reduce the dimension of the problem and thus the number of controlled variable combinations. There are 20 remained candidate variables in this point. But there might be situations where the remaining number of possibilities is still large, in which case one can try to perform a local analysis that can lead to a good selection which can be found by using maximum scaled gain method. They are not guaranteed to give the best solution but due to their practicality and ease of use, they become very attractive in practice. Table 4.10 show 20 remained candidate variables.

Table 4.10 Remained candidate variables

	Controlled variables	Note
Y8	Mixer outlet methane mole fraction	-
Y21	Reactor outlet temperature	°F
Y23	Reactor outlet hydrogen mole fraction	-
Y24	Reactor outlet methane mole fraction	-
Y25	Reactor outlet benzene mole fraction	-
Y26	Reactor outlet toluene mole fraction	-
Y27	Reactor outlet diphenyl mole fraction	-

Y28	Toluene conversion at reactor outlet	-
Y29	Benzene conversion at reactor outlet	-
Y34	Separator overhead vapor hydrogen mole fraction	-
Y35	Separator overhead vapor methane mole fraction	-
Y41	Separator liquid outlet benzene mole fraction	-
Y42	Separator liquid outlet toluene mole fraction	-
Y43	Separator liquid outlet diphenyl mole fraction	-
Y47	Quencher outlet hydrogen mole fraction	-
Y48	Quencher outlet methane mole fraction	-
Y49	Quencher outlet benzene mole fraction	-
Y50	Quencher outlet toluene mole fraction	-
Y51	Quencher outlet diphenyl mole fraction	-
Y60	Compressor outlet pressure	psi

Table 4.11 shows the maximum scaled gain between candidates controlled variables that remained from pre-screening criteria and important disturbances. The controlled variables should be insensitive with disturbance (Requirement 1). For disturbance rejection, it is required to keep the output variables as close to zero (operation point) as possible. In this work, we peruse the maximum scaled gain between candidates controlled variables and disturbances. This maximum gain can only be used as a pre-screening tool to detect possible candidate controlled variables with eliminated controlled variables that large change when disturbance occurred. As can be seen in Table 4.11, we can exclude eleven candidate controlled variables. There is 9 remained candidate controlled variable in this point. And then, those controlled variables are scrutinized by the maximum scaled gain between candidates controlled variables and remained manipulated variables. We chose controlled variable large maximum gain with manipulated variable, as can be seen in Table 4.12. Table 4.12 shows the maximum scaled gain between remained controlled variables and remained manipulated variables.

Table 4.11 The maximum scaled gain between candidates controlled variables and disturbances

	Y8	Y21	Y23	Y24	Y25	Y26	Y27	Y28	Y29	Y34
D1-D2	-0.571	0.049	0.709	-0.416	0.809	-2.595	2.015	0.182	2.423	0.762
D3	0.002	-0.001	-0.002	0.001	-0.002	0.013	-0.007	-0.001	-0.003	-0.002
D4	-0.548	0.013	1.060	-0.497	-0.001	-1.778	-0.271	0.088	-0.215	1.051
D5	0.555	-0.101	-0.733	0.432	-0.753	-0.425	-0.867	-0.017	0.097	-0.780
D6	0.065	-0.095	-0.081	0.047	-0.100	0.611	-0.337	-0.036	-0.295	-0.086

	Y35	Y41	Y42	Y43	Y47	Y48	Y49	Y50	Y51	Y60
D1-D2	-0.366	0.141	-3.347	1.223	0.693	-0.430	0.708	-2.729	1.859	0.014
D3	0.001	-0.001	0.015	-0.005	-0.002	0.001	-0.002	0.013	-0.007	0.000
D4	-0.504	0.125	-1.676	-0.153	1.063	-0.495	0.020	-1.760	-0.250	-0.012
D5	0.381	-0.091	0.270	-0.159	-0.720	0.447	-0.632	-0.287	-0.718	0.899
D6	0.042	-0.031	0.686	-0.260	0.278	0.380	-3.083	-2.600	-3.613	0.048

Table 4.12 The maximum scaled gain between candidates controlled variables and remained manipulated variables.

	Y8	Y21	Y24	Y25	Y28	Y35	Y41	Y48	Y60
U3-SP	-0.246	0.776	0.007	0.623	2.239	-0.028	1.307	-0.268	-0.003
U5	0.195	-0.033	0.107	-0.320	-0.144	0.121	-0.110	0.142	0.076

4.5 Control Structure Alternatives

In this current work three control structures were designed and compared, three control structures were designed by using a maximum scaled gain method to select the candidate controlled variables. The control structures, we measured percent toluene conversion in plug flow reactor, benzene conversion in liquid outlet separator and reactor outlet temperature to cascade control reactor inlet temperature loop, namely control structure 1 (CS1), control structure 2 (CS2) and control structure 3 (CS3) respectively, as show in Figure 4.5 - 4.7. The reference control structure is Skogestad and Atonio (2006), namely reference control structure 1(REF1) as show in Figure 4.4.

4.5.1 The Reference Control Structure 1 (REF1).

Skogestad and Antonio (2006) designed 1 control structure by using a basic idea of self-optimizing control and a branch and bound algorithm for maximizing the singular value to select the candidate controlled variables. The control scheme controls 5 active constraints at its bound for economic reason. Five active constraints are fresh toluene feed rate, reactor pressure, separator temperature, aromatic ratio and quench temperature. Then, two candidate controlled variables were selected to control by a branch and bound algorithm for maximizing the singular value. Next, the regulatory control layer is to provide sufficient quality of control to enable a trained operator to keep the plant running safely without the use of the higher layers in the control system. And then, the supervisory control layer is used to keep the active constraints and un-constrained controlled variables at constant set points. More detail analysis base on RGA method which requires a linear model of the process. In summary, all of these control loops were closed the following regulatory control loop and supervisory control loop in the reaction section:

FCH: Flow control of the hydrogen feed rate (Fhyd)

PCR: Reactor inlet pressure (Pr,in) with purge flow (Fpurge)

FCTOL: Flow control of the toluene feed rate (Ftol)

TCQ: Quench outlet temperature (Tquencher) with cooling flow from the separator (Fsep,liq)

TCR: Reactor inlet temperature (Tr,in) with furnace heat duty (Qfur)

TCS: Separator temperature (Tsep) with cooler heat duty (Qcool)

LCS: Separator level uses its liquid outlet flow rate to the distillation section.

CCR2: The toluene mole fraction at the quencher outlet xquen,tol with the setpoint of the reactor temperature controller (Trmin,sp)

CCH2: The methane mole fraction at the mixer outlet xmix,met with the setpoint of the hydrogen feed rate flow controller(Fhyd,sp)

rH2: The hydrogen-to-aromatics ratio at the reactor inlet (rH2) with compressor power (Ws)

4.5.2 The Designed Control Structures (CS1, CS2 and CS3).

In this current work, we designed 3 control structures by using a basic idea of self-optimizing control and a maximum scaled gain method to select the candidate controlled variables. The control scheme controls 5 active constraints at its bound for economic reason. Five active constraints are fresh toluene feed rate, reactor pressure, separator temperature, aromatic ratio and quench temperature. Then, the maximum scaled gain between five active constraints and seven manipulated variables are calculated for paring. Next, maximum scaled gain between disturbance and candidate controlled variables are calculated for prescreening the candidate controlled variables. And then, maximum scaled gain between remain manipulated variables and candidate controlled variables are computed and considered to select controlled variable and paring them with remain manipulated variables. In all of these control structures, the same loops are used as follows:

rH2: The hydrogen mole fraction at the reactor inlet xrin,hy with the hydrogen feed rate (Fhyd)

rH2: The hydrogen-to-aromatic ratio at the reactor inlet (rH2) with the setpoint of hydrogen feed rate

PCR: Reactor inlet pressure (Pr,in) with purge flow (Fpurge)

FCTOL: Flow control of the toluene feed rate (Ftol)

TCQ: Quench outlet temperature (Tquencher) with cooling flow from the separator (Fsep,liq)

TCR: Reactor inlet temperature (Tr,in) with furnace heat duty (Qfur)

TCS: Separator temperature (Tsep) with cooler heat duty (Qcool)

LCS: Separator level uses its liquid outlet flow rate to the distillation section.

CCW: The methane mole fraction at the gas outlet separator xgas,me with compressor power (Ws)

Each control structure has different loop in cascade control of the reactor inlet temperature. The setpoint of the reactor temperature controller of each control structure are used as follows:

CS1: The percent toluene conversion at the plug flow reactor with the setpoint of the reactor temperature controller (Trin,sp)

CS2: The benzene mole fraction at the separator bottom liquid outlet with the setpoint of the reactor temperature controller (Trin,sp)

CS3: The reactor outlet temperature with the setpoint of the reactor temperature controller (Trin,sp)

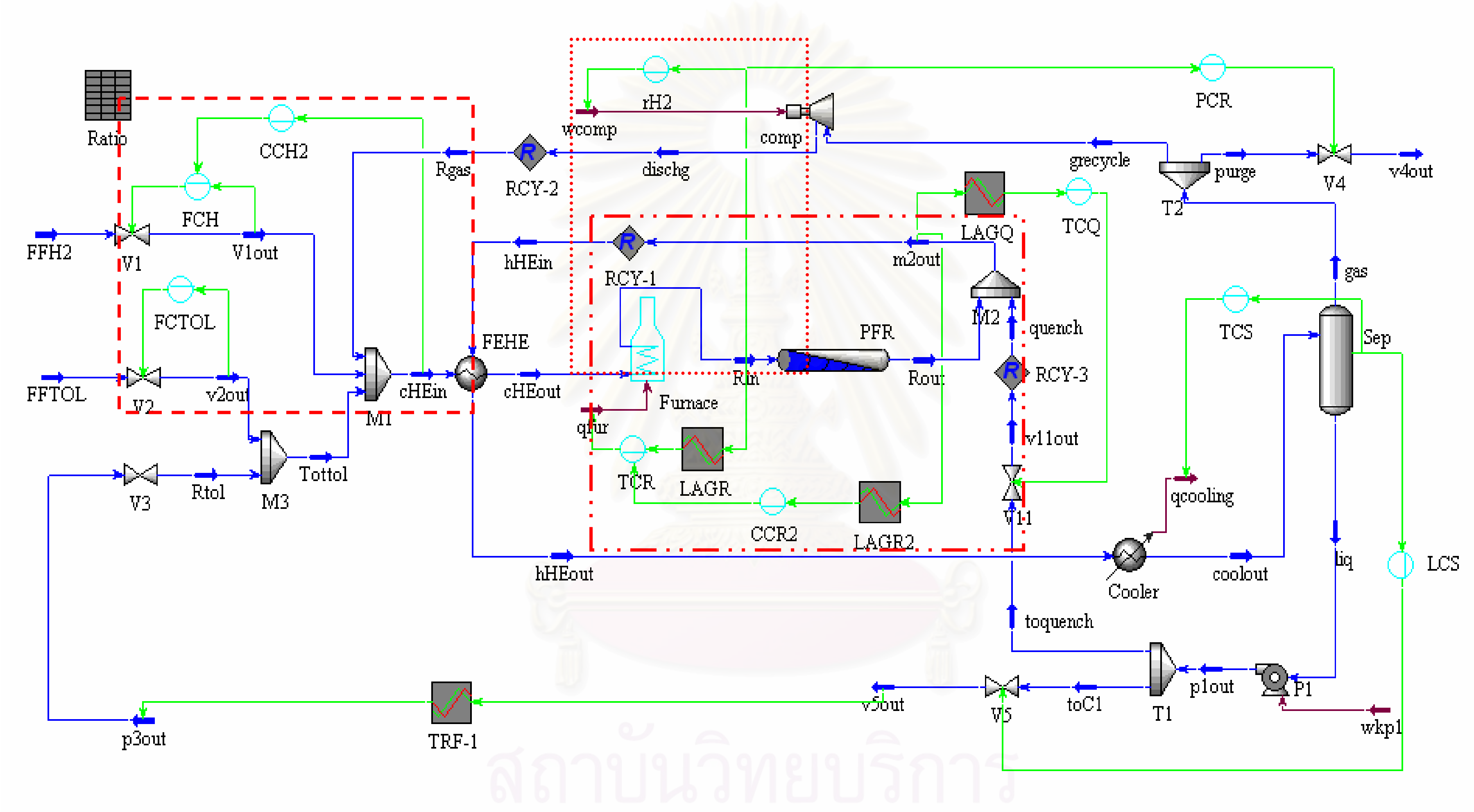


Figure 4.4 The Flowsheet of Simulation Hydrodealkylation (HDA) process of the Reference Control structure1 (REF1) (Skogestad and Antonio; 2006)

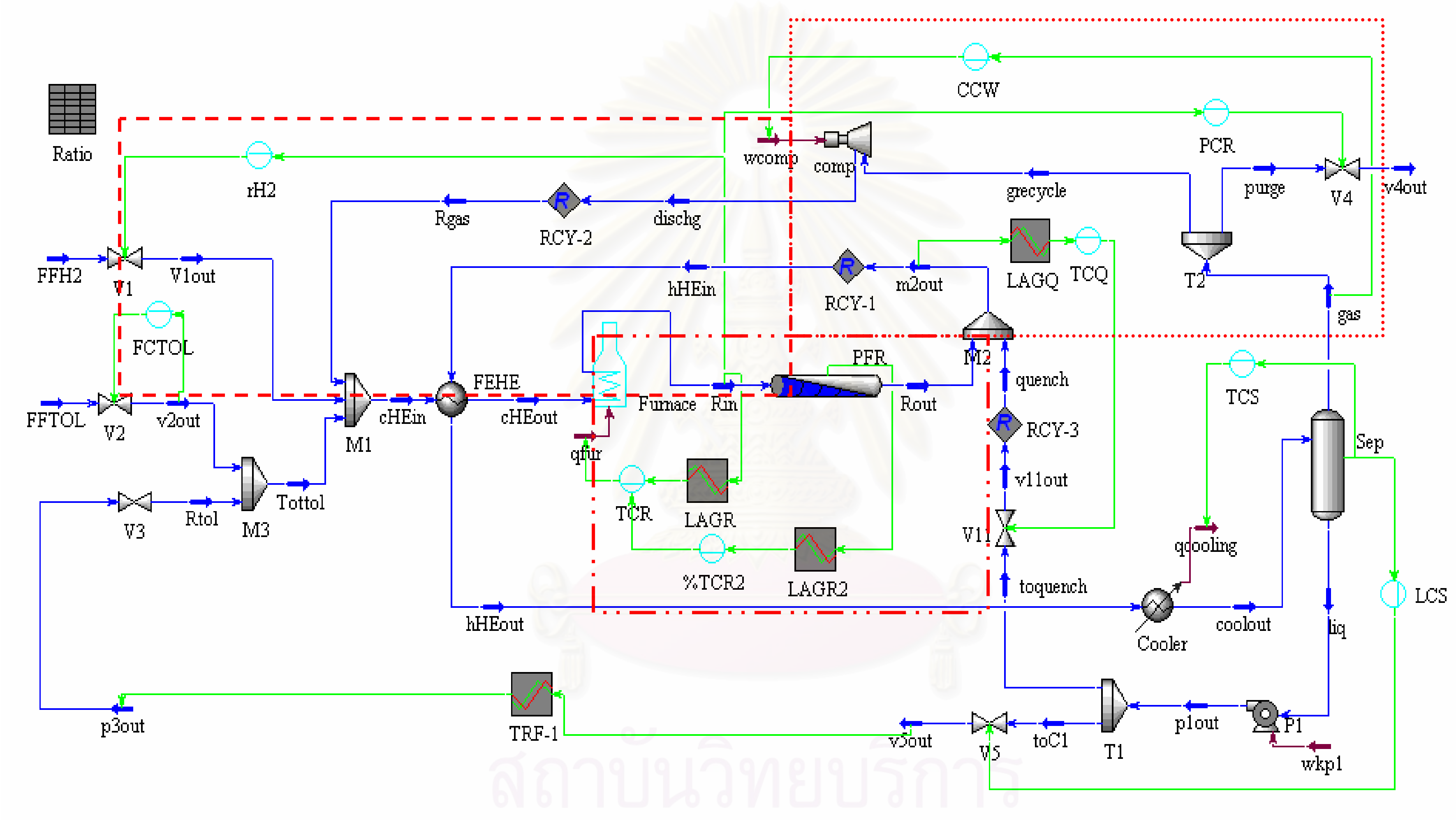


Figure 4.5 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed Control Structure 1 (CS1).

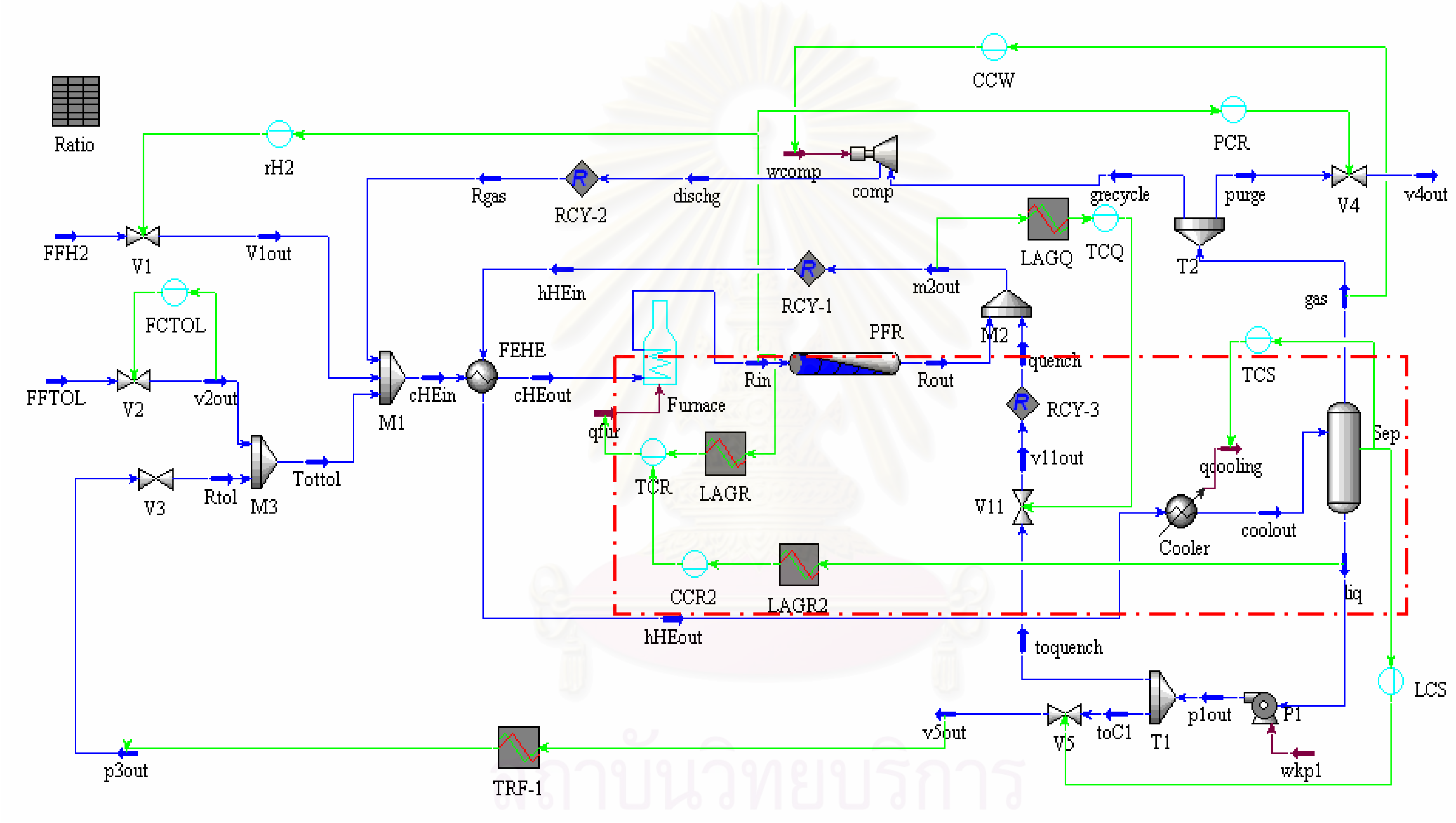


Figure 4.6 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed Control structure2 (CS2)

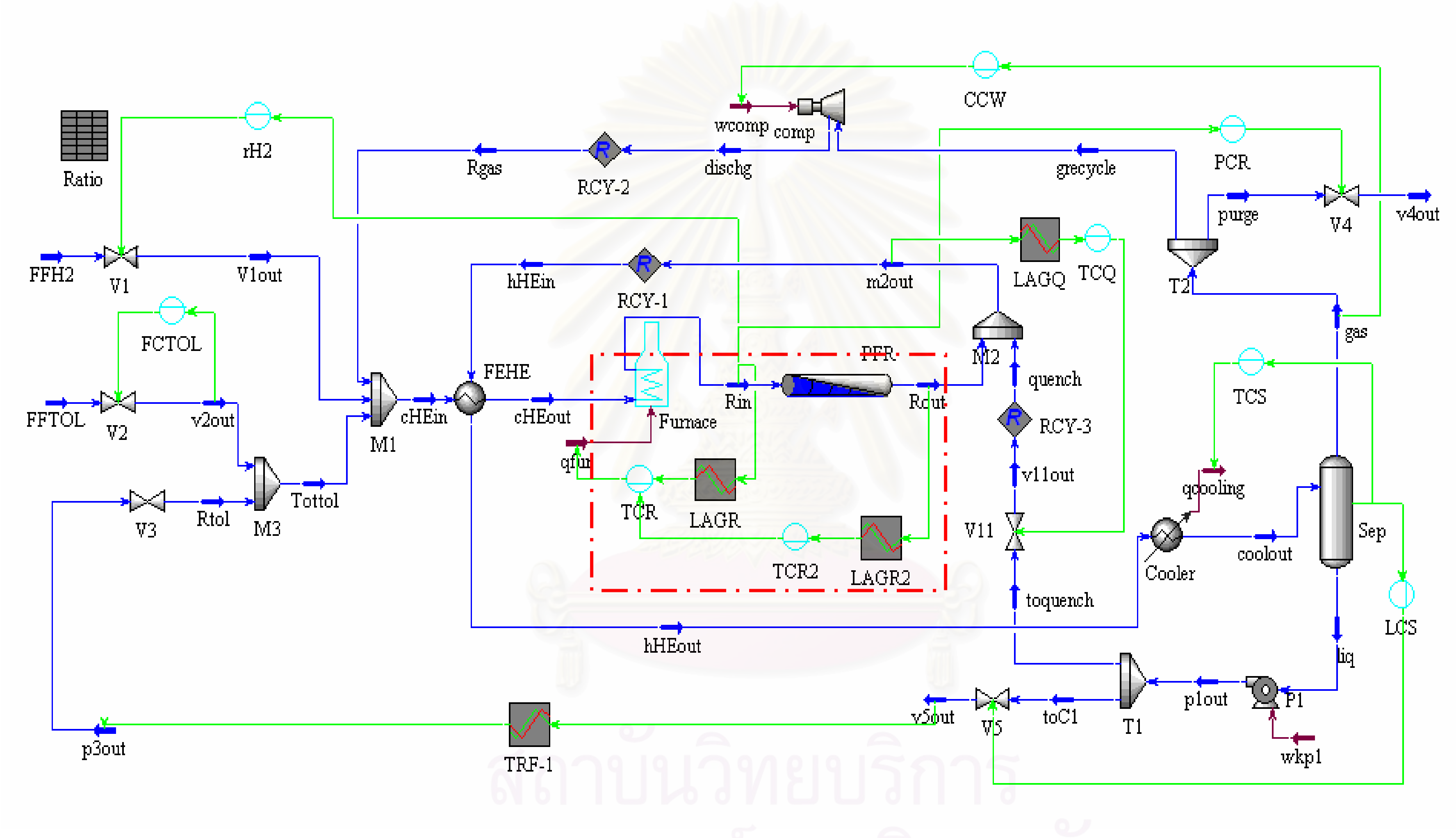


Figure 4.7 The Flowsheet of Simulation Hydrodealkylation (HDA) process of Designed Control Structure3 (CS3)

4.6 Dynamic Simulation Results

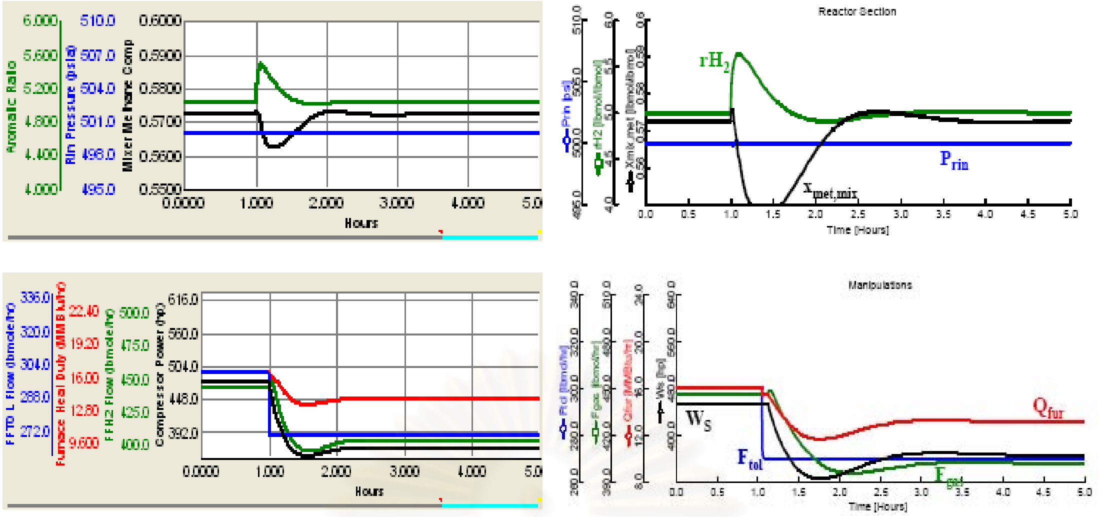
In order to illustrate the dynamic behaviors of the new control structures in reaction section of HDA process several disturbance loads were made. These three control structures were compared with reference on the paper submitted for publication in Industrial Engineering Chemistry Research by Skogestad and Antonio (2006), the result of performances and loss of our structures and Skogestad’s structures were shown in Figures 4.8 to 4.11. Results of performances and loss of our structures and Skogestad’s structures are as follows:

4.6.1 Comparison Dynamic Responses between This Works with Reference

Skogestad and Antonio (2006) designed 1 control structure by using a basic idea of self-optimizing control and a branch and bound algorithm for maximizing the singular value to select the candidate controlled variables.

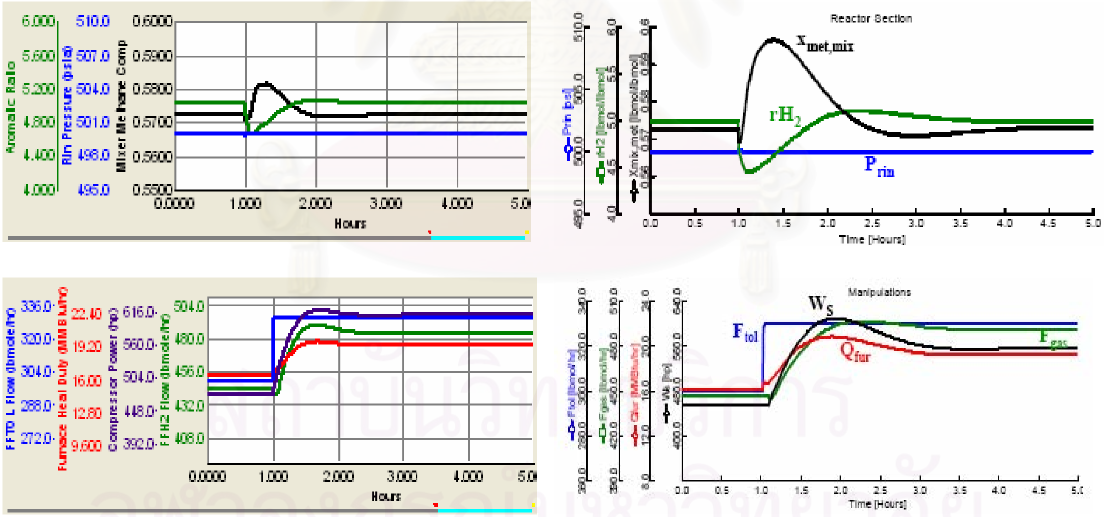
The disturbance testing is used to compare the dynamic response of this simulation (HYSYS) with Skogestad and Antonio (2006; Aspen plus). By step change in fresh toluene feed rate from 300 lbmole/hr to 270 lbmole/hr (decrease 10%) and from 300 lbmole/hr to 330 lbmole/hr (increase 10%), step change in fresh gas feed rate methane mole fraction from 0.03 to 0.08 (increase 0.05) and quench outlet temperature from 1150 oF to 1170 oF (increase 20 oF).

The dynamic response of simulation control structure in this work similar as in Skogestad’s paper. The considered variables in the first row are hydrogen-to-aromatic ratio, reactor pressure and methane mole fraction at mixer outlet. In the second row shows response of fresh feed toluene flow rate, fresh gas feed flow rate, furnace heat duty and compressor power.



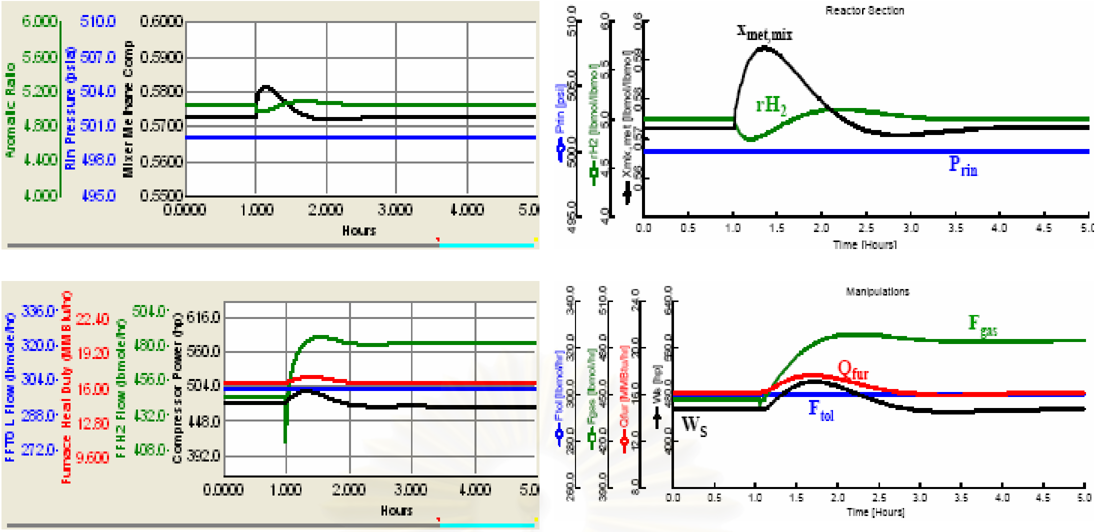
(A) (B)

Figure 4.8 Comparison dynamic responses of step change in fresh toluene feed rate from 300 lbmole/hr to 270 lbmole/hr (decrease 10%) between: (A) this work, (B) Skogestad (2006).



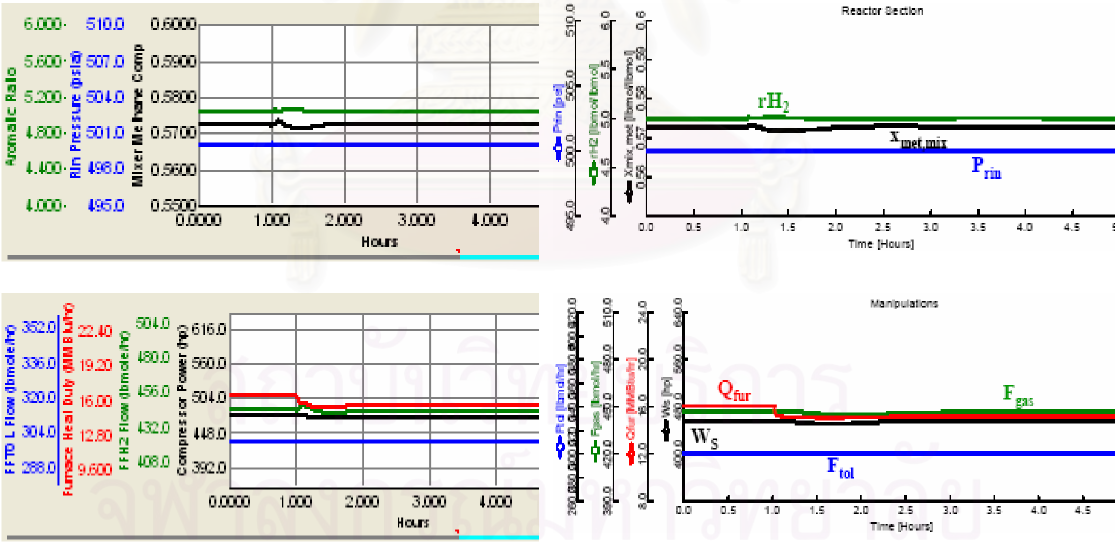
(A) (B)

Figure 4.9 Comparison dynamic responses of step change in fresh toluene feed rate from 300 lbmole/hr to 330 lbmole/hr (increase 10%) between: (A) this work, (B) Skogestad (2006).



(A) (B)

Figure 4.10 Comparison dynamic responses of step change in fresh gas feed rate methane mole fraction from 0.03 to 0.08 (increase 0.05) between: (A) this work, (B) Skogestad (2006).



(A) (B)

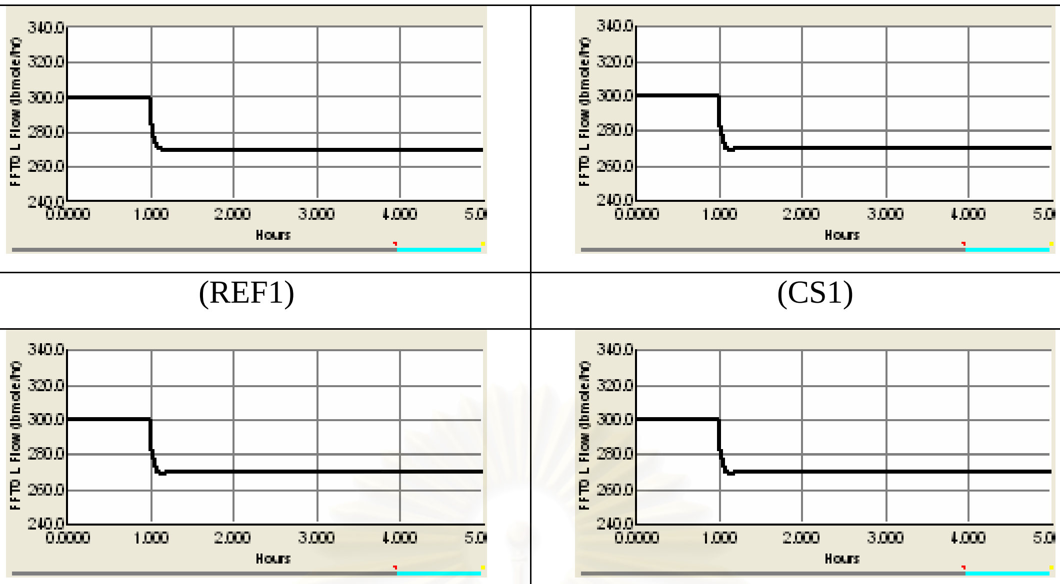
Figure 4.11 Comparison dynamic responses of step change in quench outlet temperature from 1150 oF to 1170 oF (increase 20 oF) between: (A) this work, (B) Skogestad (2006).

4.6.2 Decrease in the Fresh Toluene Feed Flowrate for Reference Control Structure (REF1) and Our Control Structure (CS1, CS2, and CS3)

Figure 4.12 shows the dynamic responses of the reaction section of the HDA process to a disturbance in the fresh toluene feed flowrates from 300 to 270 lbmole/h at time equals 1hours.

The dynamic response of each control structure when change in the fresh toluene feed flowrates for the reaction section of the HDA process were shown below. Figure4.12 when fresh toluene feed flowrate decrease (Figure4.12 (A)) fresh gas feed flowrate quickly decrease also (Figure4.12 (B)). Figure 4.12 gives simulation result for decreasing the fresh toluene feed. The reactor inlet temperature response and reactor outlet temperature are small oscillatory and it comes to new point within 2 hours. Effect from the fresh toluene feed decrease the reactor inlet temperature, the reactor outlet temperature, separator temperature and quench outlet temperature decrease because decrease fresh toluene feed flowrate affect to the production rate. The separator temperature, quench outlet temperature and reactor pressure are slightly decreased and return as before (Figure4.12 (C-H)). The furnace heat duty, cooler heat duty and compressor power quickly decrease also (Figure4.12 (I-K)).

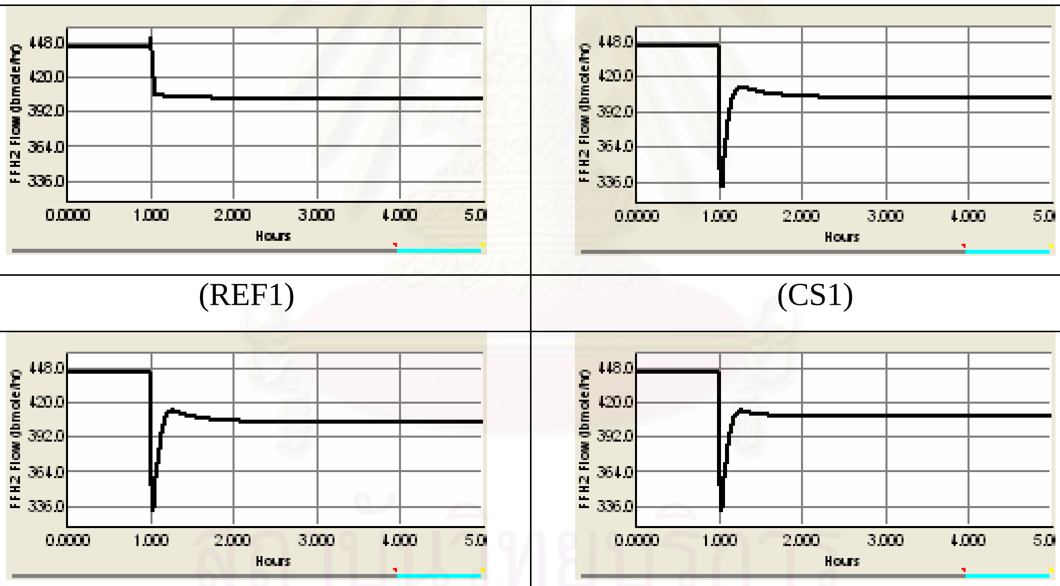
In CS1, CS2 and CS3 when decrease fresh toluene feed, this step change affects to the fresh gas feed flowrate, when toluene decrease affects to ratio of hydrogen to aromatic increase so that fresh gas feed flowrate decrease immediately and return to new point(Figure4.12(B)). The reactor inlet temperature and reactor outlet temperature in control structure 1(CS1) and CS2 are small oscillatory and slowly decrease (Figure4.12(C, D)). In the control structure 3, the reactor inlet and outlet temperature are so small oscillatory and return to old setpoint because this structure control the reactor inlet temperature with setpoint from reactor outlet temperature. Figure 4.12 (E-H) show the reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quench outlet temperature. They dynamic responses so slightly swing and come to setpoint within 30 minutes. Figure 4.12 (I-K) shows the furnace heat duty, cooler heat duty and compressor power. They dynamic responses slowly decrease because of slowly decreasing in reactor temperature.



(REF1) (CS1)

(CS2) (CS3)

(A)

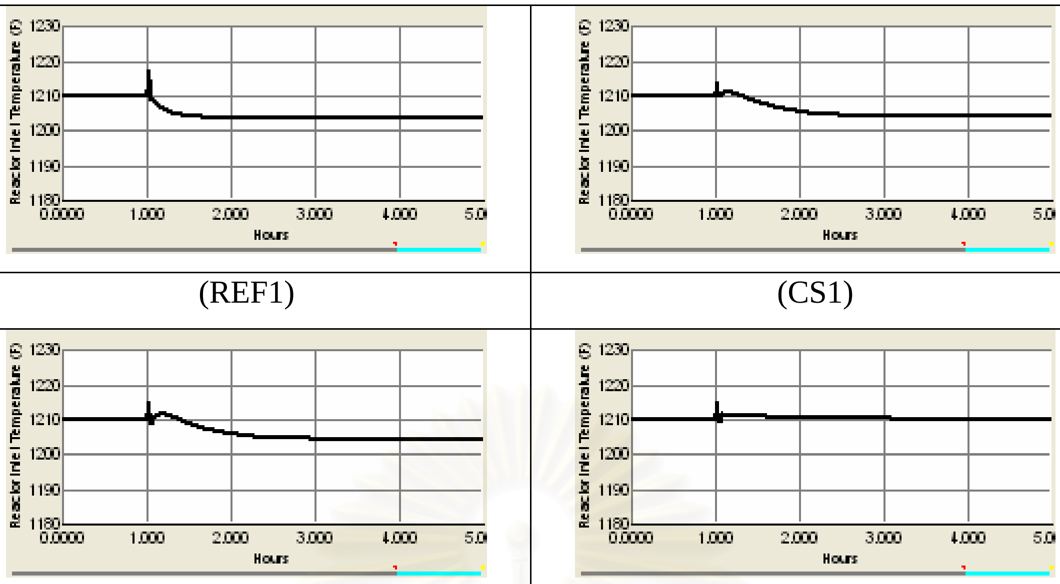


(REF1) (CS1)

(CS2) (CS3)

(B)

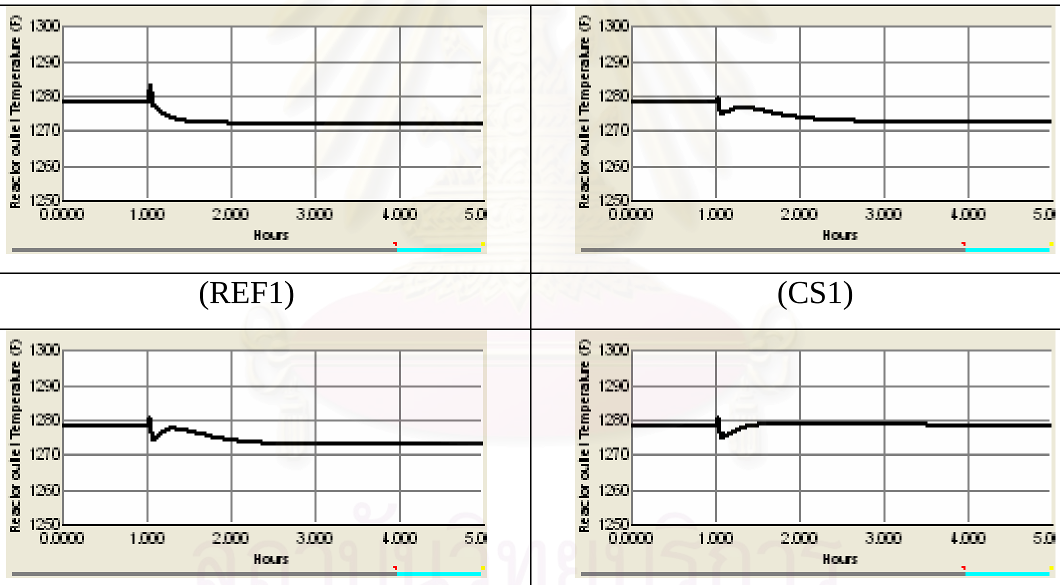
Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(C)

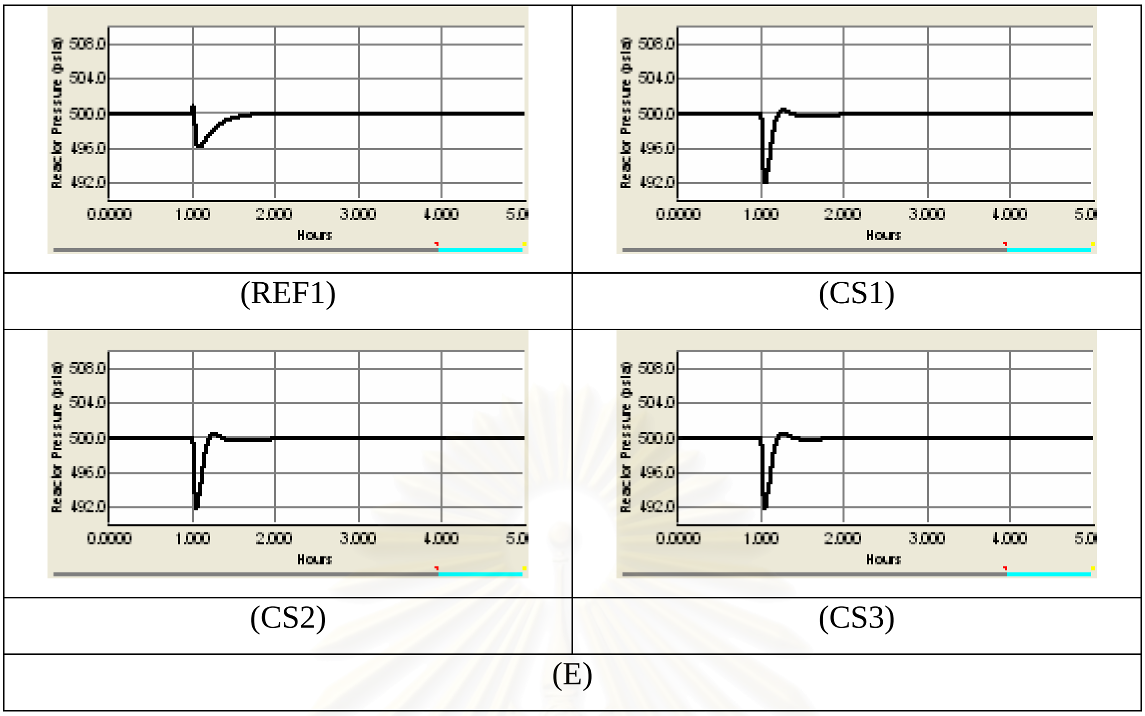


(REF1) (CS1)

(CS2) (CS3)

(D)

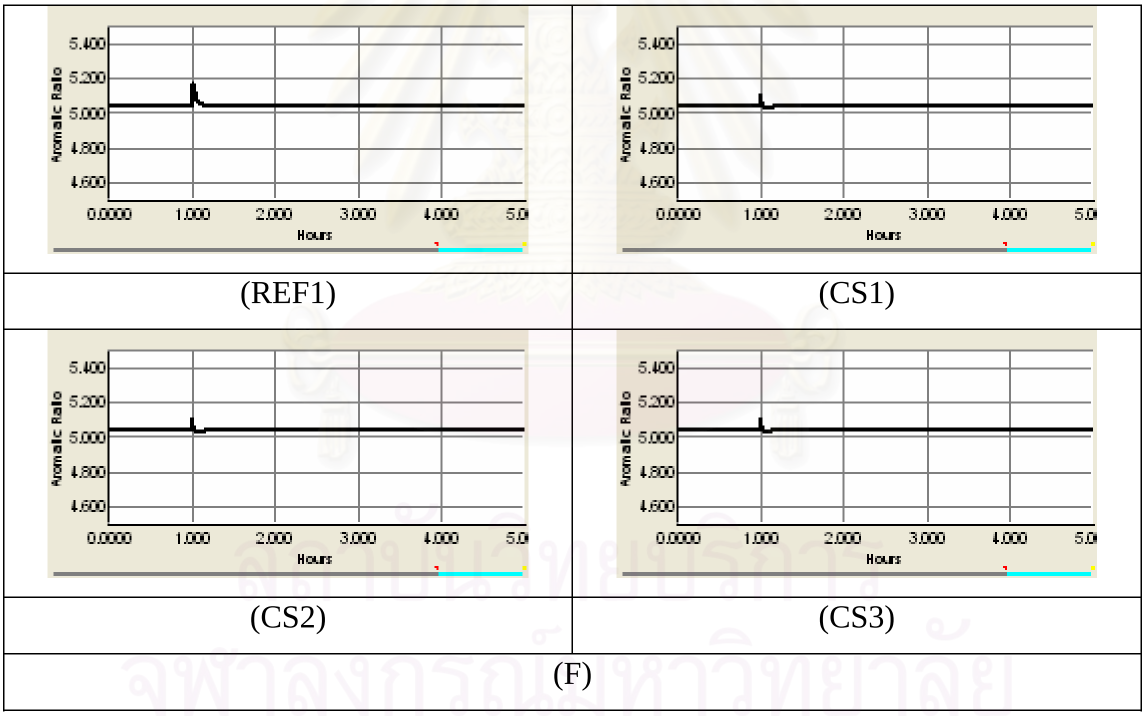
Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(E)

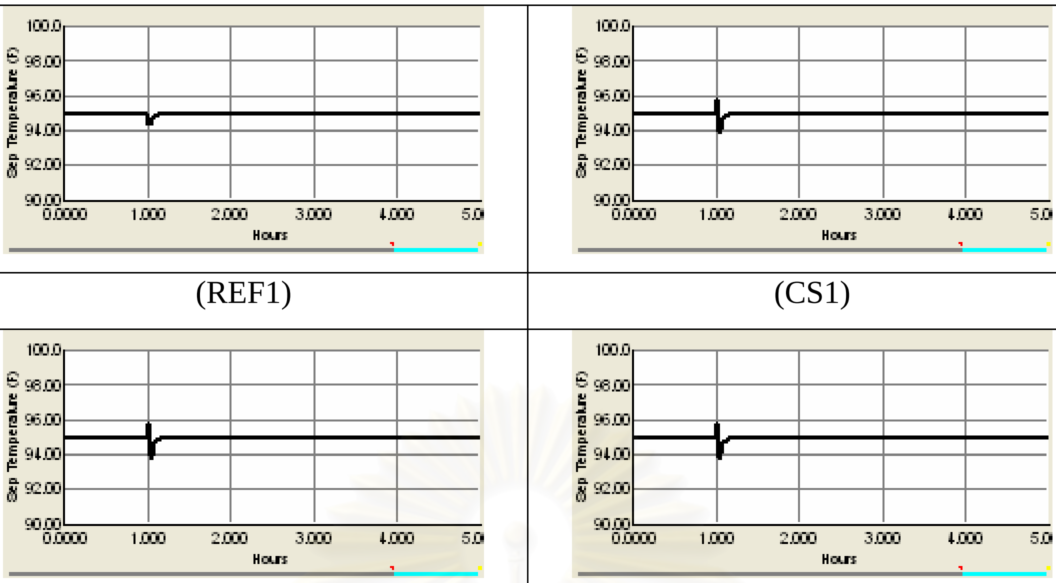


(REF1) (CS1)

(CS2) (CS3)

(F)

Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



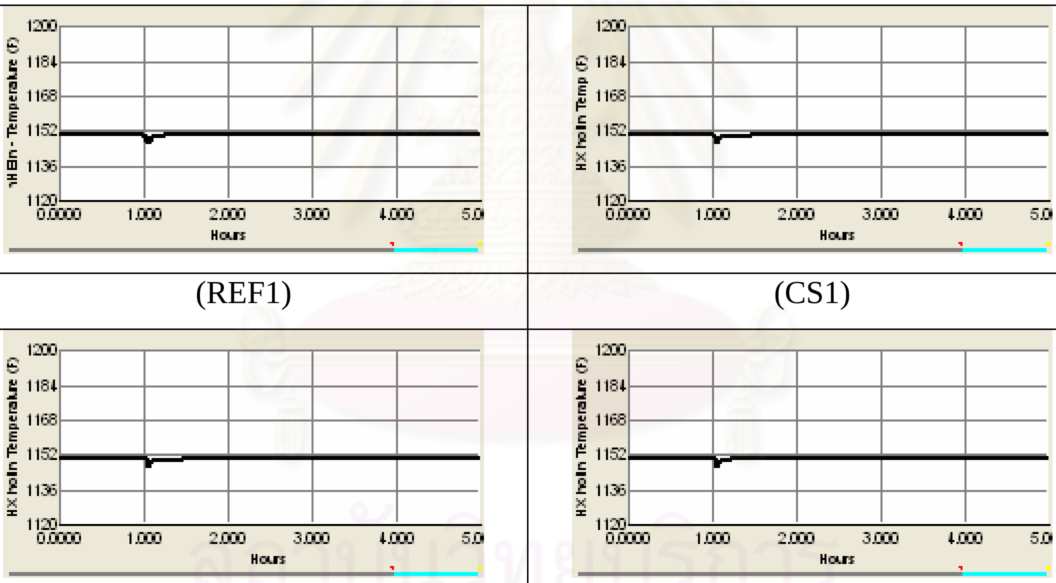
(REF1)

(CS1)

(CS2)

(CS3)

(G)



(REF1)

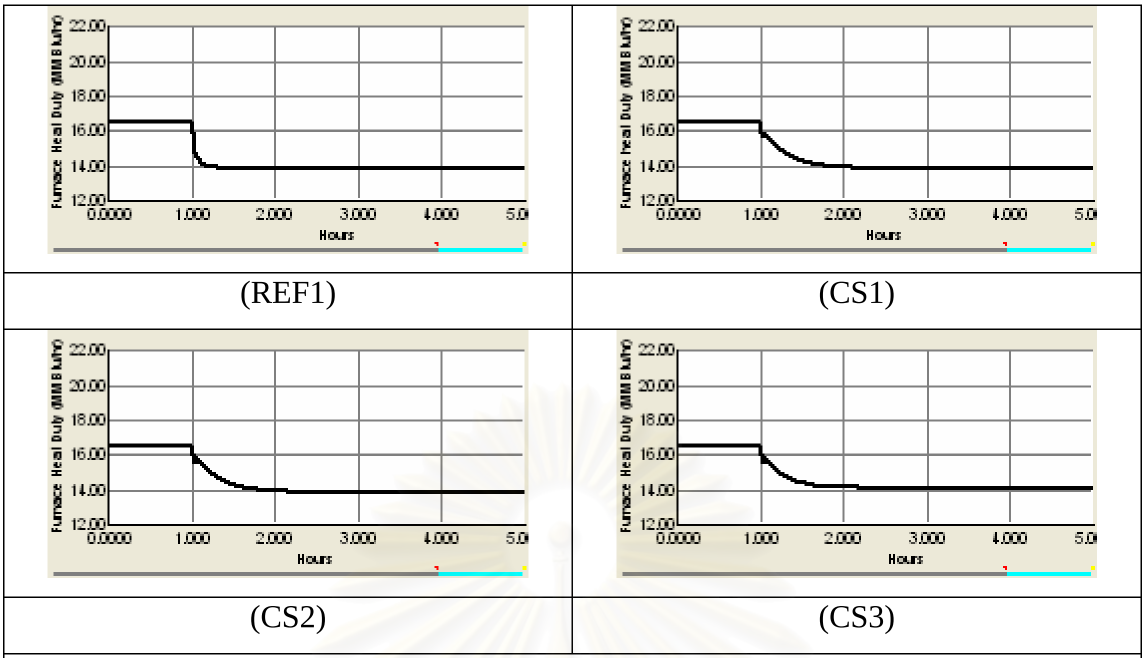
(CS1)

(CS2)

(CS3)

(H)

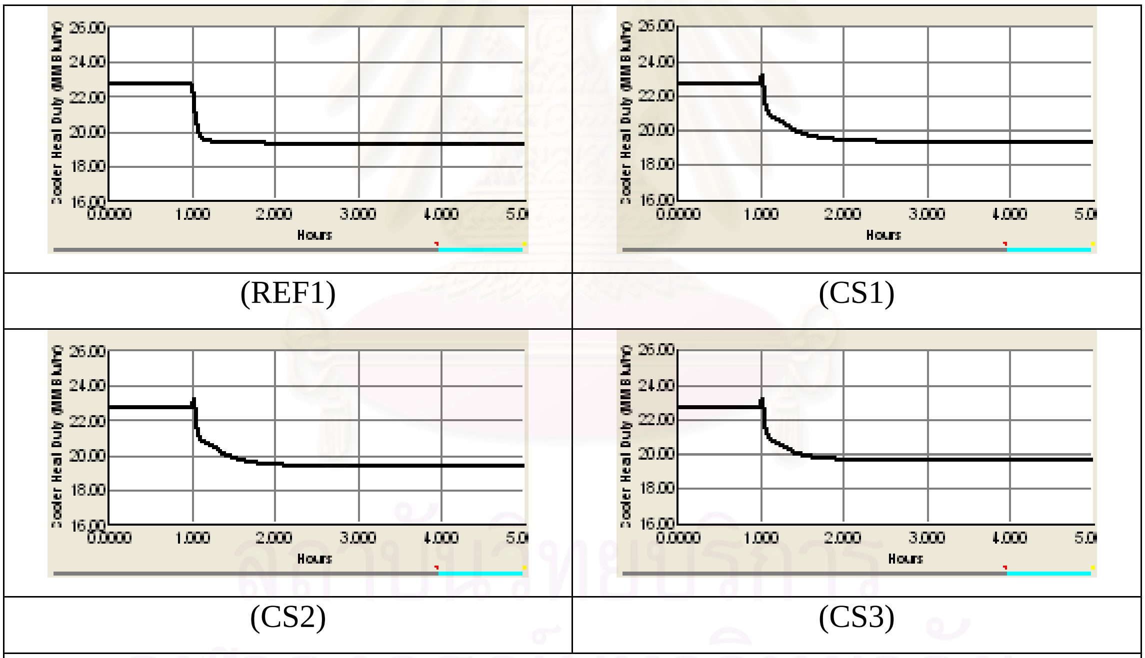
Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(I)

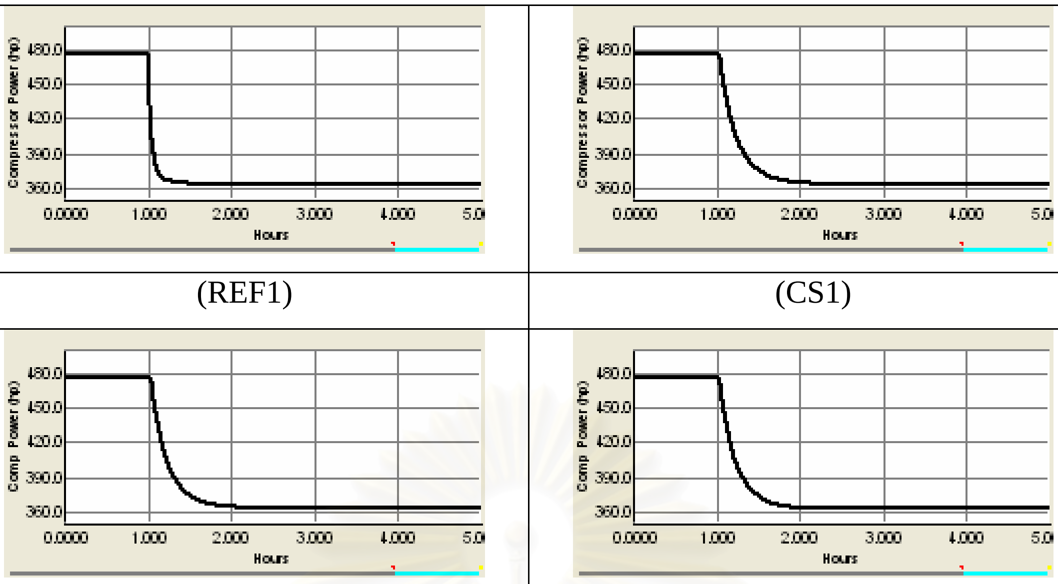


(REF1) (CS1)

(CS2) (CS3)

(J)

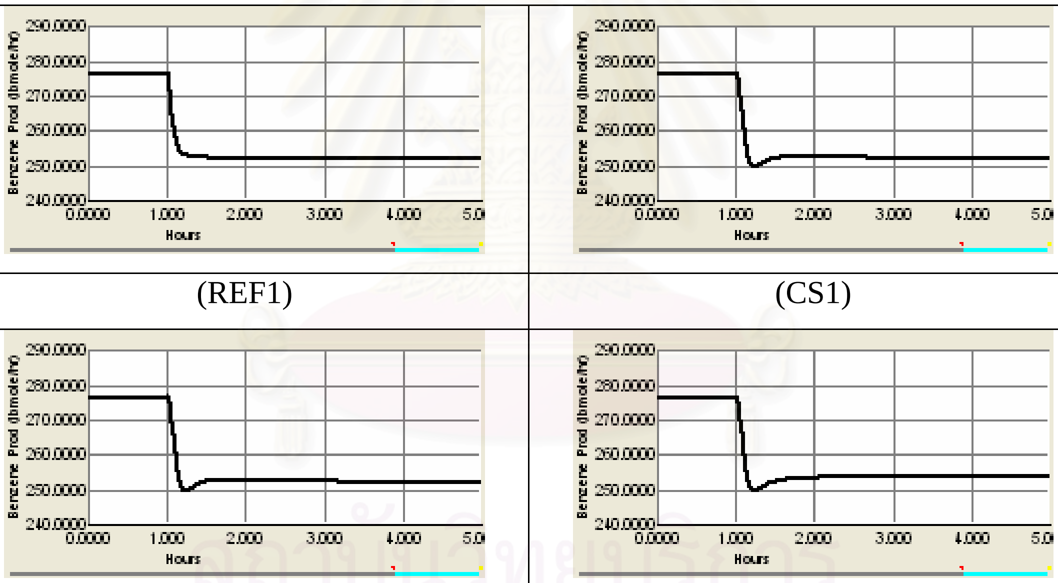
Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(K)



(REF1) (CS1)

(CS2) (CS3)

(L)

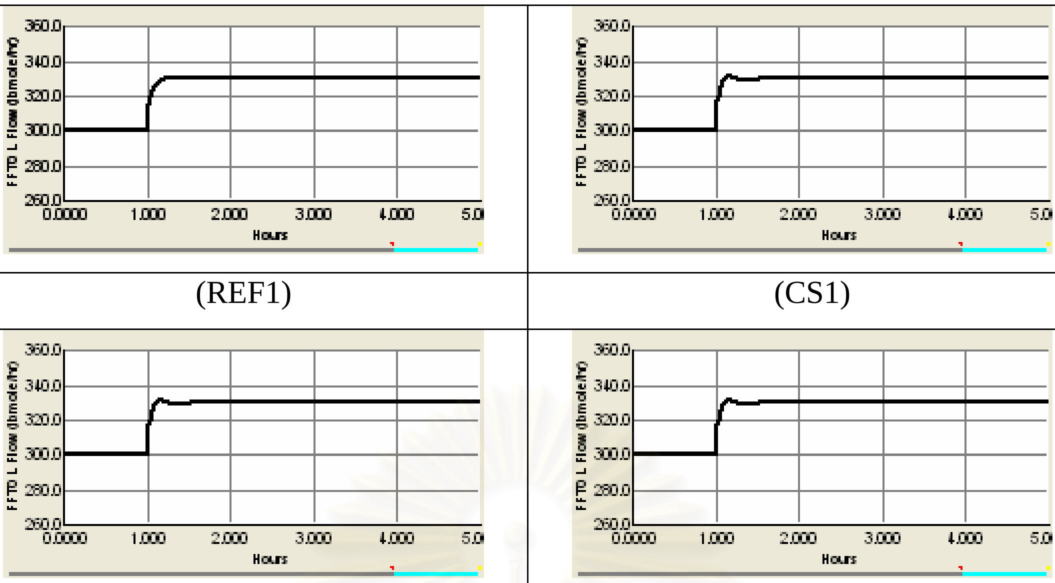
Figure 4.12 Dynamic responses of decrease 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.

4.6.3 Increase in the Fresh Toluene Feed Flowrates for Reference Control Structure (REF1) and Our Control Structure (CS1, CS2, and CS3)

Figure 4.13 shows the dynamic responses of the reaction section of the HDA process to a disturbance in the fresh toluene feed flowrates from 300 to 330 lbmole/h at time equals 1hours.

Figure4.13 (A) when fresh toluene feed flowrate increase fresh gas feed flowrate quickly increase also (Figure4.13 (B)). The reactor inlet temperature response and reactor outlet temperature are oscillatory and they come to new point within 2 hours. Effect from the fresh toluene feed increase the reactor inlet temperature, the reactor outlet temperature, separator temperature and quench outlet temperature increase because increase fresh toluene feed flowrate affect to the production rate. The separator temperature, quench outlet temperature and reactor pressure are slightly increased and return as before (Figure4.13 (C-H)). The furnace heat duty, cooler heat duty and compressor power quickly increase also (Figure4.13 (I-K)). Figure4.13 (L) the benzene production rate increase also because of increasing in toluene feed flowrate.

This step change affects to the fresh gas feed flowrate of CS1, CS2 and CS3, when toluene increase affects to ratio of hydrogen to aromatic decrease so that fresh gas feed flowrate increase immediately and return to new point(Figure4.13(B)). The reactor inlet temperature and reactor outlet temperature in control structure 1(CS1) and CS2 are small oscillatory and slowly increase (Figure4.13(C, D)). In the control structure 3, the reactor inlet and outlet temperature are so small oscillatory and return to old setpoint because this structure control the reactor inlet temperature with setpoint from reactor outlet temperature. Figure 4.13 (E-H) shows the reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quench outlet temperature. They dynamic responses so slightly swing and come to setpoint immediately. Figure 4.13 (I-K) shows the furnace heat duty, cooler heat duty and compressor power. They dynamic responses slowly increase because of slowly increasing in reactor temperature. The benzene product increase also because of increasing in toluene feed rate Figure 4.13 (L).



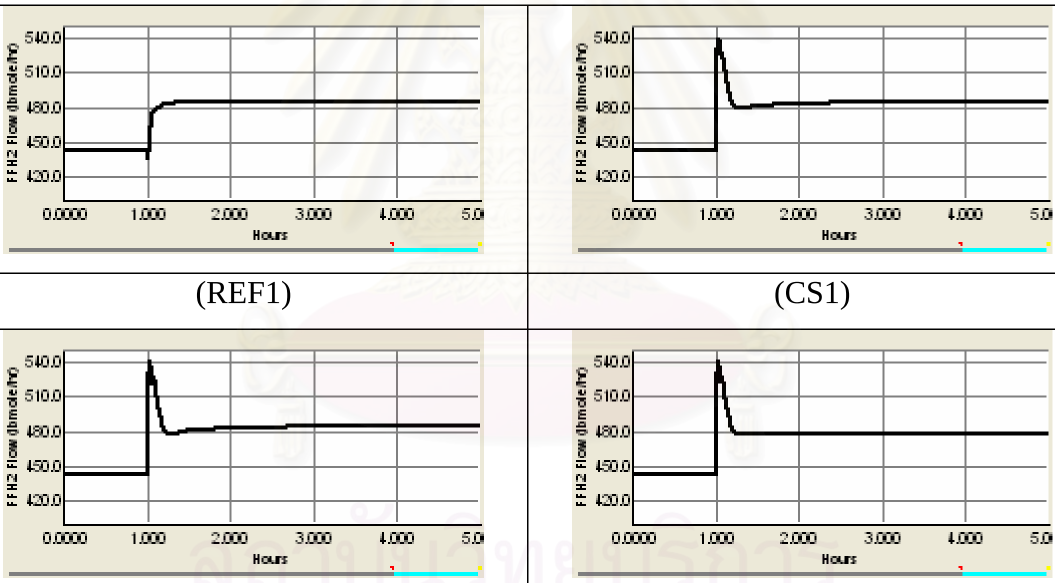
(REF1)

(CS1)

(CS2)

(CS3)

(A)



(REF1)

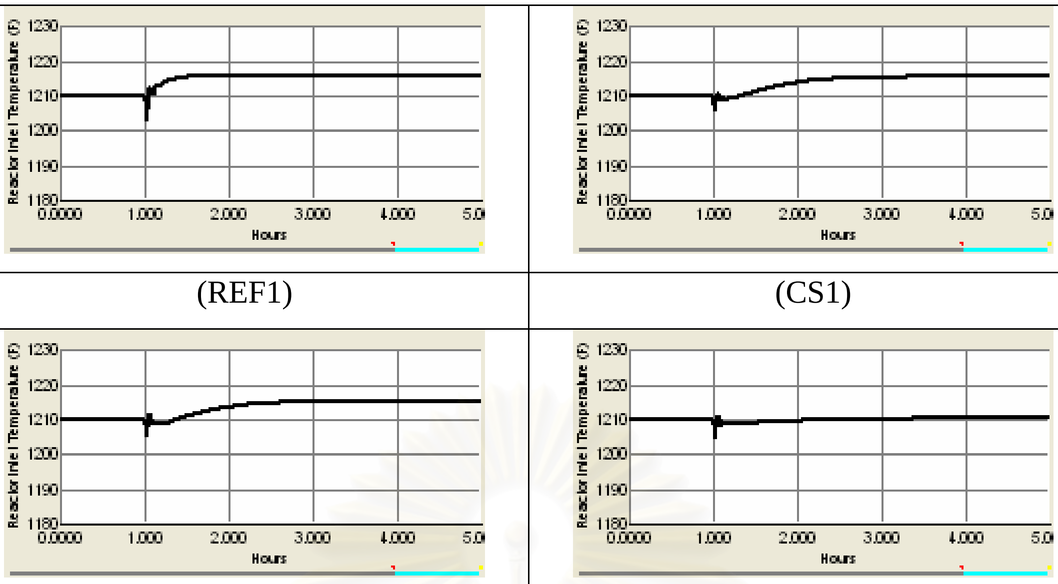
(CS1)

(CS2)

(CS3)

(B)

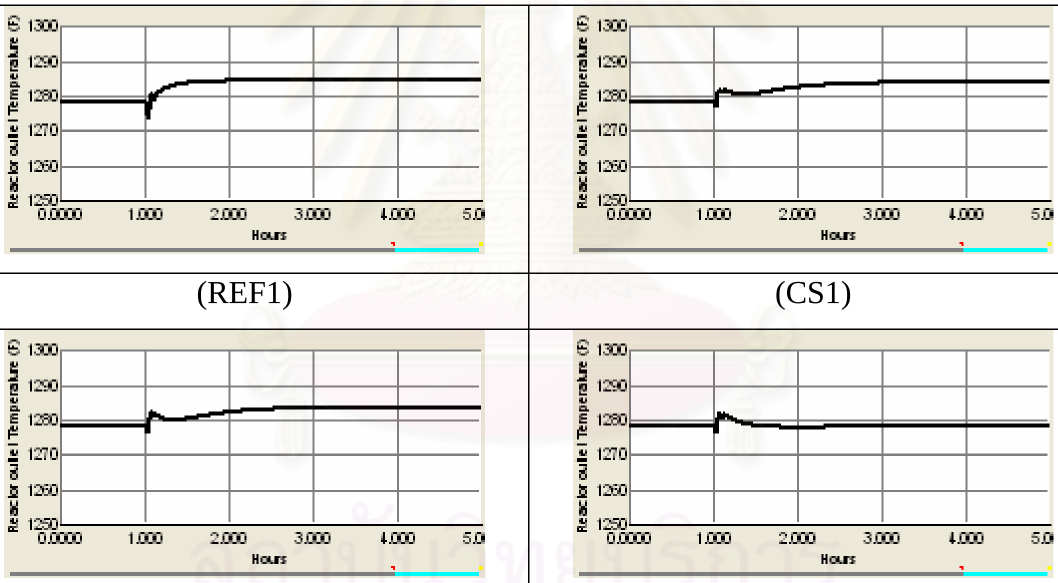
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates, (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(C)

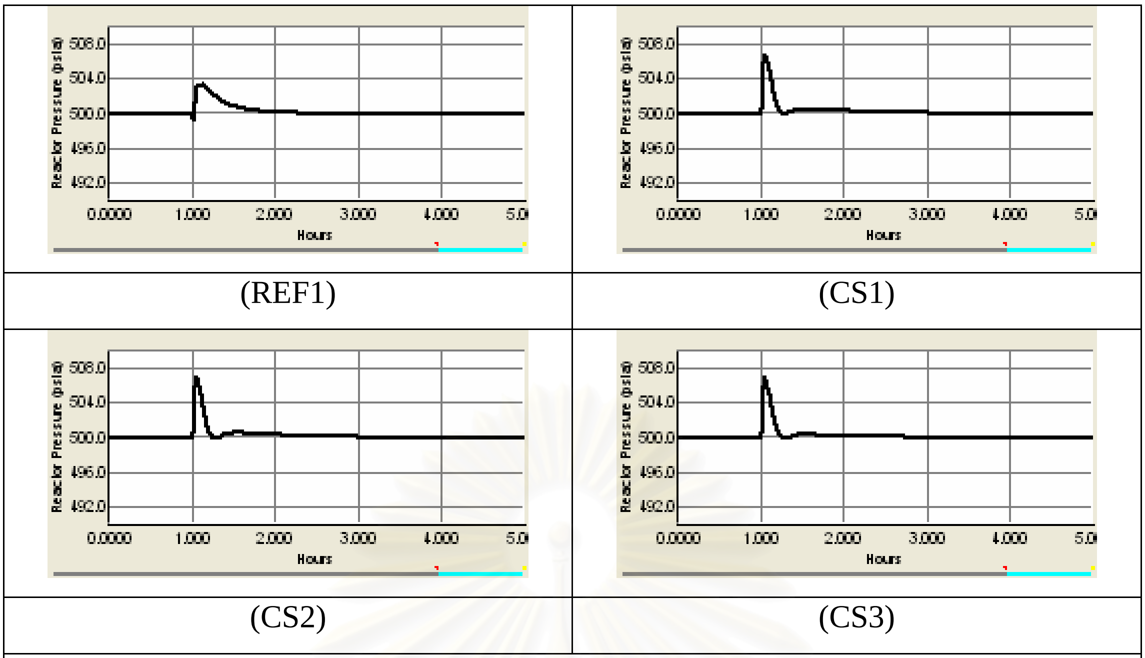


(REF1) (CS1)

(CS2) (CS3)

(D)

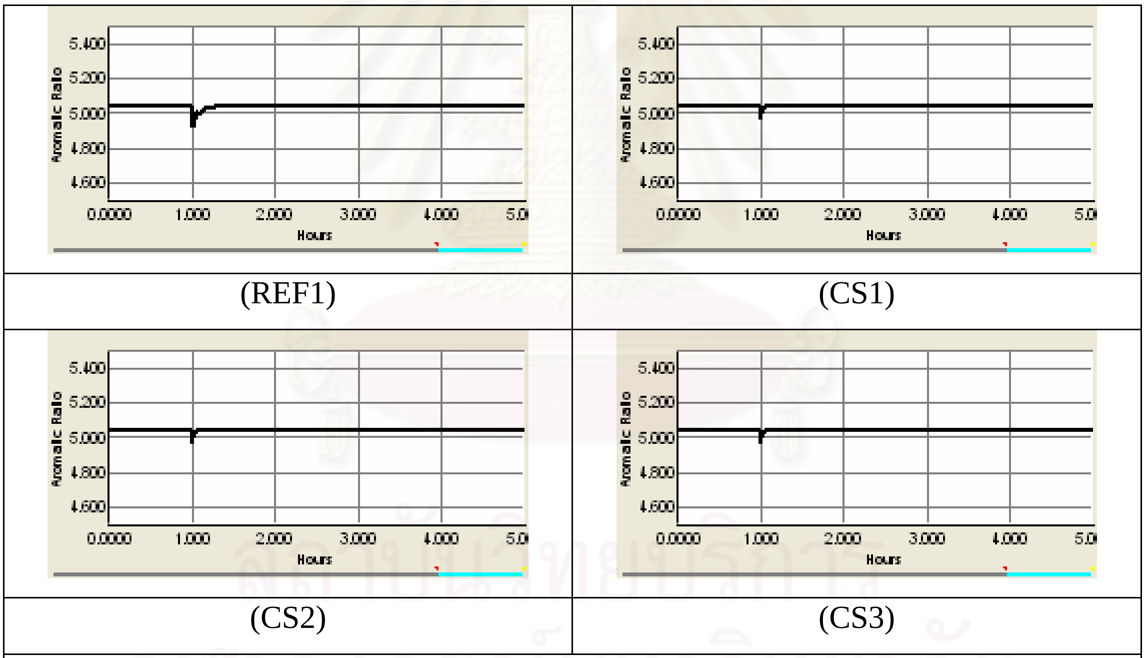
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(E)

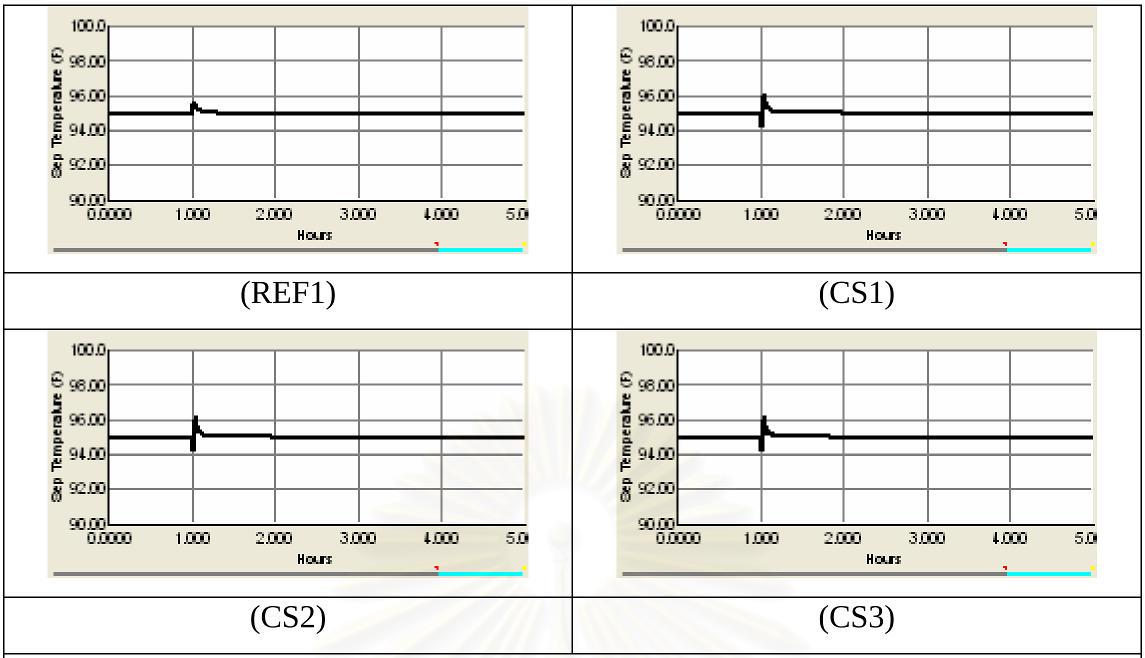


(REF1) (CS1)

(CS2) (CS3)

(F)

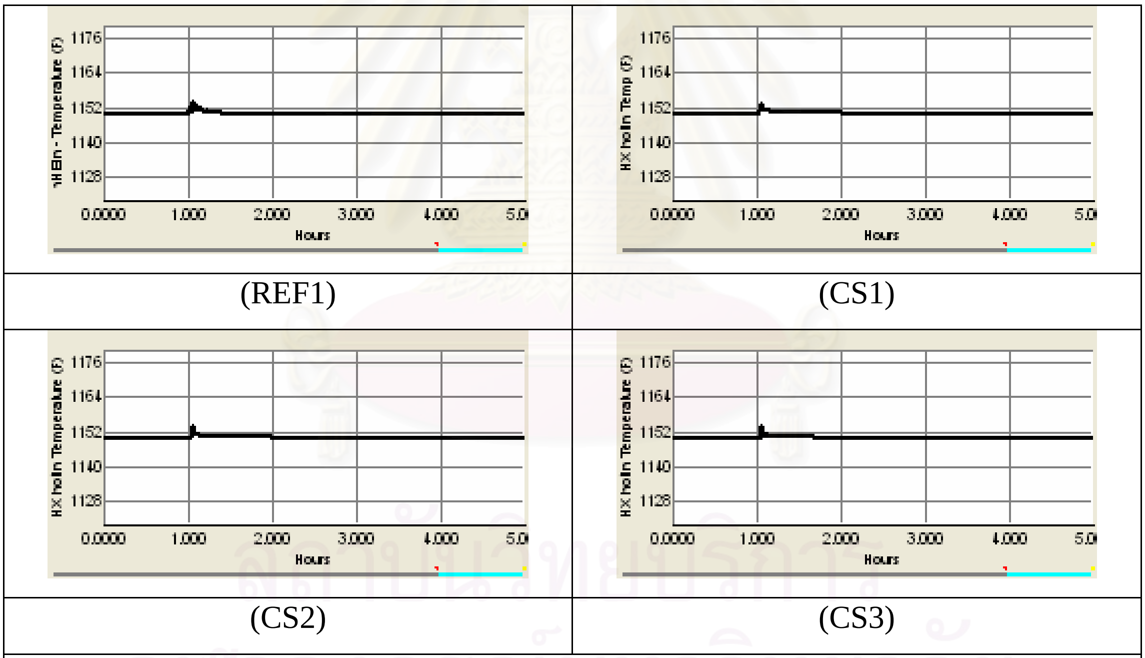
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(G)

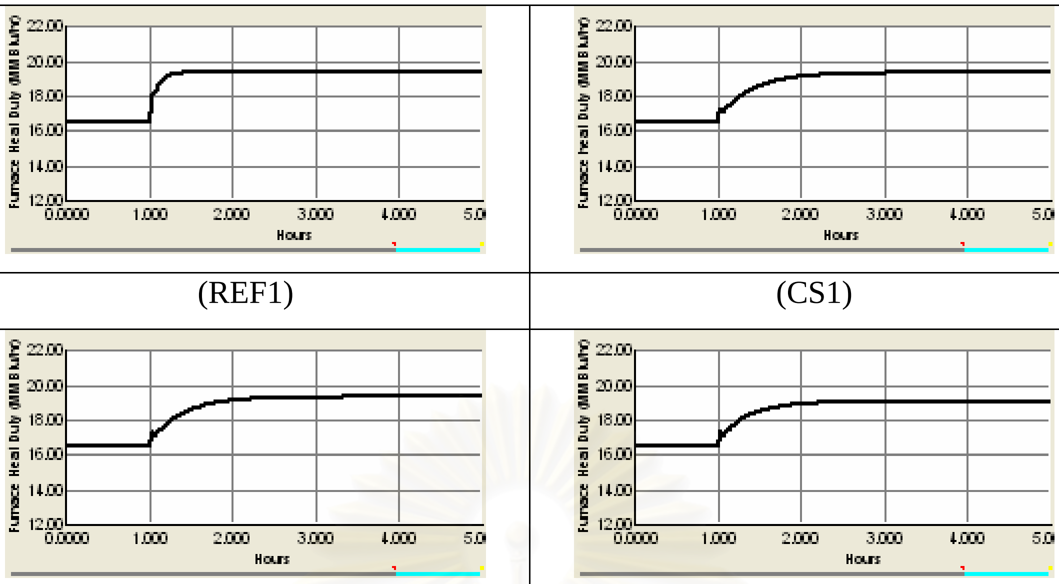


(REF1) (CS1)

(CS2) (CS3)

(H)

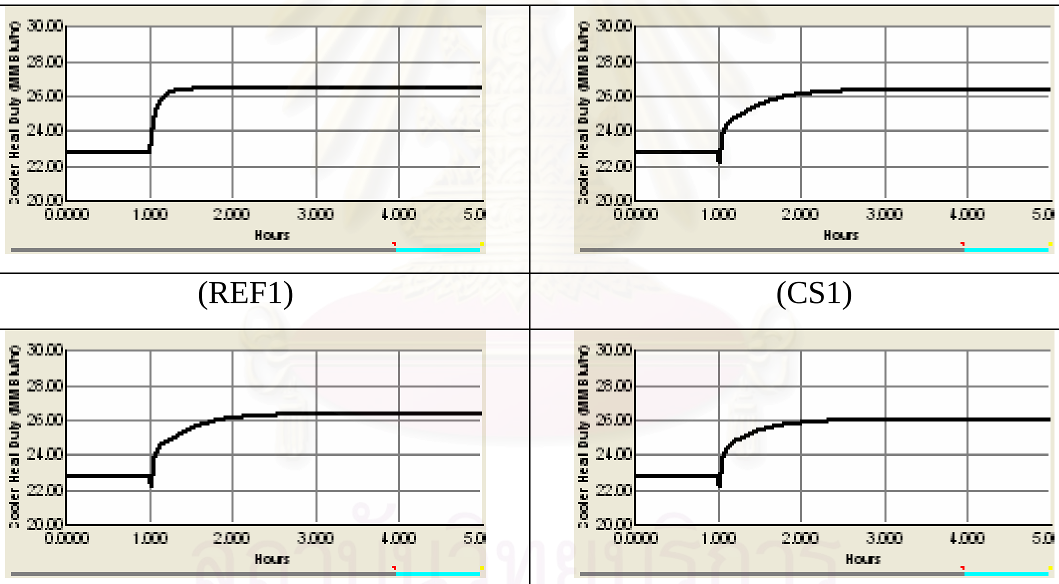
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(I)

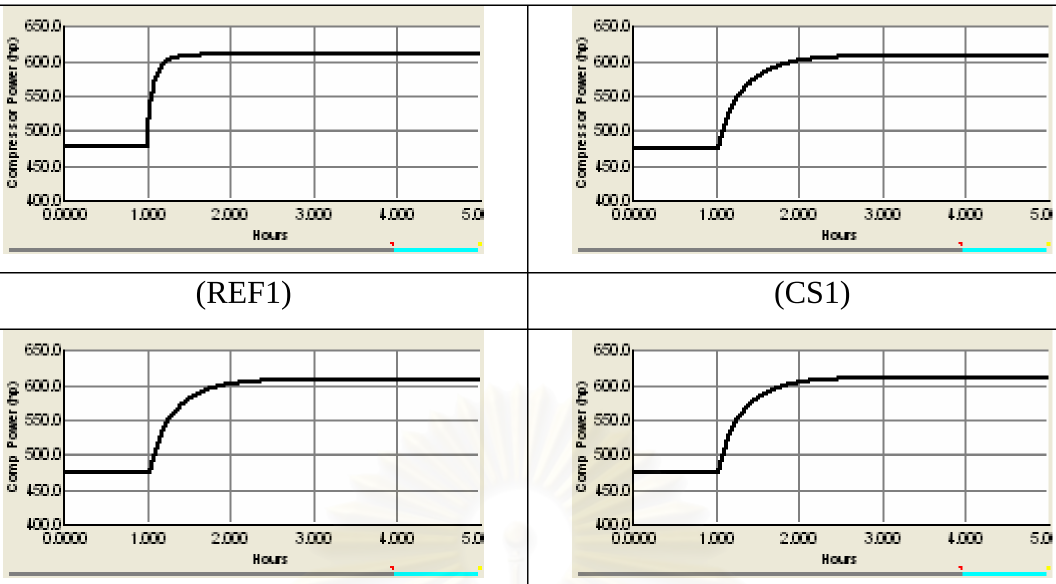


(REF1) (CS1)

(CS2) (CS3)

(J)

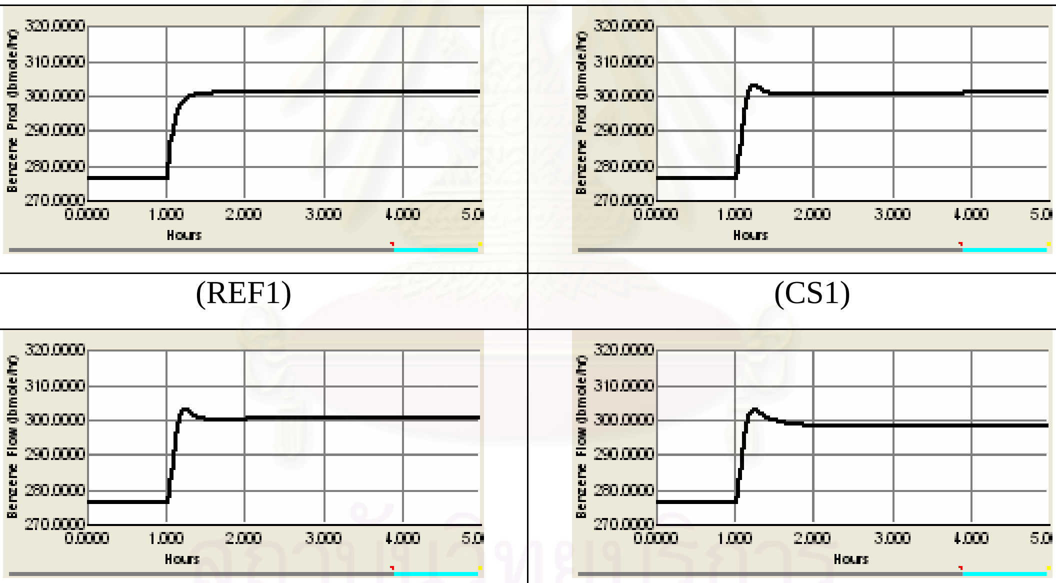
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(K)



(REF1) (CS1)

(CS2) (CS3)

(L)

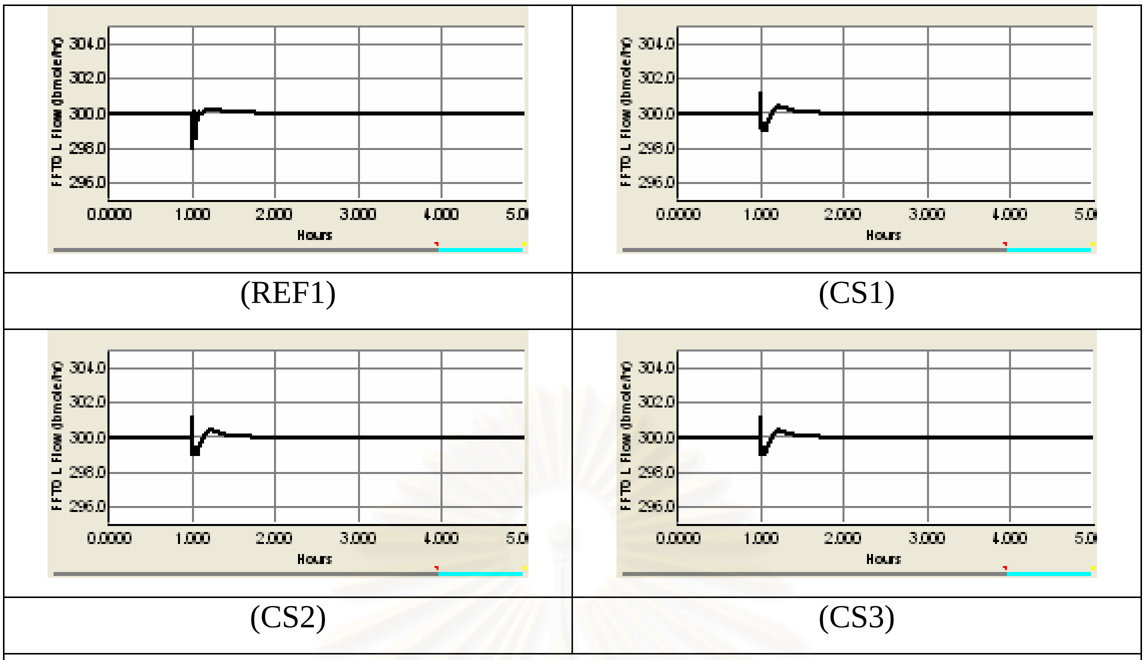
Figure 4.13 Dynamic responses of increase 10 % in fresh toluene feed rates from 300 lbmole/hr to 270 lbmole/hr for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.

4.6.4 Increase in the Fresh Gas Feed Rates Methane Mole Fraction for Reference Control Structure (REF1) and Our Control Structure (CS1, CS2, and CS3)

Figure 4.14 shows the dynamic responses of the reaction section of the HDA process to a disturbance in the fresh gas feed rates methane mole fraction from 0.03 to 0.08 at time equals 1hours.

Figure4.14 (A) the fresh feed toluene is oscillatory and retune to its setpoint. The fresh gas feed rate decrease and increase immediately and come to new point because increasing in methane mole fraction direct affect to fresh feed hydrogen in the reference control structure (Figure4.14 (B)). The increasing in methane mole fraction in fresh feed hydrogen affect to reactor inlet temperature, reactor outlet temperature, reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quench outlet temperature. They dynamic response small swing and return to their old setpoint (Figure4.14(C-H)). Figure4.14 (I-J) show dynamic response of furnace heat duty and cooler heat duty. The response of furnace heat duty and cooler heat duty small oscillate but compressor power decrease immediately and oscillate because of increasing in methane mole fraction (Figure4.14K).

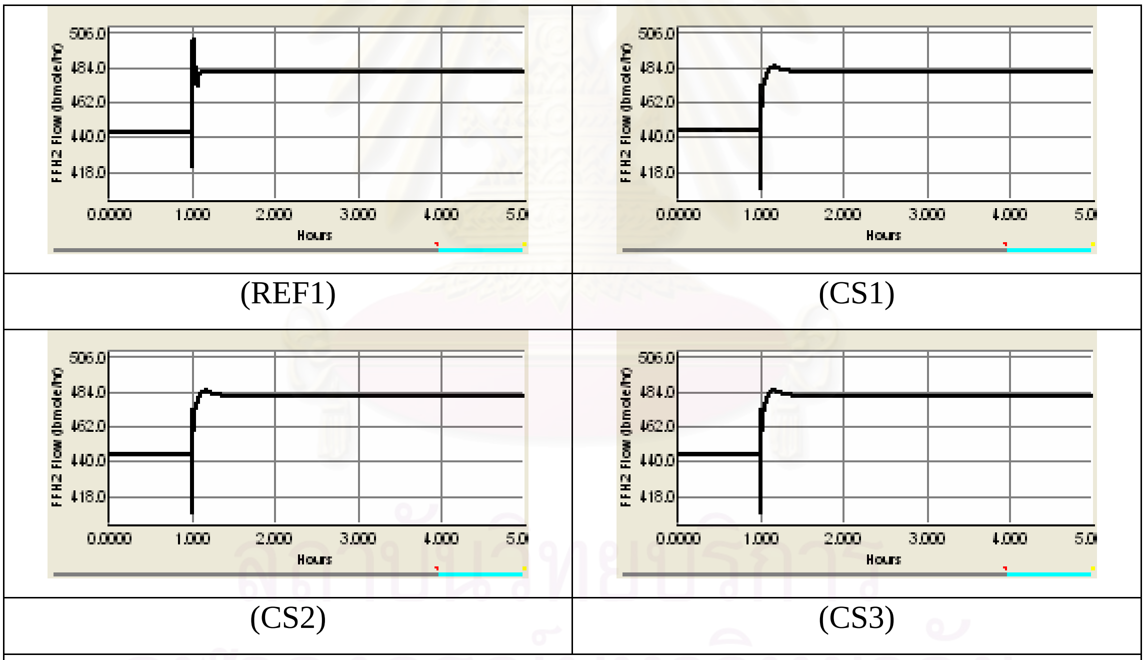
For CS1, CS2 and CS3 the fresh feed toluene (Figure4.14 (A)) is slowing oscillatory and retune to its setpoint. The fresh gas feed rate decrease immediately and increase comes to new point (Figure4.14 (B)). The increasing in methane mole fraction in fresh feed hydrogen has small affect to reactor inlet temperature, reactor outlet temperature, reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quenches outlet temperature. Their dynamic response swing rarely and return to their old setpoint (Figure4.14(C-H)). The furnace heat duty and cooler heat duty are rarely oscillatory but the compressor power slow decrease to new point because of increasing in methane mole fraction (Figure4.14 (I-K)).



(REF1) (CS1)

(CS2) (CS3)

(A)

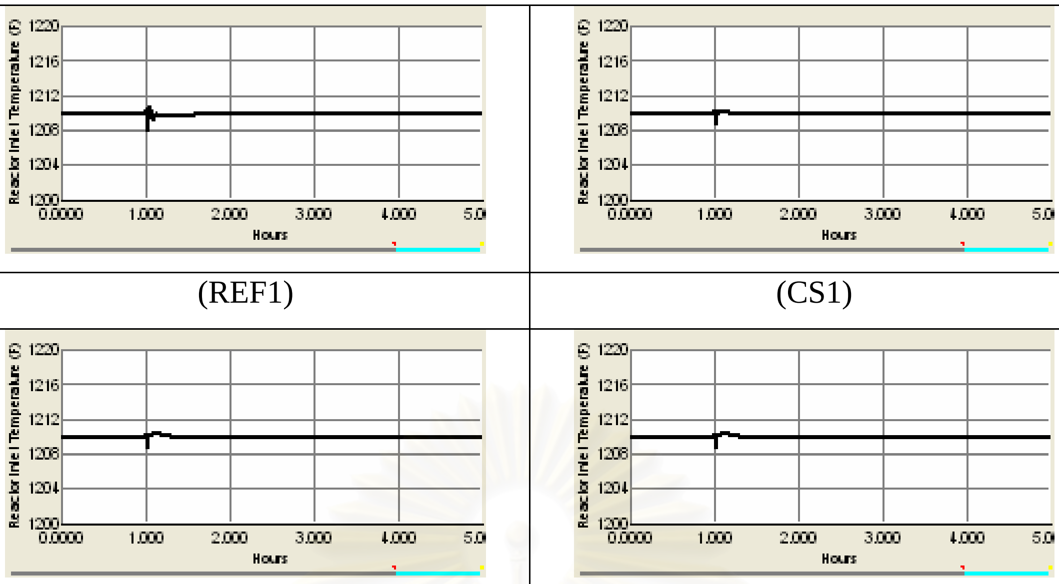


(REF1) (CS1)

(CS2) (CS3)

(B)

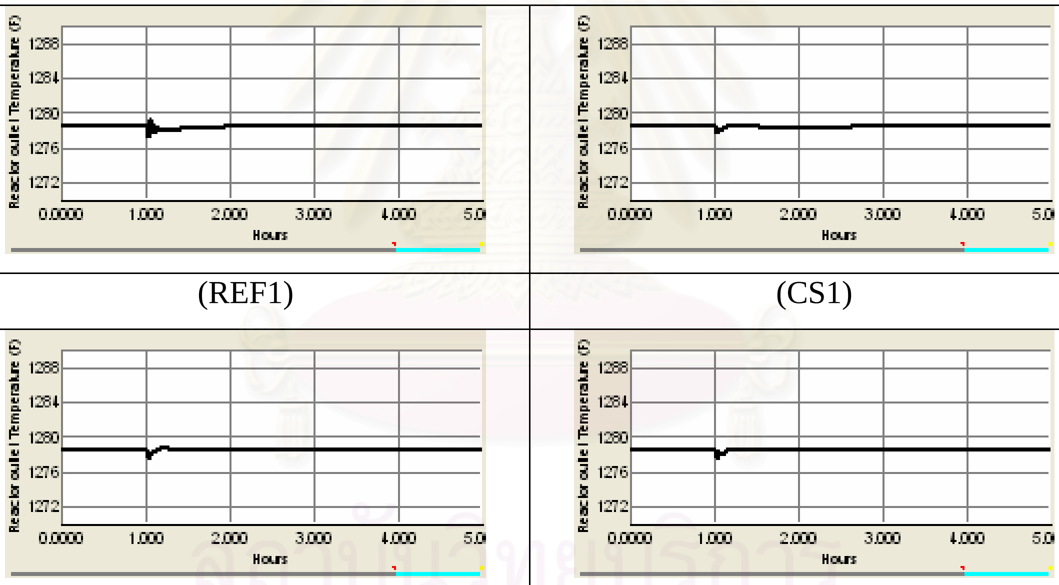
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(C)

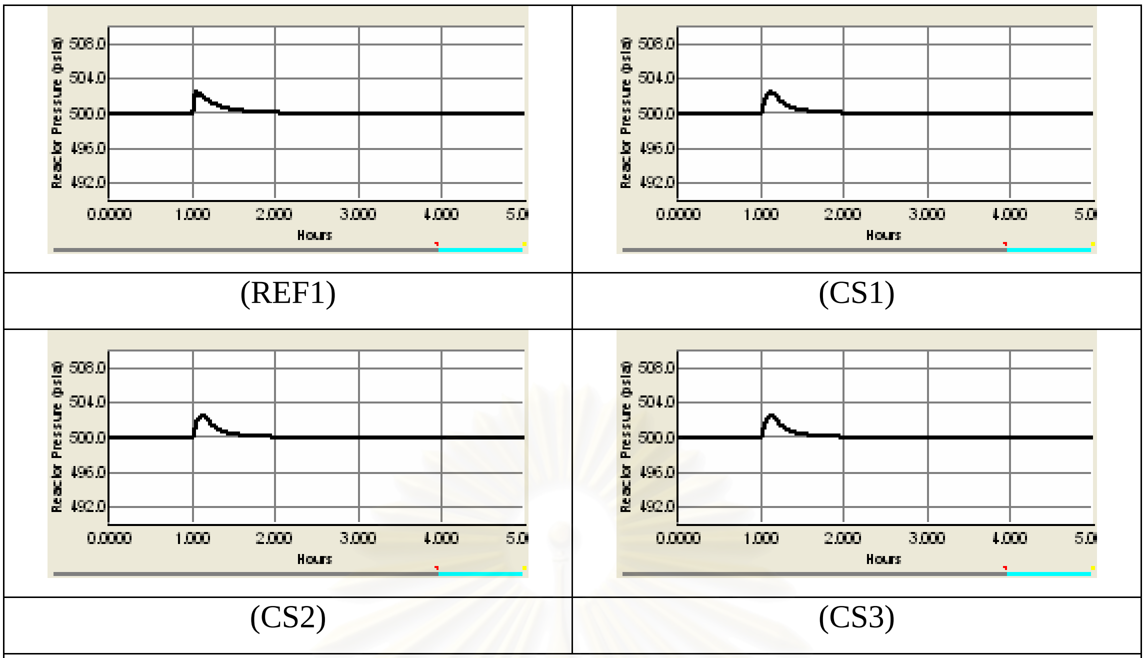


(REF1) (CS1)

(CS2) (CS3)

(D)

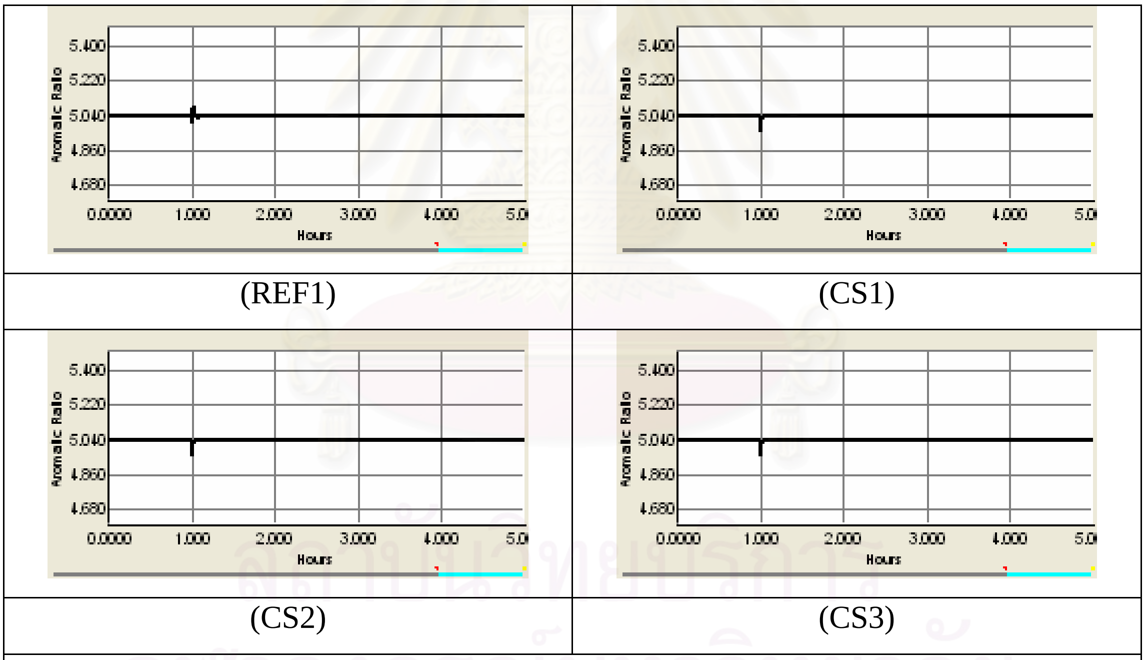
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(E)

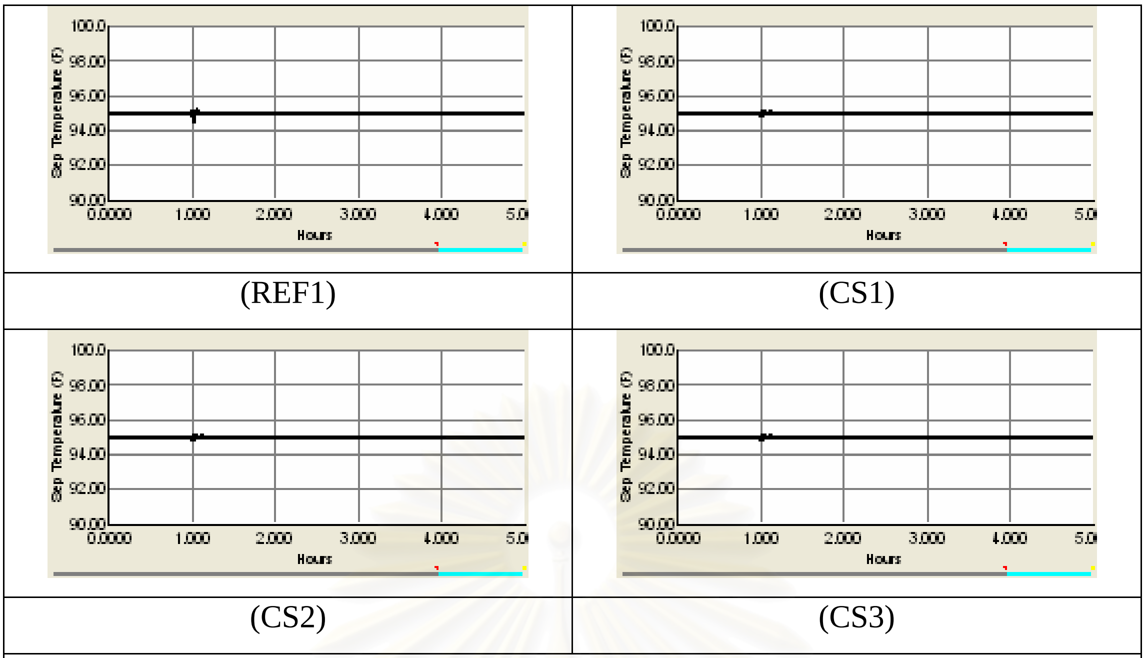


(REF1) (CS1)

(CS2) (CS3)

(F)

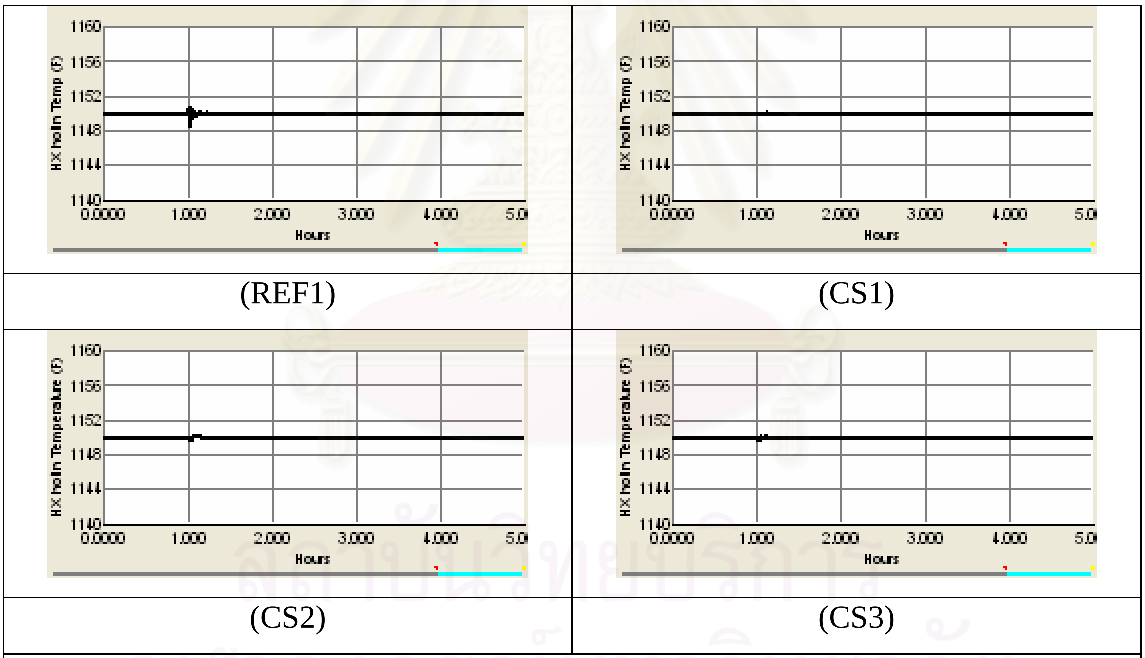
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(G)

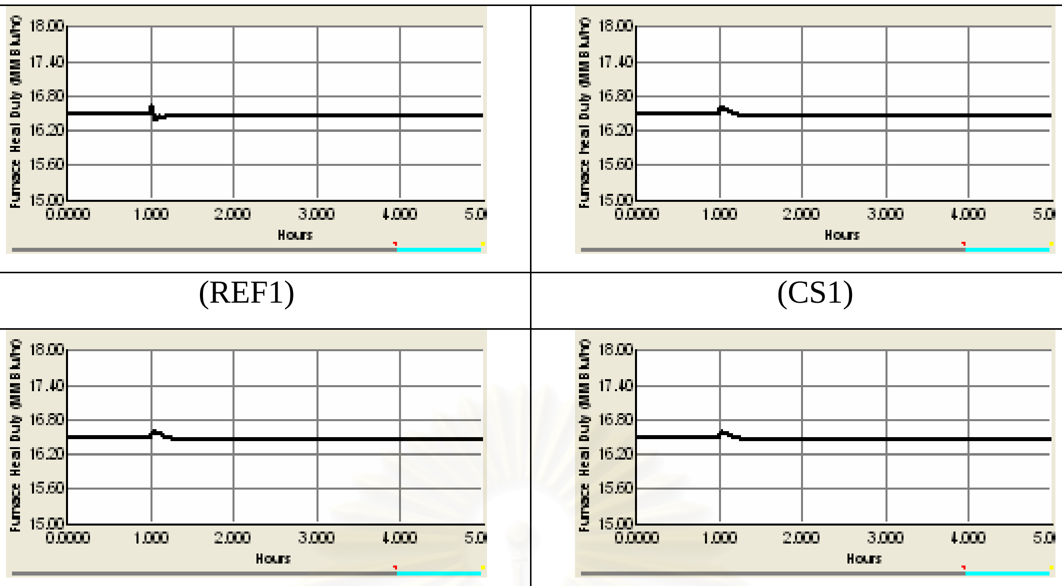


(REF1) (CS1)

(CS2) (CS3)

(H)

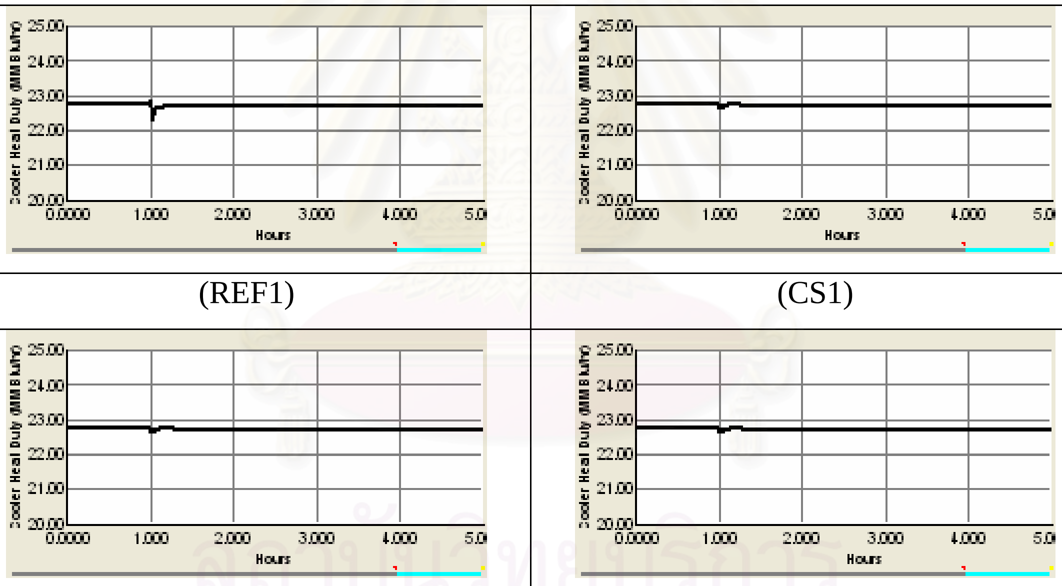
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(I)

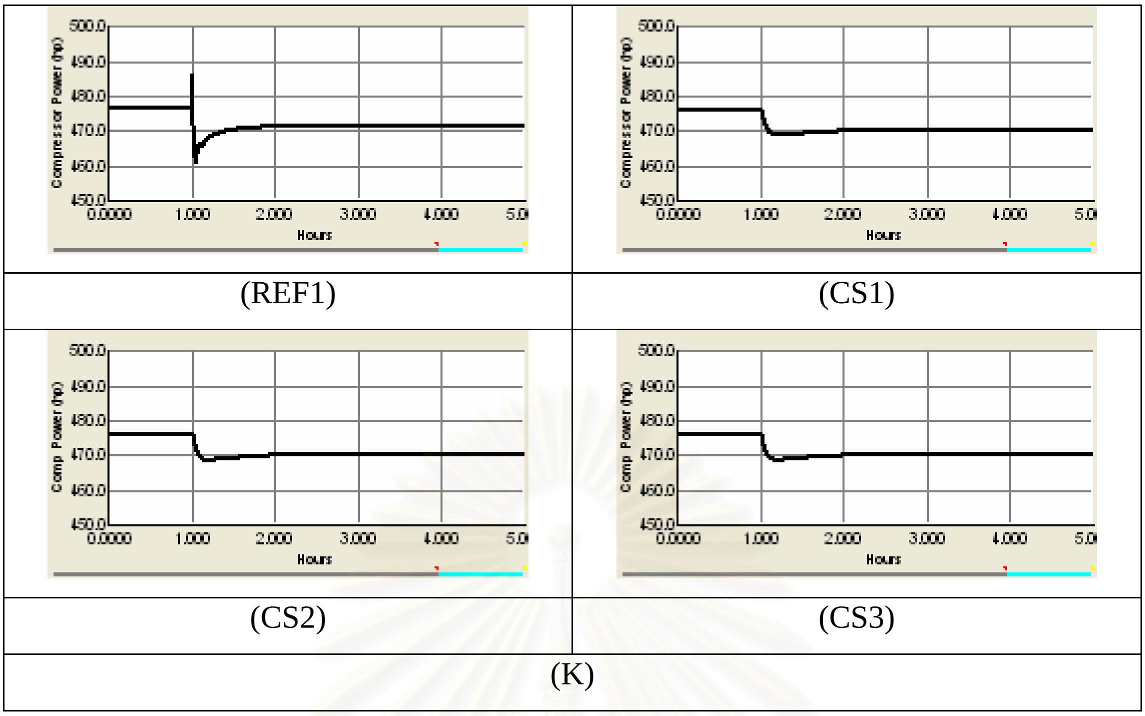


(REF1) (CS1)

(CS2) (CS3)

(J)

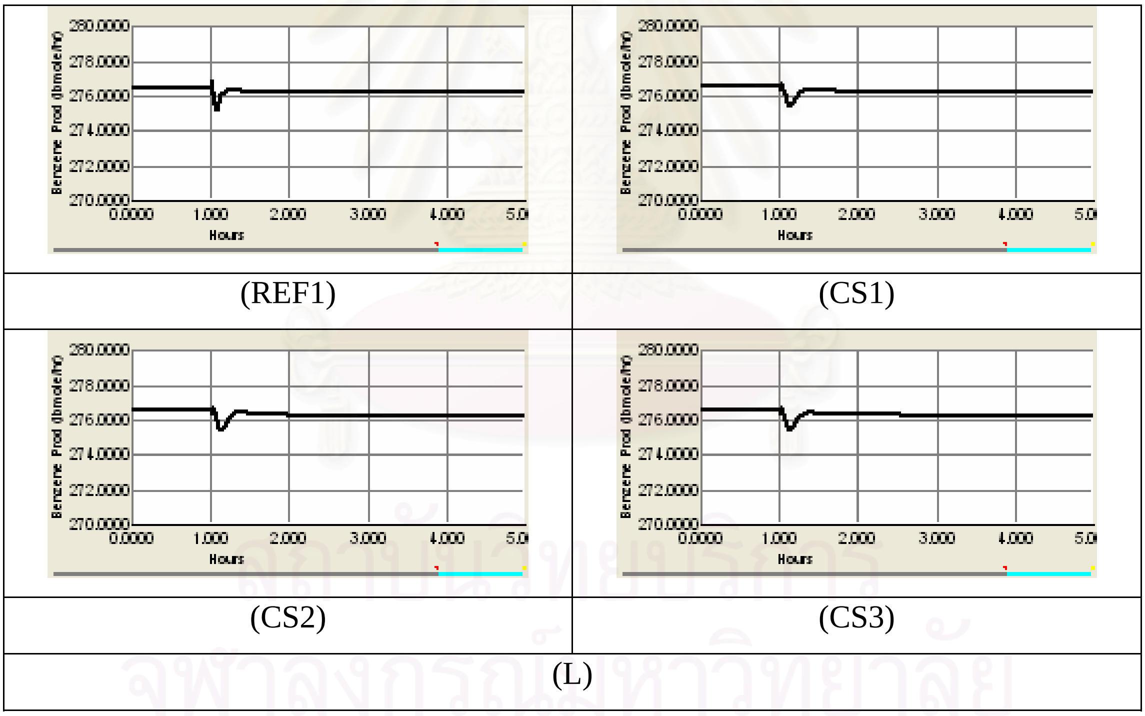
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(K)



(REF1) (CS1)

(CS2) (CS3)

(L)

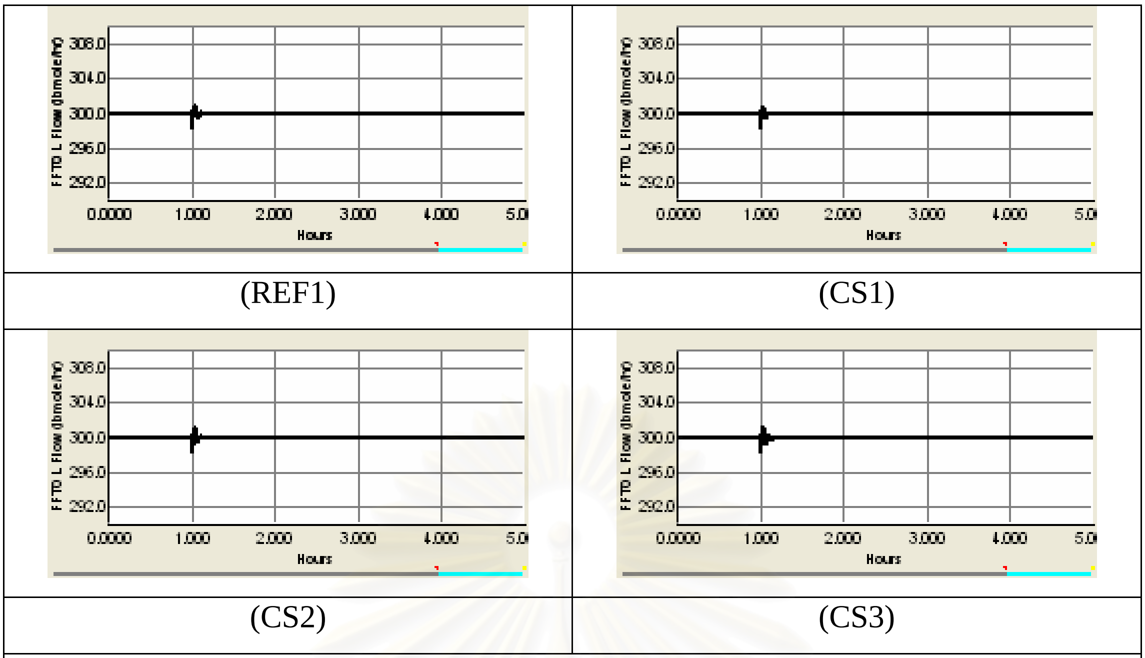
Figure 4.14 Dynamic responses of increase 0.05 in fresh gas feed rates methane mole fraction from 0.03 to 0.08 for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.

4.6.5 Increase in the Quench outlet Temperature for Reference Control Structure (REF1) and Our Control Structure (CS1, CS2, and CS3)

Figure 4.15 shows the dynamic responses of the reaction section of the HDA process to a disturbance in the quench outlet temperature from 1150 oF to 1170 oF at time equals 1hours.

Figure 4.15 (A-B) the fresh feed toluene flowrate and fresh feed hydrogen are small oscillatory. Figure 4.15(H) increasing in quench outlet temperature setpoint affect to oscillation of the response of reactor inlet temperature, reactor outlet temperature, reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quenches outlet temperature. Their dynamic response swing and return to their old setpoint (Figure4.15(C-H)). The furnace heat duty and cooler heat duty decrease immediately and oscillate before come to new point. The compressor power oscillates before slow decrease to new point (Figure4.15 (I-K)).

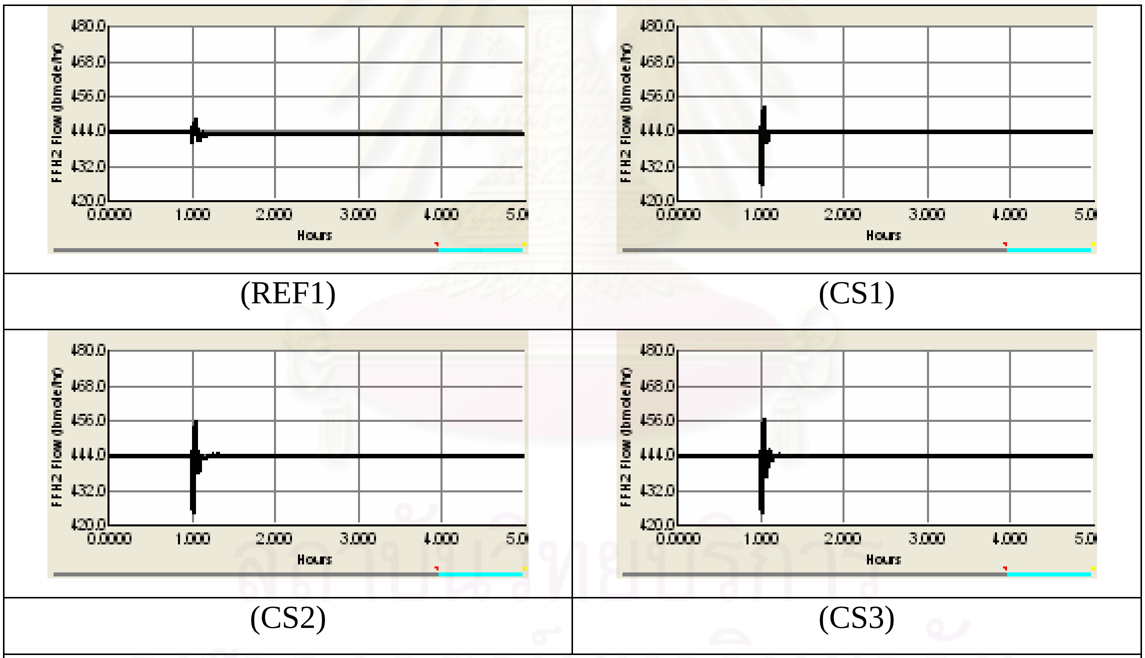
For CS1, CS2 and CS3, the fresh feed toluene flowrate is small oscillatory. The fresh feed hydrogen is also oscillatory. The control structure 1 is oscillating smaller than CS2 and CS3 (Figure 4.15(A-B)). Figure 4.15(H) increasing in quench outlet temperature setpoint affect to oscillation of the response of reactor inlet temperature, reactor outlet temperature, reactor pressure, hydrogen-to-aromatic ratio, separator temperature and quenches outlet temperature. Their dynamic response swing short time and return to their old setpoint (Figure4.15(C-H)). The furnace heat duty and cooler heat duty decrease immediately and small oscillate before come to new point. The compressor power slow decrease to new point (Figure4.15 (I-K)).



(REF1) (CS1)

(CS2) (CS3)

(A)

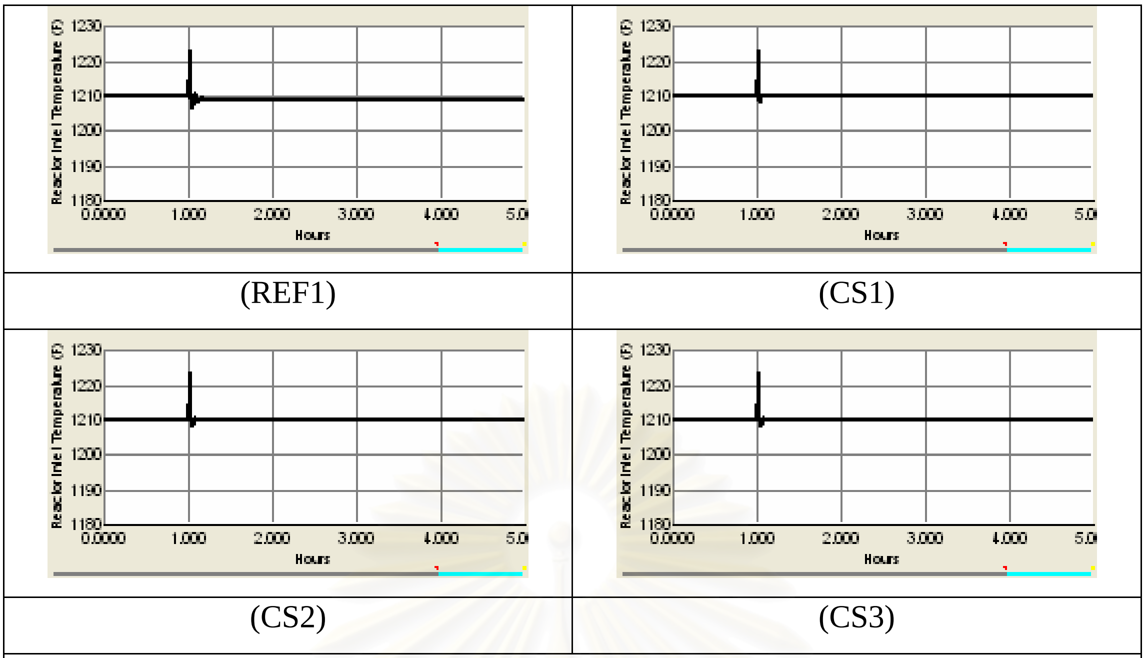


(REF1) (CS1)

(CS2) (CS3)

(B)

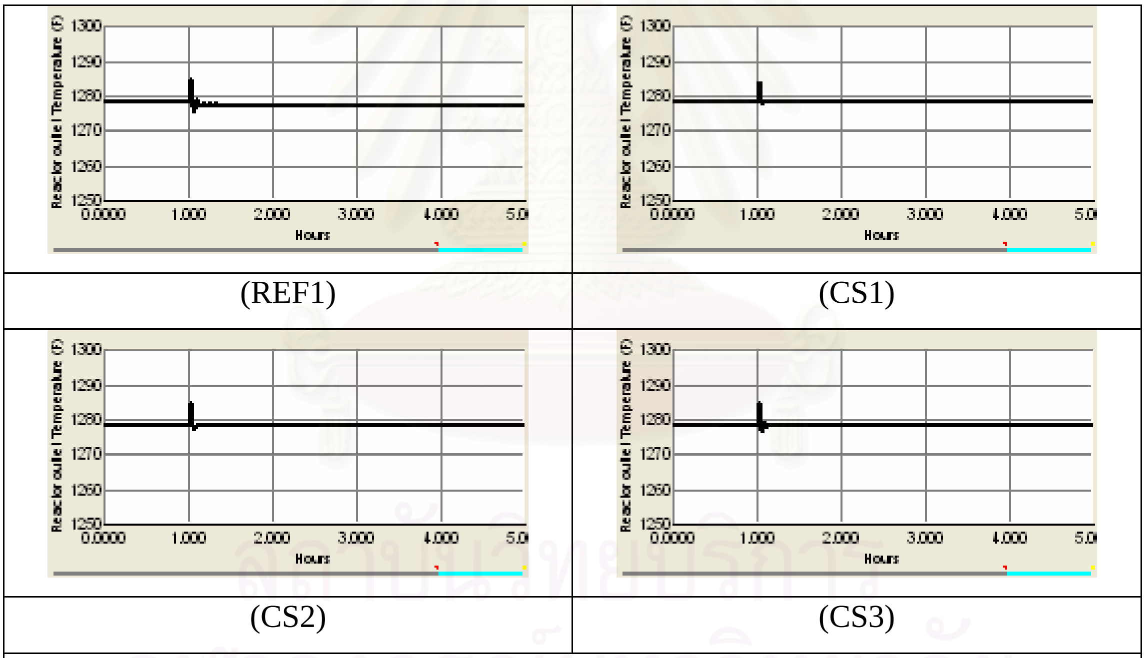
Figure 4.15 Dynamic responses of increase 20 $_o$F in quench outlet temperature from 1150 $_o$F to 1170 $_o$F for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(C)

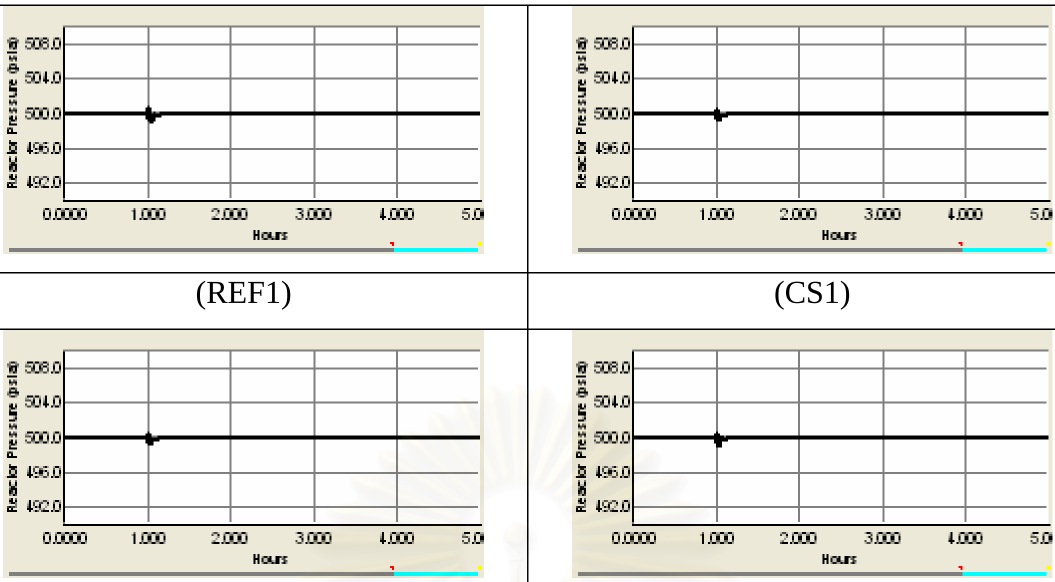


(REF1) (CS1)

(CS2) (CS3)

(D)

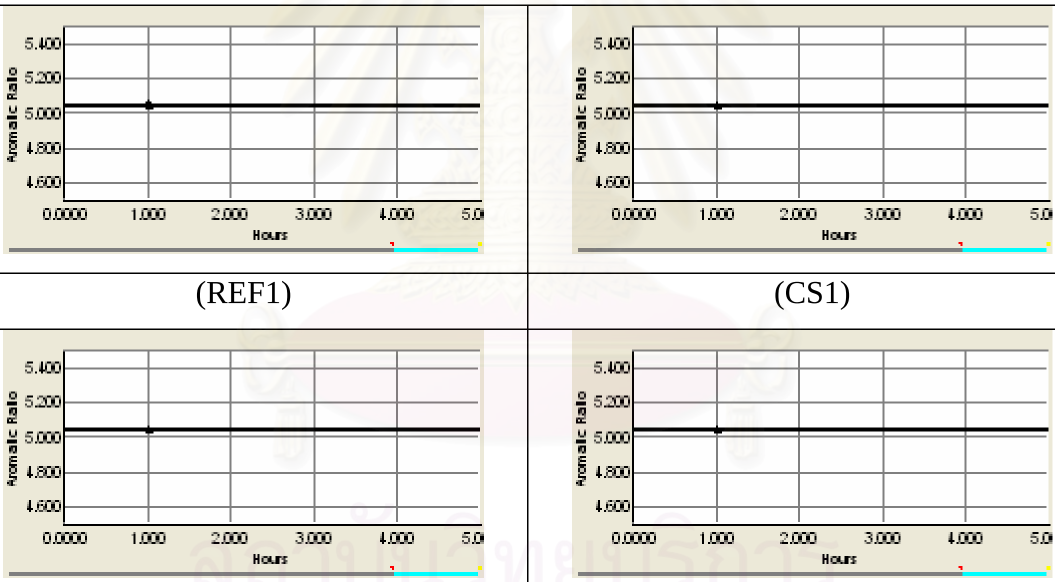
Figure 4.15 Dynamic responses of increase 20 ₒF in quench outlet temperature from 1150 ₒF to 1170 ₒF for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(E)

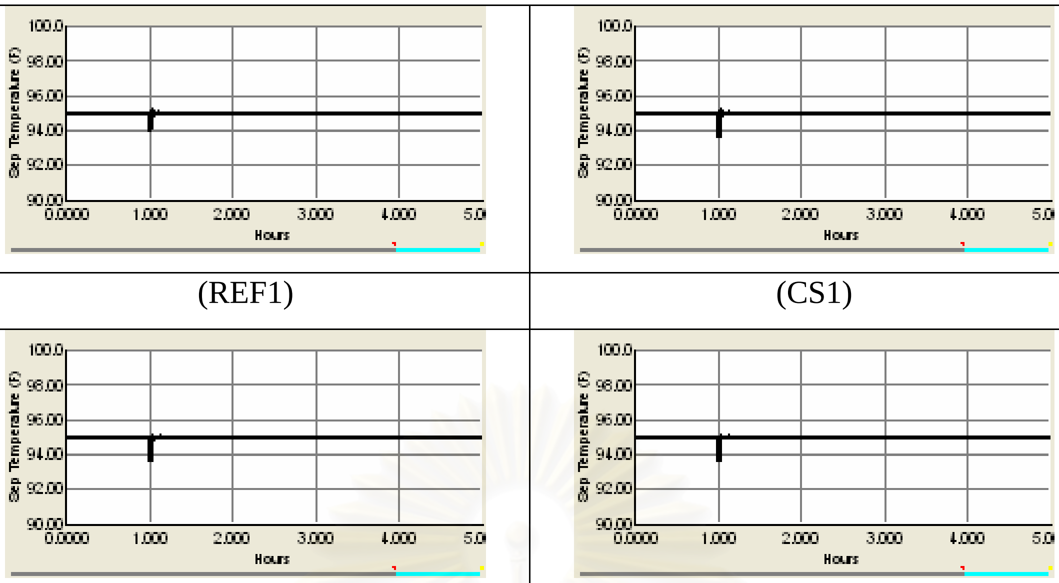


(REF1) (CS1)

(CS2) (CS3)

(F)

Figure 4.15 Dynamic responses of increase 20 °F in quench outlet temperature from 1150 °F to 1170 °F for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



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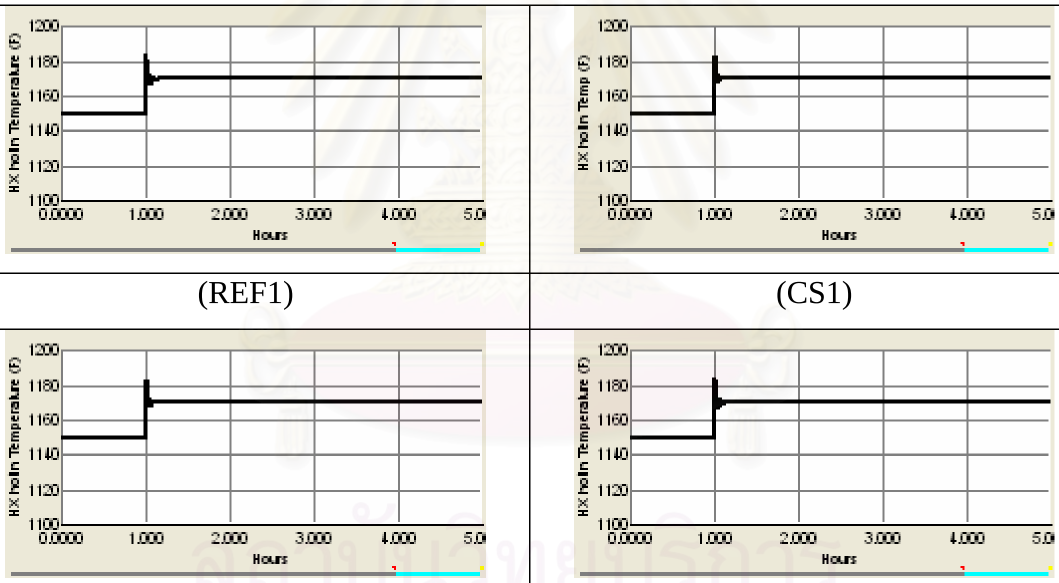
(G)

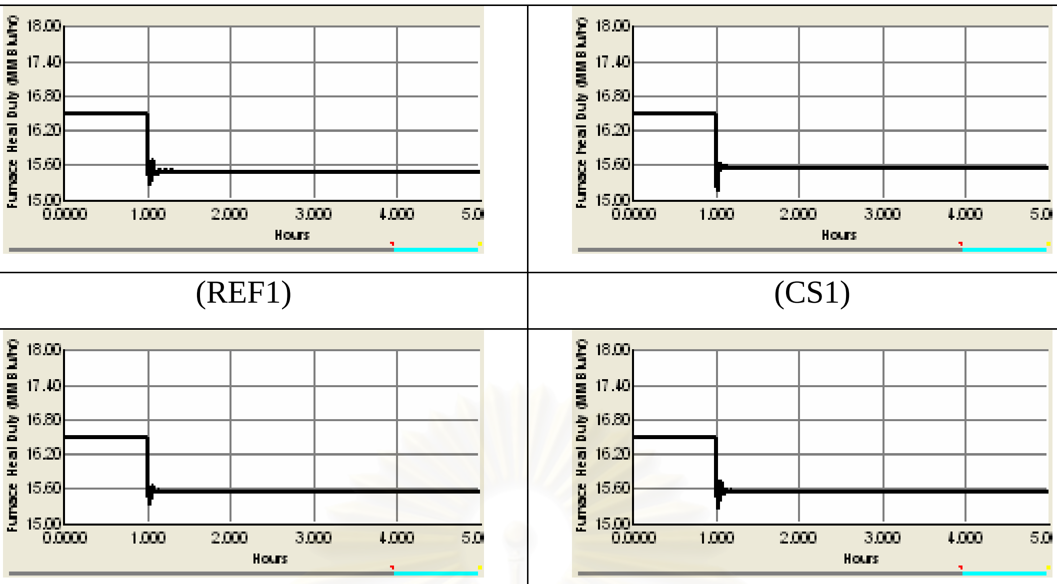


(REF1) (CS1)

(CS2) (CS3)

(H)

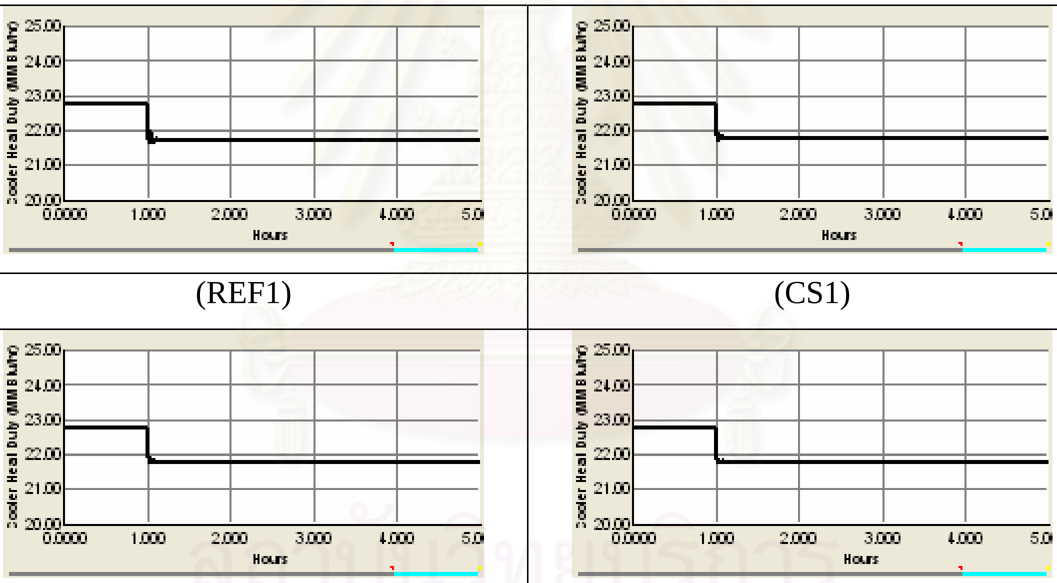
Figure 4.15 Dynamic responses of increase 20 $_{o}$F in quench outlet temperature from 1150 $_{o}$F to 1170 $_{o}$F for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(I)

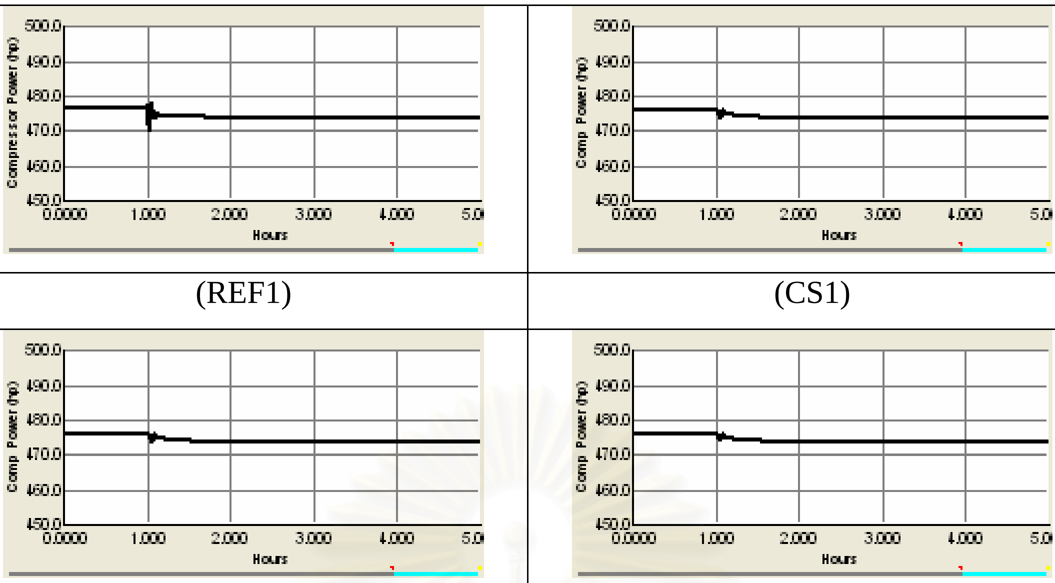


(REF1) (CS1)

(CS2) (CS3)

(J)

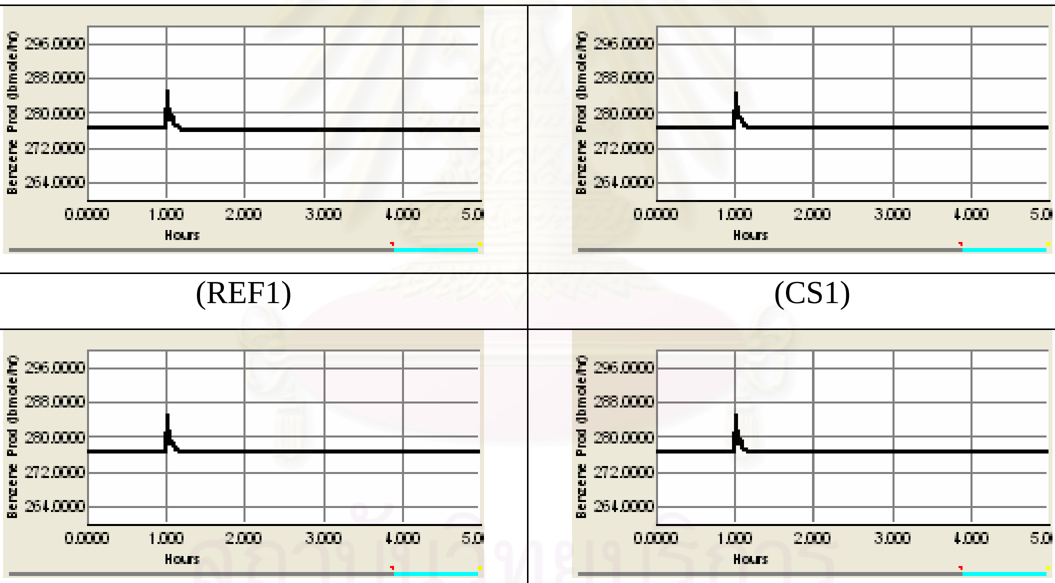
Figure 4.15 Dynamic responses of increase 20 $_{o}$F in quench outlet temperature from 1150 $_{o}$F to 1170 $_{o}$F for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.



(REF1) (CS1)

(CS2) (CS3)

(K)



(REF1) (CS1)

(CS2) (CS3)

(L)

Figure 4.15 Dynamic responses of increase 20 $_{o}$F in quench outlet temperature from 1150 $_{o}$F to 1170 $_{o}$F for; (A) fresh toluene feed rates (B) fresh gas feed rates, (C) reactor inlet temperature, (D) reactor outlet temperature, (E) reactor pressure, (F) hydrogen-to-aromatic ratio at inlet reactor, (G) separator temperature, (H) Quench outlet temperature, (I) furnace heat duty, (J) cooler heat duty, (K) compressor power, (L) benzene product.

4.7 Evaluation of the dynamic performance

The estimation of the minimum achievable variance of SISO controlled variable from "normal" closed- loop data. Since then, minimum variance control has been widely used as a benchmark for assessing control loop performance. However, minimum variance control based performance assessment methods cannot adequately evaluate the performance for controllers with constraints explicitly incorporated or for controllers where transient response and deterministic disturbance regulation are concerned. For assessing constrained control loop performance the proposed dynamic performance index is focused on time related characteristics of the controller's response to set-point changes or deterministic disturbances. There exist several candidate performance measures such as settling time and integral absolute error (IAE). Integral absolute error is widely used for the formulation of a dynamic performance as written below:

$$IAE = \int \left|\varepsilon(t)\right| dt$$

In this study, IAE method is used to evaluate the dynamic performance of the designed control system. Table 4.13, 4.15-4.17 shows the IAE results for the change in the dynamic disturbance in reaction section of HDA process with control loops in different control structure (REF1, CS1, CS2 and CS3) respectively, Table 4.14, 4.18-4.20 shows the IAE results for the change in the dynamic disturbance with variation of considered controlled variables from their setpoints in different control structure (REF1, CS1, CS2 and CS3) respectively.

4.7.1 Evaluation of the Dynamic Performance for REF1 Reference Control Structure Case

Table 4.13-4.14 shows the IAE results for the change in four dynamic disturbance loads in reaction section of HDA process. Four dynamic disturbance loads consist of decreasing in fresh feed toluene flowrate, increasing in fresh feed toluene flowrate, increasing in fresh gas feed methane mole fraction and increasing in quench outlet temperature setpoint respectively (Dyn1, Dyn2, Dyn3 and Dyn4).

Table 4.13 shows the IAE values of control loops between control variables and control setpoints. For in the reference control structure (REF1) has nine control loops excepted level loops but in our control structure (CS1-CS3) have eight control loops. The value of IAE in the reference control structure some loops is smaller than our control structure especially in fresh feed toluene when increase feed flowrate (Dyn2) but when increase methane mole fraction in gas feed, the value of IAE in the reference control structure is larger than our control structure. However, the summation value of IAE value in reference control structure more than our control structure because our control structures have smaller control loops than the reference control structure.

Table 4.14 shows the IAE values of reference control structure between considered control variables and their nominal setpoints. The considered controlled variables consist of fresh feed toluene flowrate, reactor inlet pressure, quench outlet temperature, separator temperature, hydrogen-to-aromatic ratio, reactor inlet temperature, reactor outlet temperature, methane composition in gas stream outlet separator, toluene conversion in plug flow reactor, toluene composition in quench outlet flow, methane composition outlet mixer and benzene composition in liquid stream outlet separator. The reference control structure has high value of IAE in reactor inlet temperature and reactor outlet temperature loops.

Table 4.13 The IAE values of control loops between control variables and control setpoints of the reference control structure.

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	45.839	19.564	6.900	3.503
Reactor Pressure	62.412	70.654	41.375	5.243
Quench Temp	16.607	24.644	2.163	21.011
Sep Temp	2.571	2.737	0.740	1.218
Reactor inlet Temp	19.564	20.824	2.623	11.539
rH2	0.031	0.036	0.008	0.003
Toluene in Quench	0.016	0.015	0.002	0.003
Methane in Mixer	0.001	0.001	0.005	0.001
FFH2	56.804	90.016	98.805	10.361
SUM	203.845	228.491	152.620	52.883

Table 4.14 The IAE values of the reference control structure between considered control variables and their nominal setpoints.

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	45.839	19.564	6.900	3.503
Reactor Pressure	62.412	70.654	41.375	5.243
Quench Temp	16.607	24.644	2.163	21.011
Sep Temp	2.571	2.737	0.740	1.218
rH2	0.031	0.036	0.008	0.003
Reactor inlet Temp	1441.300	1325.700	33.982	277.070
Reactor outlet Temp	1447.700	1325.300	15.221	278.050
Methane in gas	0.045	0.038	0.018	0.034
Toluene conversion	0.354	0.334	0.044	0.862
Toluene in Quench	0.016	0.015	0.002	0.003
Methane in Mixer	0.001	0.001	0.005	0.001
Benzene in liq	0.288	0.277	0.014	0.480
SUM	3017.164	2769.299	100.472	587.479

4.7.2 Evaluation of the Dynamic Performance for CS1, CS2 and CS3 Our Control Structure Case

Table 4.15-4.20 shows the IAE results for the change in four dynamic disturbance loads in reaction section of HDA process. Four dynamic disturbance loads consist of decreasing in fresh feed toluene flowrate, increasing in fresh feed toluene flowrate, increasing in fresh gas feed methane mole fraction and increasing in quench outlet temperature setpoint respectively (Dyn1, Dyn2, Dyn3 and Dyn4).

Table 4.15-4.17 shows the IAE values of control loops between control variables and control setpoints. For in our control structures (CS1-CS3) have eight control loops. The value of IAE in the control structure1 (CS1) similar as the control structure2 (CS2) and the summation of IAE value in the control structure1 (CS1) smaller than in the control structure2 (CS2) except in dynamic disturbance 2 CS2 a little smaller than CS1. However, the summation value of both control structure CS1 and CS2 smaller than the control structure3 (CS3) because the control structure 3 control reactor outlet temperature. The reactor outlet temperature has the IAE value more than toluene conversion in pug flow reactor and benzene composition in liquid stream outlet separator.

Table 4.18-4.19 shows the IAE values of our control structures between considered control variables and their nominal setpoints. The considered controlled variables consist of fresh feed toluene flowrate, reactor inlet pressure, quench outlet temperature, separator temperature, hydrogen-to-aromatic ratio, reactor inlet temperature, reactor outlet temperature, methane composition in gas stream outlet separator, toluene conversion in plug flow reactor, toluene composition in quench outlet flow, methane composition outlet mixer and benzene composition in liquid stream outlet separator. The control structure1 has high value of IAE in reactor inlet temperature and reactor outlet temperature loops more than the control structure2 and the control structure3. Particularly, the control structure3 is lowest value of IAE in reactor inlet temperature and reactor outlet temperature loops because this structure controls the reactor inlet temperature with setpoint of reactor outlet temperature. The IAE values of the other loops of each control structure do not more difference. The IAE value of reactor temperature loops affect to the summation of IAE value more than the other loops.

Table 4.15 The IAE values of control loops between control variables and control setpoints of the control structure1 (CS1).

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.798	68.537	10.381	3.877
Reactor Pressure	63.969	68.592	41.381	3.184
Quench Temp	16.896	24.857	0.628	18.397
Sep Temp	6.121	6.353	0.562	1.683
Reactor inlet Temp	19.990	21.403	1.696	7.785
rH2	0.008	0.008	0.005	0.001
Toluene conversion	0.371	0.343	0.019	0.049
Methane in gas	0.341	0.401	0.025	0.008
SUM	154.494	190.495	54.697	34.984

Table 4.16 The IAE values of control loops between control variables and control setpoints of the control structure2 (CS2).

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.740	67.935	10.404	4.656
Reactor Pressure	64.349	68.353	41.428	3.361
Quench Temp	16.867	24.719	0.907	19.433
Sep Temp	6.189	6.413	0.577	1.623
Reactor inlet Temp	20.020	21.514	1.678	8.579
rH2	0.008	0.009	0.005	0.002
Benzene in liq	0.269	0.247	0.016	0.010
Methane in gas	0.322	0.379	0.025	0.008
SUM	154.763	189.568	55.039	37.672

Table 4.17 The IAE values of control loops between control variables and control setpoints of the control structure3 (CS3).

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.365	68.614	10.340	5.460
Reactor Pressure	57.722	57.866	41.490	3.271
Quench Temp	14.012	20.003	0.629	19.753
Sep Temp	5.718	5.930	0.534	1.662
Reactor inlet Temp	18.462	20.230	1.668	10.551
rH2	0.007	0.008	0.005	0.002
Reactor outlet Temp	73.715	91.468	8.928	12.447
Methane in gas	0.325	0.385	0.024	0.008
SUM	216.326	264.505	63.618	53.153

Table 4.18 The IAE values of the control structure1 (CS1) between considered control variables and their nominal setpoints.

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.798	68.537	10.381	3.877
Reactor Pressure	63.969	68.592	41.381	3.184
Quench Temp	16.896	24.857	0.628	18.397
Sep Temp	6.121	6.353	0.562	1.683
rH2	0.008	0.008	0.005	0.001
Reactor inlet Temp	1151.300	1031.600	36.844	11.313
Reactor outlet Temp	1218.600	1104.900	15.157	11.370
Methane in gas	0.341	0.401	0.025	0.008
Toluene conversion	0.371	0.343	0.019	0.049
Toluene in Quench	0.053	0.050	0.003	0.065
Methane in Mixer	0.459	0.532	0.047	0.011
Benzene in liq	0.236	0.215	0.020	0.022
SUM	2505.153	2306.389	105.072	49.980

Table 4.19 The IAE values of the control structure2 (CS2) between considered control variables and their nominal setpoints.

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.740	67.935	10.404	4.656
Reactor Pressure	64.349	68.353	41.428	3.361
Quench Temp	16.867	24.719	0.907	19.433
Sep Temp	6.189	6.413	0.577	1.623
rH2	0.008	0.009	0.005	0.002
Reactor inlet Temp	1098.100	986.380	30.817	11.987
Reactor outlet Temp	1141.000	1035.500	10.124	15.761
Methane in gas	0.322	0.379	0.025	0.008
Toluene conversion	0.615	0.586	0.048	0.120
Toluene in Quench	0.073	0.069	0.003	0.066
Methane in Mixer	0.422	0.491	0.048	0.012
Benzene in liq	0.269	0.247	0.016	0.010
SUM	2374.953	2191.080	94.400	57.039

Table 4.20 The IAE values of the control structure3 (CS3) between considered control variables and their nominal setpoints.

	Dyn1	Dyn2	Dyn3	Dyn4
FFTOL	46.365	68.614	10.340	5.460
Reactor Pressure	57.722	57.866	41.490	3.271
Quench Temp	14.012	20.003	0.629	19.753
Sep Temp	5.718	5.930	0.534	1.662
rH2	0.007	0.008	0.005	0.002
Reactor inlet Temp	79.713	90.459	19.432	14.613
Reactor outlet Temp	73.715	91.468	8.928	12.447
Methane in gas	0.325	0.385	0.024	0.008
Toluene conversion	3.476	3.869	0.077	0.132
Toluene in Quench	0.320	0.357	0.005	0.064
Methane in Mixer	0.511	0.576	0.050	0.012
Benzene in liq	1.905	2.338	0.023	0.032
SUM	283.789	341.874	81.537	57.455

4.8 Economic analysis for HDA process

This section evaluates economics of a HDA process. The term economics refers to the evaluation of the operating costs associated with the operation of a HDA process. The methods consider the continuing costs associated with the daily operation of the process and the benefit obtained from benzene product are combined into meaningful economic criteria are provided.

In this work, we evaluate economic of each control structure by using benzene product and operational (energy) cost when disturbance occurs. Four dynamic disturbances used to evaluate operational cost in 5 hours. The utility consumptions are shown in Table 4.21. The furnace heat duty when decrease in fresh toluene feed flowrate (Dyn1), the utility consumption of the reference control structure smaller than our control structure (Figure 4.16). The furnace heat duty when increase in fresh toluene feed flowrate (Dyn2) and methane composition in fresh gas feed (Dyn3), the utility consumption of the reference control structure more than our control structures (Figure 4.17-4.18). However, the summations of the utility consumption of the reference control structure more than our control structures.

Table 4.22 show utility saving of control structure CS1, CS2 and CS3 from the reference control structure. The utility consumption of control structure CS1, CS2 and CS3 decrease from the reference control structure and save cost average estimate 800$/5hr.

Table 4.21 the utility consumptions of four control structure (REF1, CS1, CS2, and CS3) when change in four dynamic disturbances in 5 hour.

		Dyn1	Dyn2	Dyn3	Dyn4	SUM
Furnace Heat Duty(MBtu)	REF1	7.1807	9.3771	8.2338	7.8436	32.6352
	CS1	7.2473	9.2746	8.2275	7.8658	32.6152
	CS2	7.2509	9.2733	8.2287	7.8669	32.6198
	CS3	7.3412	9.1850	8.2289	7.8657	32.6208
Cooler Heat Duty(MBtu)	REF1	10.0181	12.8059	11.3522	10.9603	45.1365
	CS1	10.0924	12.6913	11.3455	10.9875	45.1167
	CS2	10.0973	12.6888	11.3469	10.9889	45.1219
	CS3	10.2048	12.5762	11.3472	10.9874	45.1156
Compressor Power(Mhp)	REF1	0.6966	1.0460	0.8491	0.8537	3.4454
	CS1	0.7045	1.0307	0.8480	0.8534	3.4366
	CS2	0.7039	1.0316	0.8480	0.8533	3.4368
	CS3	0.7029	1.0345	0.8480	0.8533	3.4387

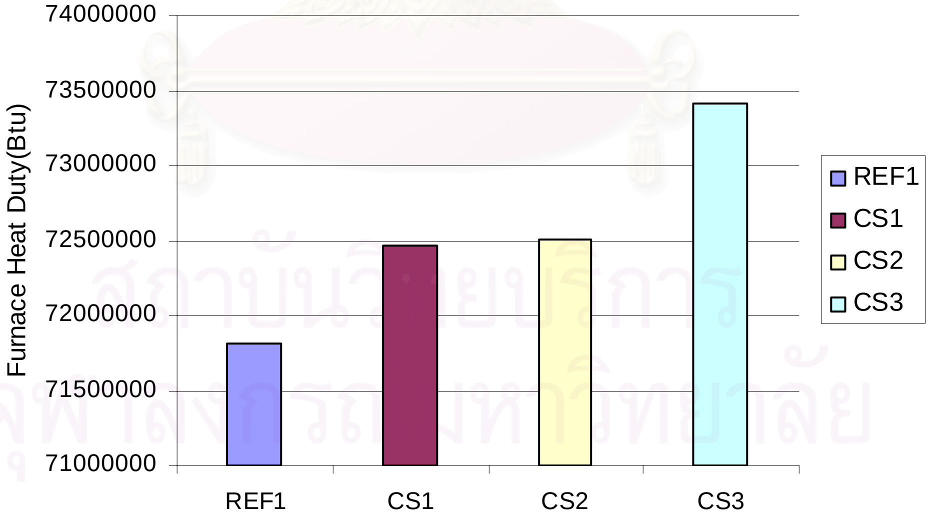


Figure 4.16 Furnace heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when decrease 10% in fresh feed toluene flowrate.

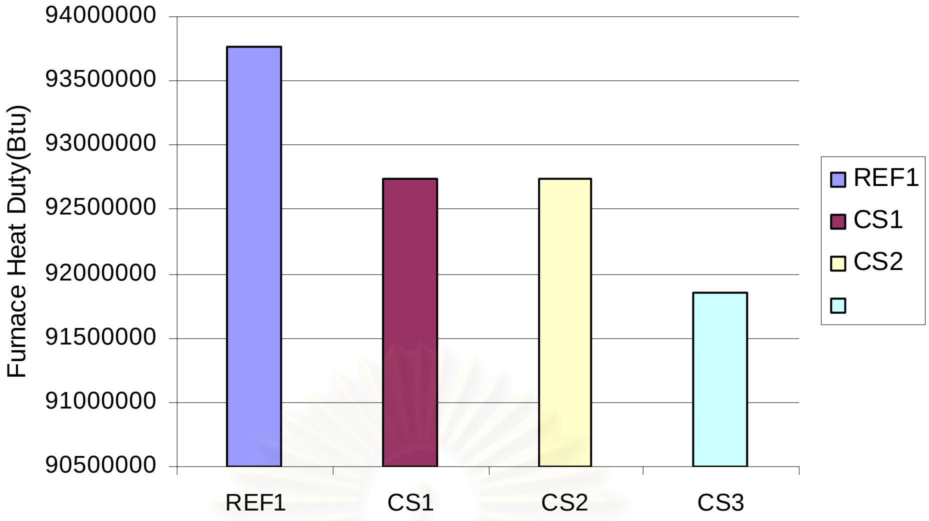


Figure 4.17 Furnace heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 10% in fresh feed toluene flowrate.

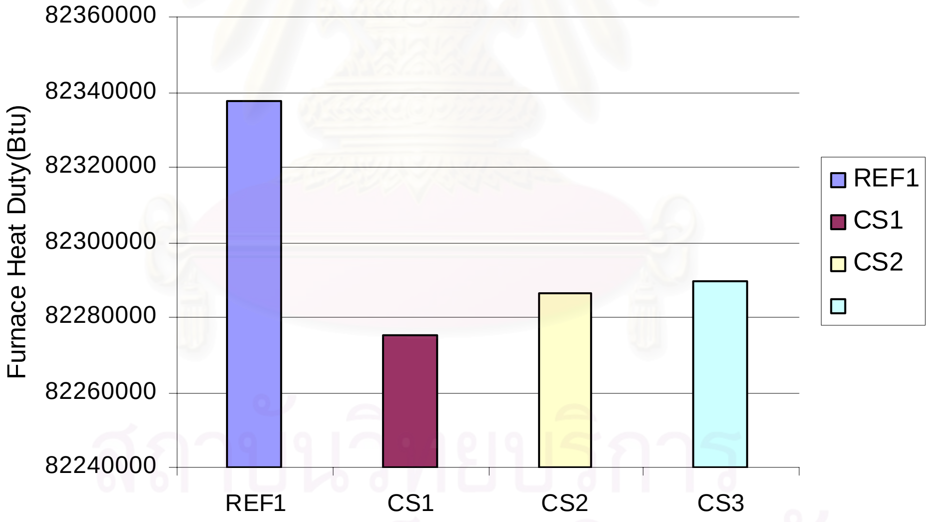


Figure 4.18 Furnace heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 0.05 in fresh gas feed methane mole fraction

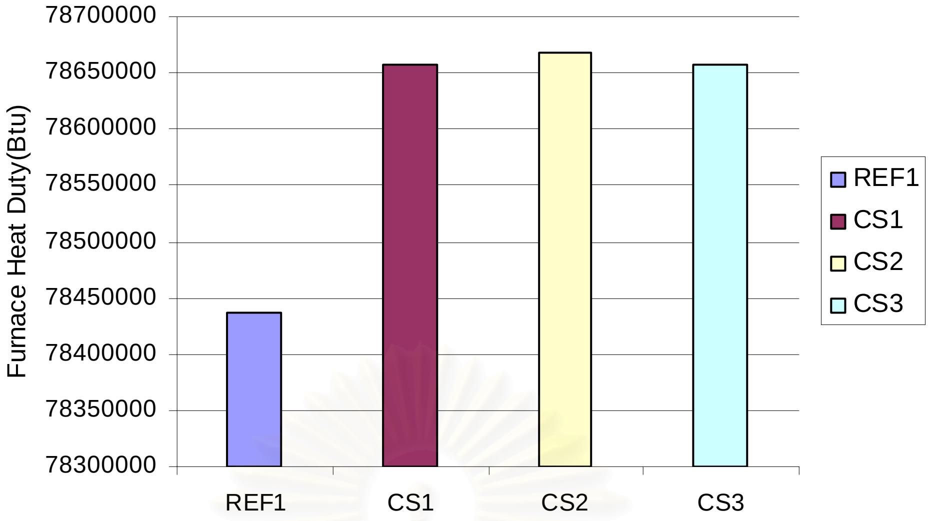


Figure 4.19 Furnace heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 20 ₒF in quench outlet temperature.

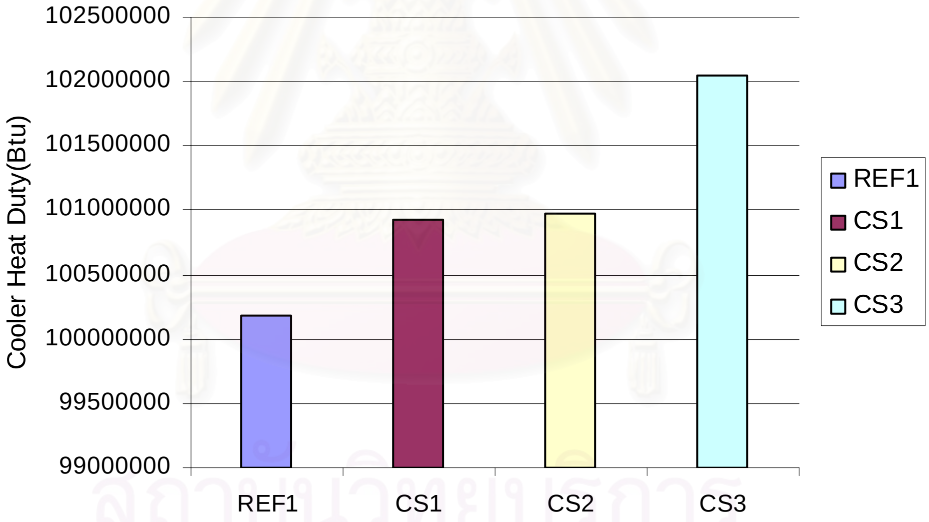


Figure 4.20 Cooler heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when decrease 10% in fresh feed toluene flowrate.

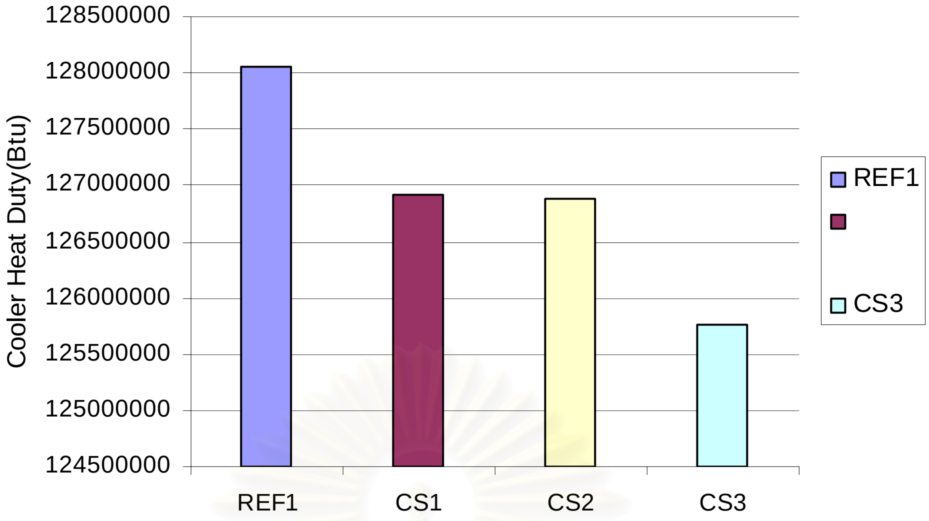


Figure 4.21 Cooler heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 10% in fresh feed toluene flowrate.

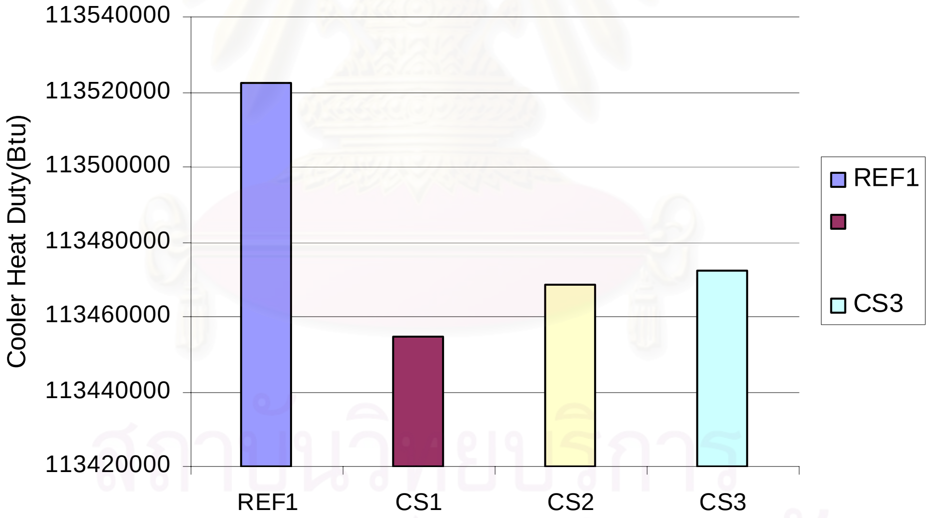


Figure 4.22 Cooler heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 0.05 in fresh gas feed methane mole fraction

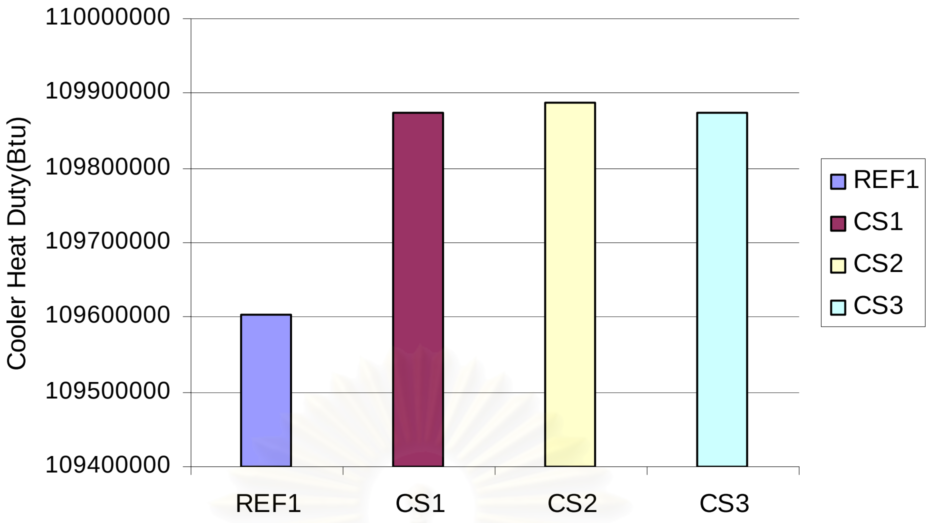


Figure 4.23 Cooler heat duty consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 20 ₒF in quench outlet temperature.

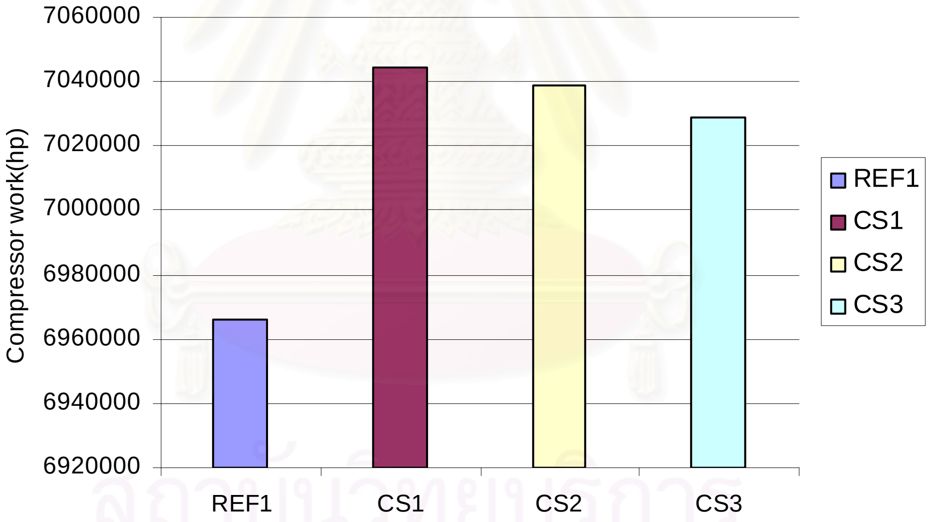


Figure 4.24 Compressor work consumptions of four control structure (REF1, CS1, CS2, and CS3) when decrease 10% in fresh feed toluene flowrate.

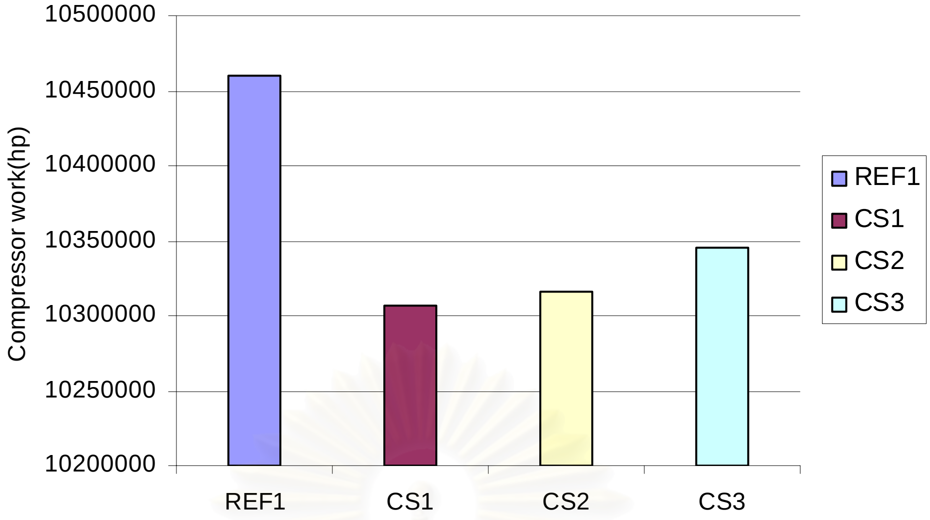


Figure 4.25 compressor work consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 10% in fresh feed toluene flowrate.

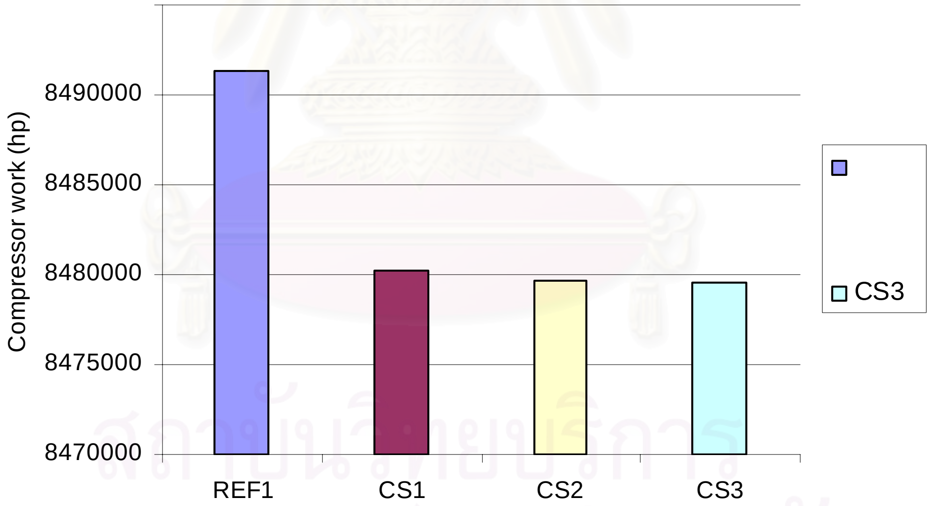


Figure 4.26 Compressor work consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 0.05 in fresh gas feed methane mole fraction

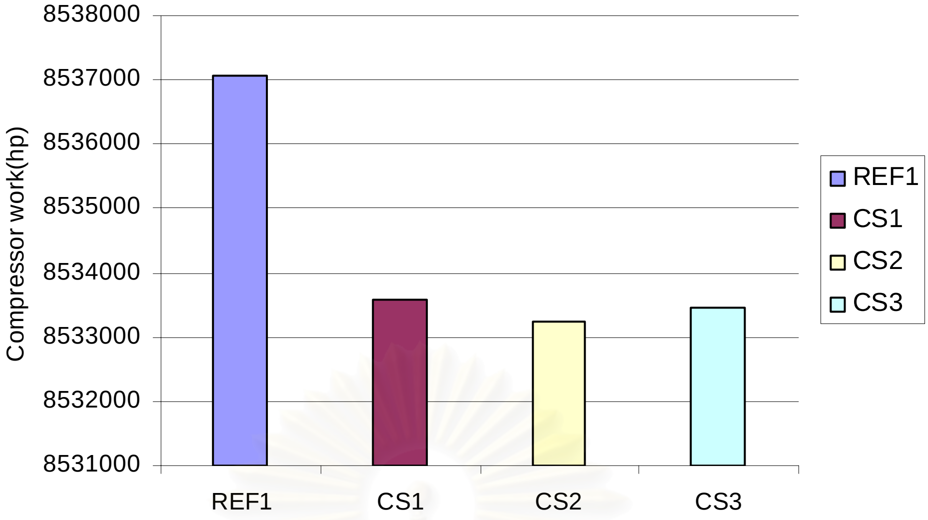


Figure 4.27 Compressor work consumptions of four control structure (REF1, CS1, CS2, and CS3) when increase 20 ₒF in quench outlet temperature.

Table 4.22 the utility saving of control structure CS1, CS2 and CS3 from the reference control structure (REF1) when change in four dynamic disturbances.

		Furnace Heat Duty($)	Cooler Heat Duty($)	Compressor Power($)
Dyn1	CS1	+2.6627	+0.1740	+3293.1994
	CS2	+2.8083	+0.1854	+3053.6268
	CS3	+6.4190	+0.4372	+2646.8064
Dyn2	CS1	-4.0990	-0.2683	-6418.1830
	CS2	-4.1509	-0.2742	-6021.5110
	CS3	-7.6830	-0.5377	-4826.8716
Dyn3	CS1	-0.2489	-0.0158	-466.9064
	CS2	-0.2037	-0.0125	-490.1828
	CS3	-0.1926	-0.0117	-492.7123
Dyn4	CS1	+0.8855	+0.0637	-146.3738
	CS2	+0.9290	+0.0668	-160.7821
	CS3	+0.8825	+0.0635	-151.5499

(+) cost increase from the reference control structure

(-) cost decrease from the reference control structure

Table 4.23 the summation of utility consumptions and utility saving of control structure CS1, CS2 and CS3 decrease from REF1 when change in four dynamic disturbances.

	Utility consumptions of CS1 decrease from REF1	Utility consumptions of CS2 decrease from REF1	Utility consumptions of CS3 decrease from REF1
Furnace Heat Duty(Btu)	199926.3889	154309.8611	143533.0556
Cooler Heat Duty(Btu)	198251.6667	147015.9722	208240.6944
Compressor Power(hp)	89006.2800	86163.0750	67245.8900
	Utility saving of CS1 from REF1	Utility saving of CS2 from REF1	Utility saving of CS3 from REF1
Furnace Heat Duty($)	0.7997	0.6172	0.5741
Cooler Heat Duty($)	0.0464	0.0344	0.0488
Compressor Power($)	3738.2638	3618.8491	2824.3274
SUM($)	3739.1099	3619.5008	2824.9503

The benefit obtained from utility saving from reference control structure is given in Table 4.23 The summation of energy cost savings from the furnace heat duty, cooler heat duty and compressor power cost of our control structure more than the reference control structure when four dynamic disturbances occurs.

Table 4.24 the benzene product at inlet separator section (lbmole), loss of benzene product from steady state (lbmole) and percent loss of benzene product from steady state (%) of control structure REF1, CS1, CS2 and CS3 when change in four dynamic disturbances.

		Dyn1	Dyn2	Dyn3	Dyn4
Benzene Molar Flow (lbmole) (SS=1382.2109)	REF1	1286.1485	1477.0721	1380.9746	1380.9775
	CS1	1286.6553	1476.8309	1381.0467	1382.5252
	CS2	1286.9644	1476.2386	1381.0101	1382.4768
	CS3	1291.1840	1468.5538	1381.1514	1382.5214
Loss Benzene (lbmole)	REF1	-95.9724	94.9513	-1.1463	-1.1433
	CS1	-95.5557	94.6199	-1.1642	0.3142
	CS2	-95.1566	94.1176	-1.1103	0.3559
	CS3	-91.0270	86.3428	-1.0596	0.3105
%Loss from Steady-state	REF1	-6.94%	+6.87%	-0.08%	-0.08%
	CS1	-6.91%	+6.85%	-0.08%	+0.02%
	CS2	-6.88%	+6.81%	-0.08%	+0.03%
	CS3	-6.59%	+6.25%	-0.08%	+0.02%

From Table4.24 when decrease fresh toluene feed flowrate, benzene product at inlet separation section of the reference control structure decrease more than our control structures. Decreasing of benzene product of the control structure3 (CS3) is the smallest in the all of control structures. However, when increase fresh toluene feed flowrate, benzene product at inlet separation section of the reference control structure increase more than our control structures and increasing of benzene product of control structure3 (CS3) is the smallest in the all of control structures also. That mean, the references structure more deviation in benzene product more than designed structure. Change in quench outlet temperature, benzene product of reference control structure decreases but benzene product of our control structures increase slightly.

Table 4.25 Deviation of Furnace heat duty, Cooler heat duty and compressor power from steady state and percent loss of Furnace heat duty, Cooler heat duty and compressor power from steady state (%) of control structure REF1, CS1, CS2 and CS3 when change in four dynamic disturbances.

		Dyn1	Dyn2	Dyn3	Dyn4
Furnace Heat Duty deviate from steady state(MBtu)	REF1	-1.0668	1.1297	-0.0137	-0.4038
	CS1	-0.9948	1.0326	-0.0145	-0.3763
	CS2	-0.9916	1.0308	-0.0139	-0.3757
	CS3	-0.9009	0.9430	-0.0131	-0.3764
%Loss from Steady-state	REF1	-12.934%	13.697%	-0.166%	-4.896%
	CS1	-12.070%	12.528%	-0.176%	-4.565%
	CS2	-12.031%	12.506%	-0.169%	-4.558%
	CS3	-10.930%	11.441%	-0.159%	-4.566%
Cooler Heat Duty deviate from steady state(MBtu)	REF1	-1.3540	1.4338	-0.0199	-0.4118
	CS1	-1.2739	1.3250	-0.0208	-0.3788
	CS2	-1.2696	1.3219	-0.0200	-0.3780
	CS3	-1.1615	1.2100	-0.0191	-0.3788
%Loss from Steady-state	REF1	-11.906%	12.608%	-0.175%	-3.621%
	CS1	-11.208%	11.657%	-0.183%	-3.332%
	CS2	-11.169%	11.629%	-0.176%	-3.326%
	CS3	-10.219%	10.645%	-0.168%	-3.333%
Compressor power deviate from steady state(hp)	REF1	-0.1611	0.1883	-0.0086	-0.0040
	CS1	-0.1522	0.1740	-0.0087	-0.0033
	CS2	-0.1528	0.1750	-0.0087	-0.0034
	CS3	-0.1538	0.1778	-0.0087	-0.0034
%Loss from Steady-state	REF1	-18.782%	21.951%	-0.999%	-0.466%
	CS1	-17.771%	20.310%	-1.013%	-0.390%
	CS2	-17.837%	20.422%	-1.019%	-0.393%
	CS3	-17.951%	20.753%	-1.021%	-0.392%

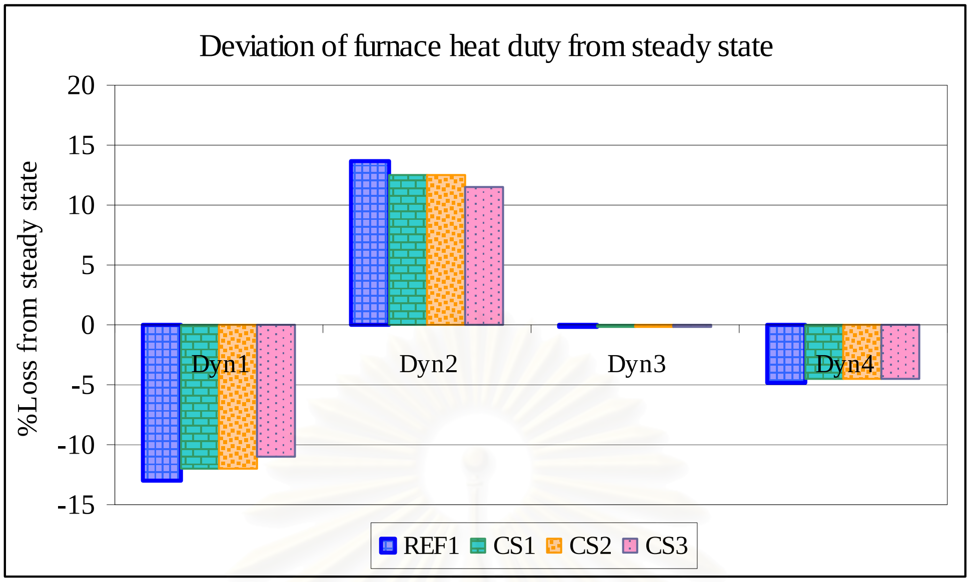


Figure 4.28 Deviation of furnace heat duty (%) from steady state of four control structure (REF1, CS1, CS2, and CS3) when four disturbance occur.

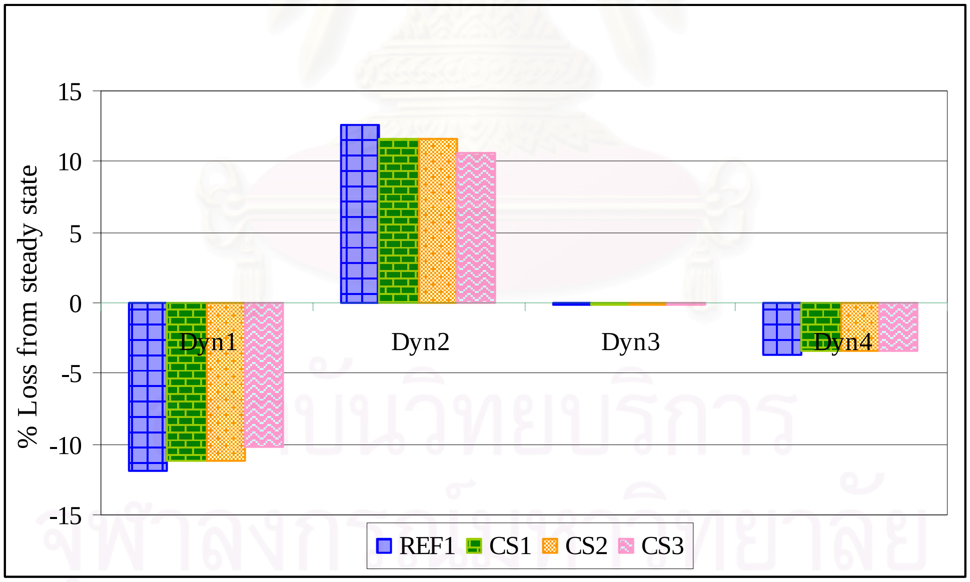


Figure 4.29 Deviation of cooler heat duty (%) from steady state of four control structure (REF1, CS1, CS2, and CS3) when four disturbance occur.

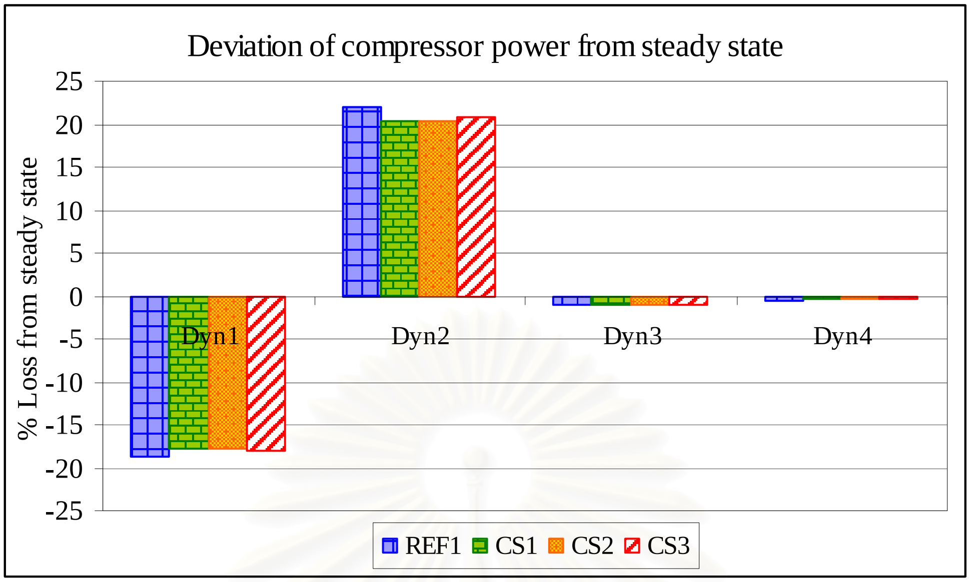


Figure 4.30 Deviation of Compressor power (%) from steady state of four control structure (REF1, CS1, CS2, and CS3) when four disturbance occur.

As can be seen in Figure 4.28, furnace heat duty of the reference control structure is more deviates from steady state than our control structures. The control structure 3(CS3) is the smallest deviation in the all of control structures. Figure 4.29-4.30 shows the deviation of cooler heat duty and compressor power. The reference control structure is more deviates from steady state than our control structures. That mean, the references structure more deviation in furnace heat duty, cooler heat duty and compressor power more than designed structure.

CHAPTER V

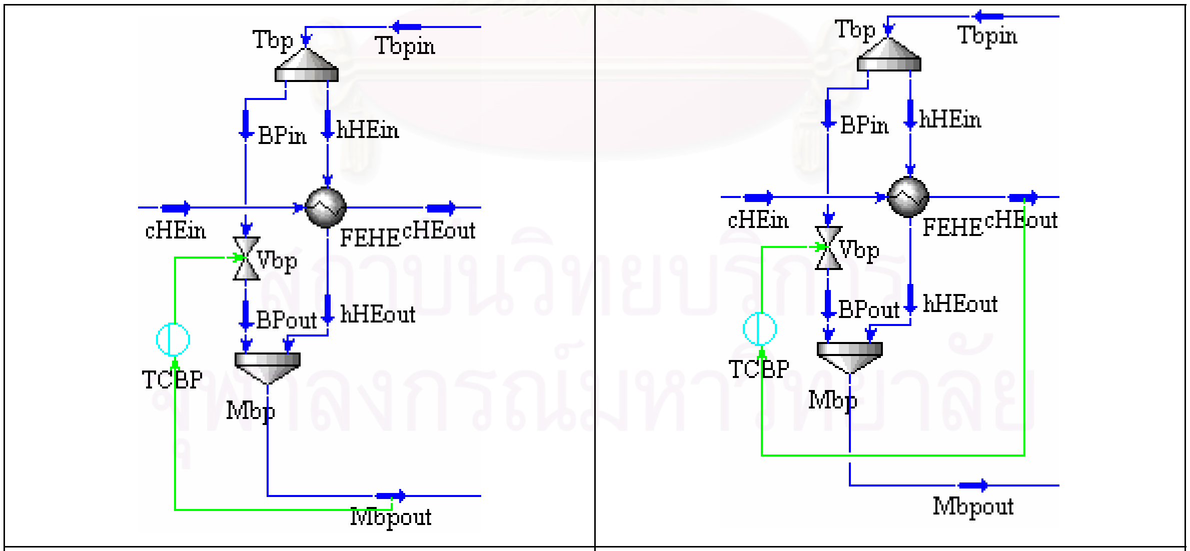
REACTOR FEED-EFFLUENT EXCHANGE SYSTEM

We start with the design and control of the FEHE system in the HDA process. The HDA process requires a furnace for all design cases since the reactor effluent stream is quench down to the reactor feed temperature to prevent by-product formation in the heat exchanger.

5.1 Control of Process-to-process Exchanger

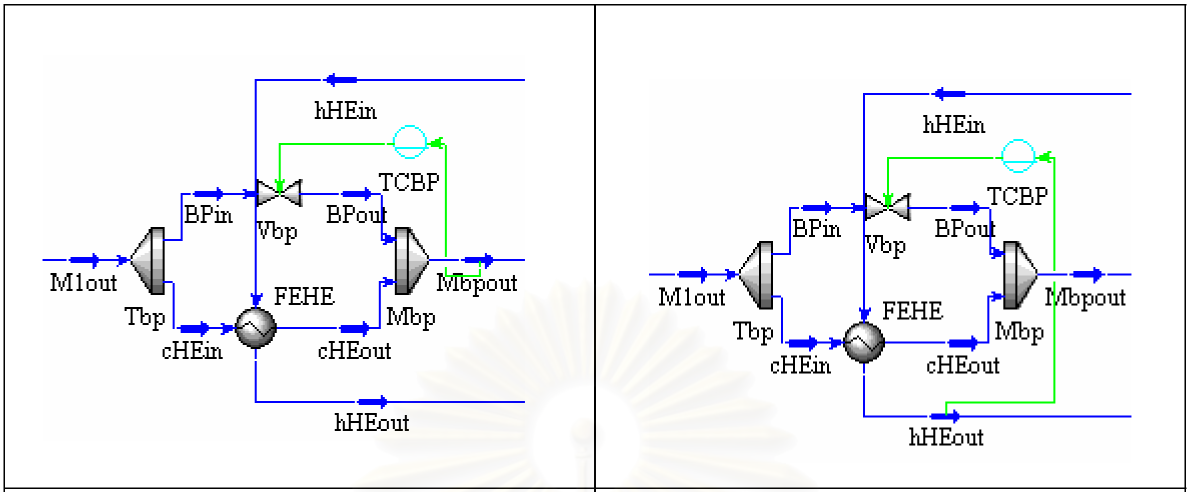
Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provided we can independently manipulate the two inlet flow rates.

In this current work four common alternatives about the bypass location and the control point were compared by using control structure namely reference control structure 1(REF1), Skogestad and Atonio (2006), as show in Figure 5.1-5.2.



(a) (b)

Figure 5.1: Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream (BP1); (b) controlling cold stream and bypassing hot stream (BP2)



(c) (d)

Figure 5.2: Bypass control of process-to-process heat exchangers. (c) Controlling and bypassing cold stream (BP3); (d) controlling hot stream and bypassing cold stream (BP4).

5.2 Dynamic Simulation Results for Four Alternatives of the Bypass Location and the Control Point of the Reference Control Structure1.

In order to evaluated the dynamic behaviors of the bypass control of process-to-process heat exchangers given by Skogestad and Atonio (2006) in HDA process alternative 1, several disturbance loads were made. The dynamic responses of four alternatives of the bypass location and the control point are shown in Figures 5.2-5.4. The pictures represent the dynamic behavior of the controlling and bypassing hot stream; controlling cold stream and bypassing hot stream; controlling and bypassing cold stream; controlling hot stream and bypassing cold stream respectively.

The disturbance testing is used to compare the dynamic response of four alternative of bypass control with Skogestad and Antonio (2006). By step change in the disturbance load of cold stream (Reactor feed stream), the disturbance load of hot stream (Reactor product stream) and change in the fresh toluene feed flowrates. Results for the disturbance load changes are as follows:

5.2.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Figure5.3 shows the dynamic responses of four alternative of bypass control of the reference control structure1 to a change in the disturbance load of cold stream (reactor feed stream). In order to make this disturbance, first the fresh feed toluene temperature is decreased from 100 to 80 $_{\circ}$F at time equals 60 minutes, and the temperature is increased from 80 to 120 $_{\circ}$F at time equals 180 minutes, then its temperature is returned to its nominal value of 100 $_{\circ}$F at time equals 300 minutes.

When disturbance load of cold stream change effect to cold steam inlet FEHE directly (Figure5.3a), thus it will result in slightly oscillated in reactor inlet temperature and reactor outlet temperature. The cold stream outlet FEHE (Figure5.3g) of bypassing and controlling at hot stream more oscillate than other alternatives. That response has effect to reactor inlet temperature (Figure5.3b), reactor outlet temperature (Figure5.3c) and quenches outlet temperature (Figure5.3d). The response of the controlling and bypassing cold (BP3) stream and the bypassing hot stream and controlling cold stream (BP2) have smaller oscillated than other structures. Controlling at cold stream small vacillate than controlling at hot stream. Controlling at cold stream spent small furnace heat duty (Figure5.3i) but lost cooler heat duty (Figure5.3j) differs from controlling at hot stream.

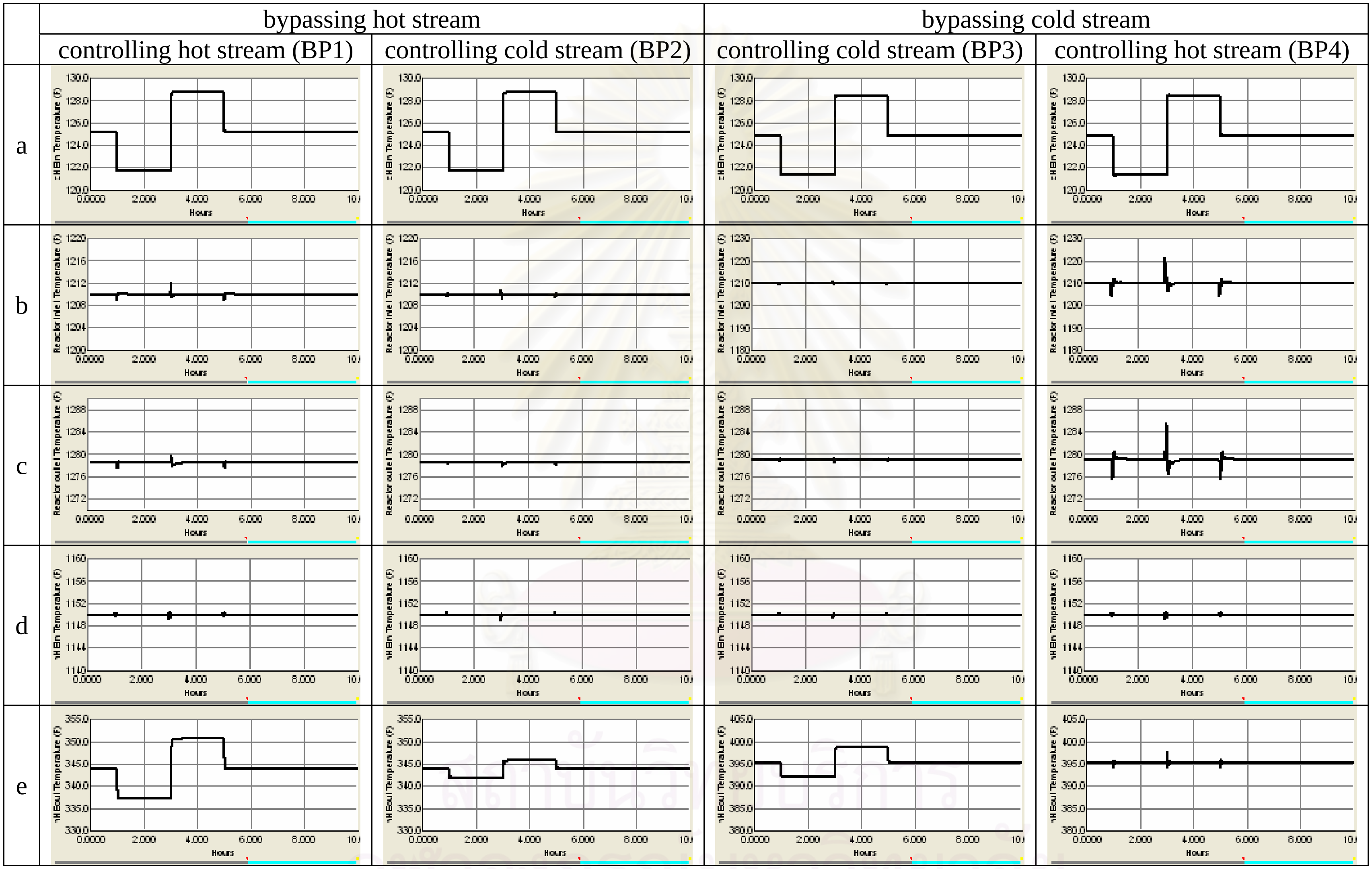


Figure 5.3 Dynamic responses of four alternative of bypass control to change in the disturbance load of cold stream.

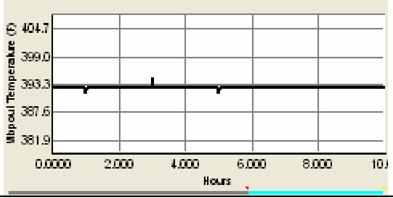
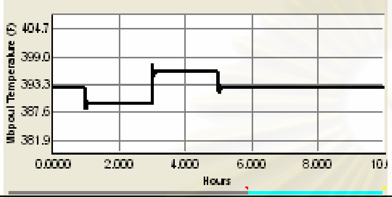
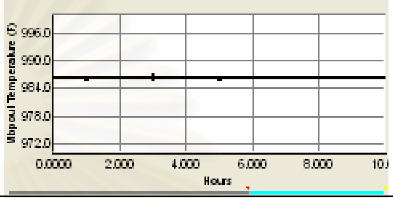
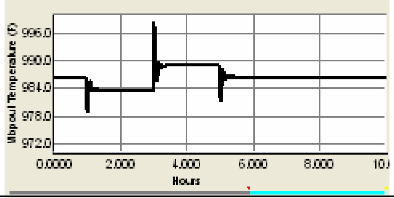
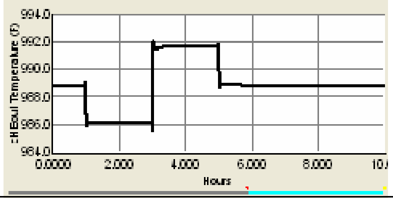
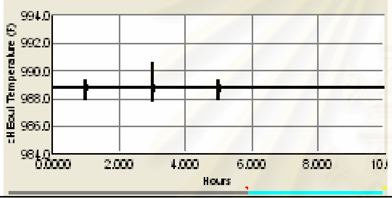
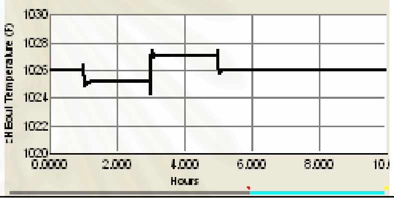
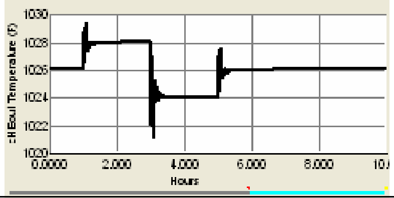
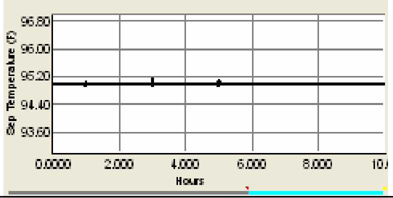
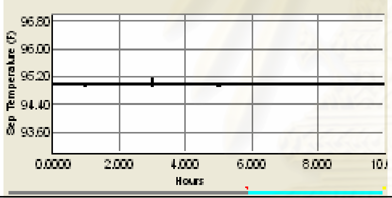
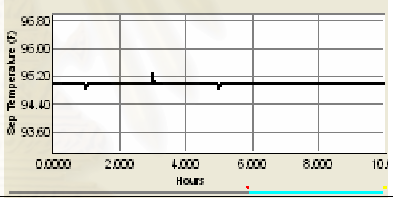
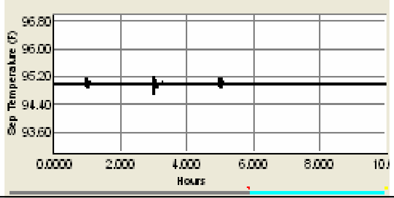
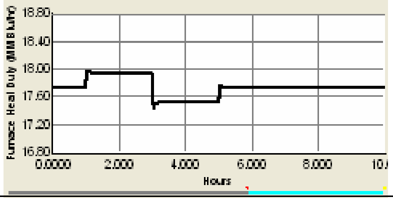
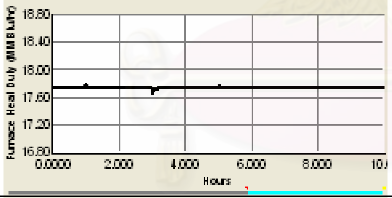
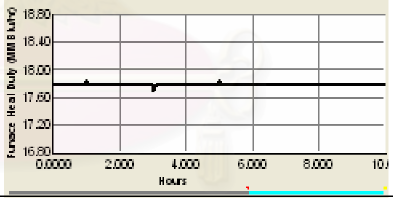
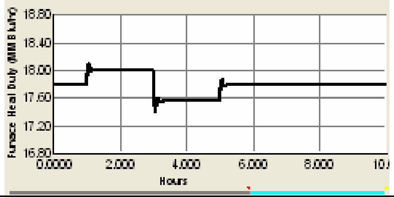
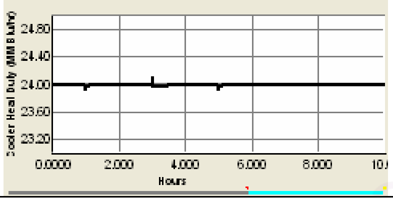
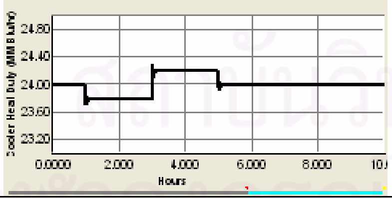
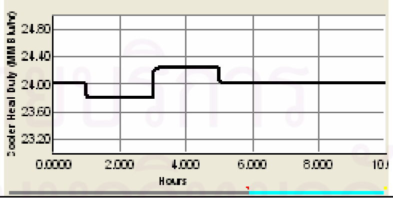
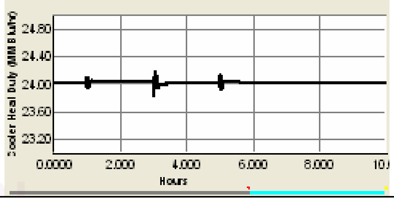
	bypassing hot stream		bypassing cold stream	
	controlling hot stream (BP1)	controlling cold stream (BP2)	controlling cold stream (BP3)	controlling hot stream (BP4)
f				
g				
h				
i				
j				

Figure 5.3 Dynamic responses of four alternative of bypass control to change in the disturbance load of cold stream

5.2.2 Change in the Disturbance Load of Hot Stream (Reactor Product Stream)

Figure5.4 shows the dynamic responses of four alternative of bypass control of the reference control structure1 to a change in the disturbance load of hot stream (Reactor product stream). In order to make this disturbance, first the hot inlet temperature of FEHE (i.e. stream hHEin in Figure 5.1) is decreased from 1150 to 1130 $_\circ$F at time equals 60 minutes, and the temperature is increased from 1130 to 1170 $_\circ$F at time equals 180 minutes, then its temperature is returned to its nominal value of 1150 $_\circ$F at time equals 300 minutes.

As can be seen, when change in the hot inlet temperature of FEHE (Figure 5.4d), thus hot outlet temperature and cold outlet temperature more oscillated. Then, there are effect to swing in reactor inlet temperature (Figure 5.4b), reactor outlet temperature (Figure 5.4c) and separator temperature (Figure 5.4h). Controlling hot stream (BP1 and BP4) more oscillate than other alternatives. Hot stream outlet FEHE (Figure 5.4e) of controlling at cold stream (BP2 and BP3) more swing because we do not control them. Controlling at hot stream (BP1 and BP4) more lost in furnace heat duty (Figure 5.4i) and in cooler heat duty (Figure 5.4j).

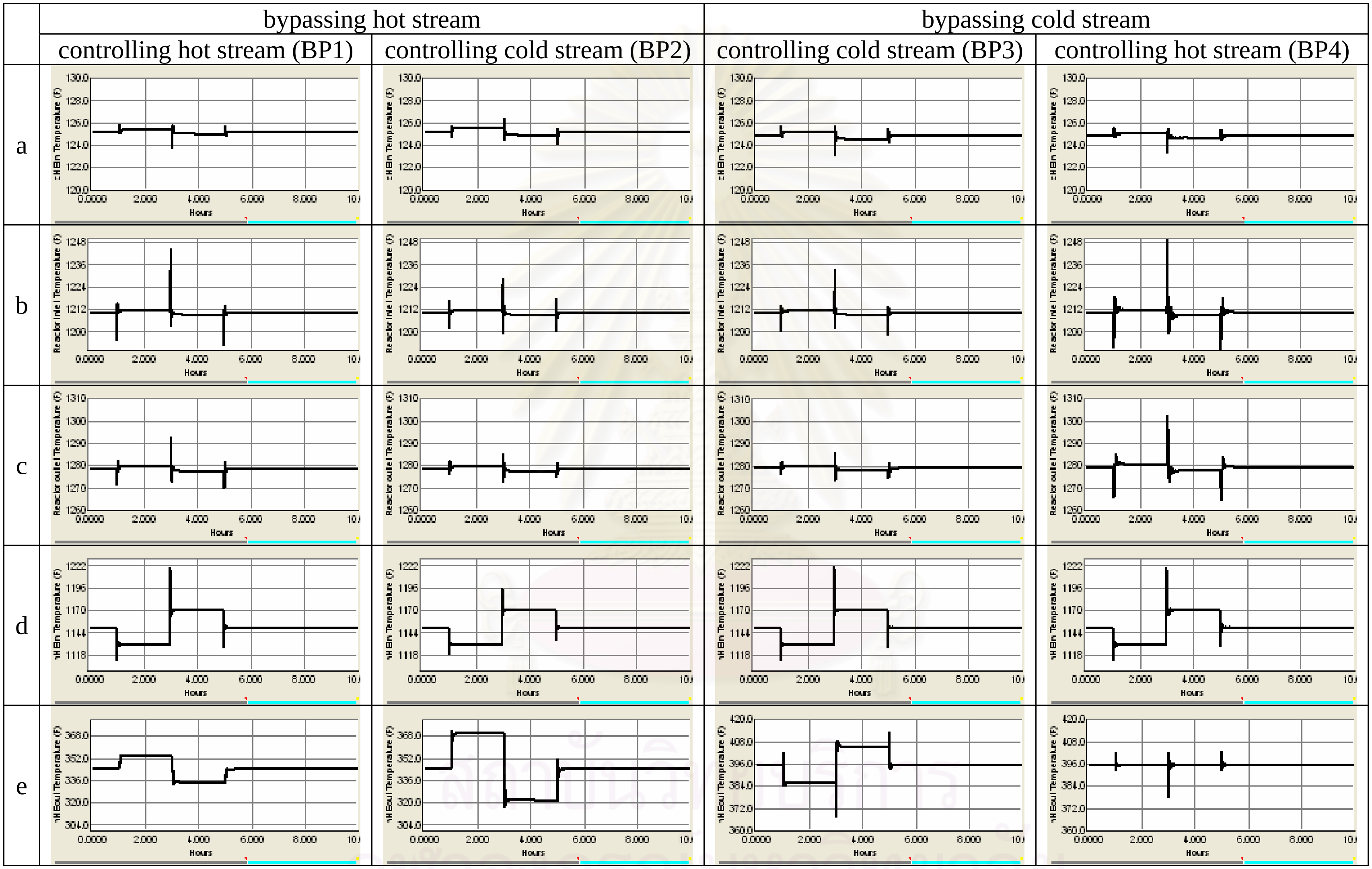


Figure 5.4 Dynamic responses of four alternative of bypass control to change in the disturbance load of hot stream.

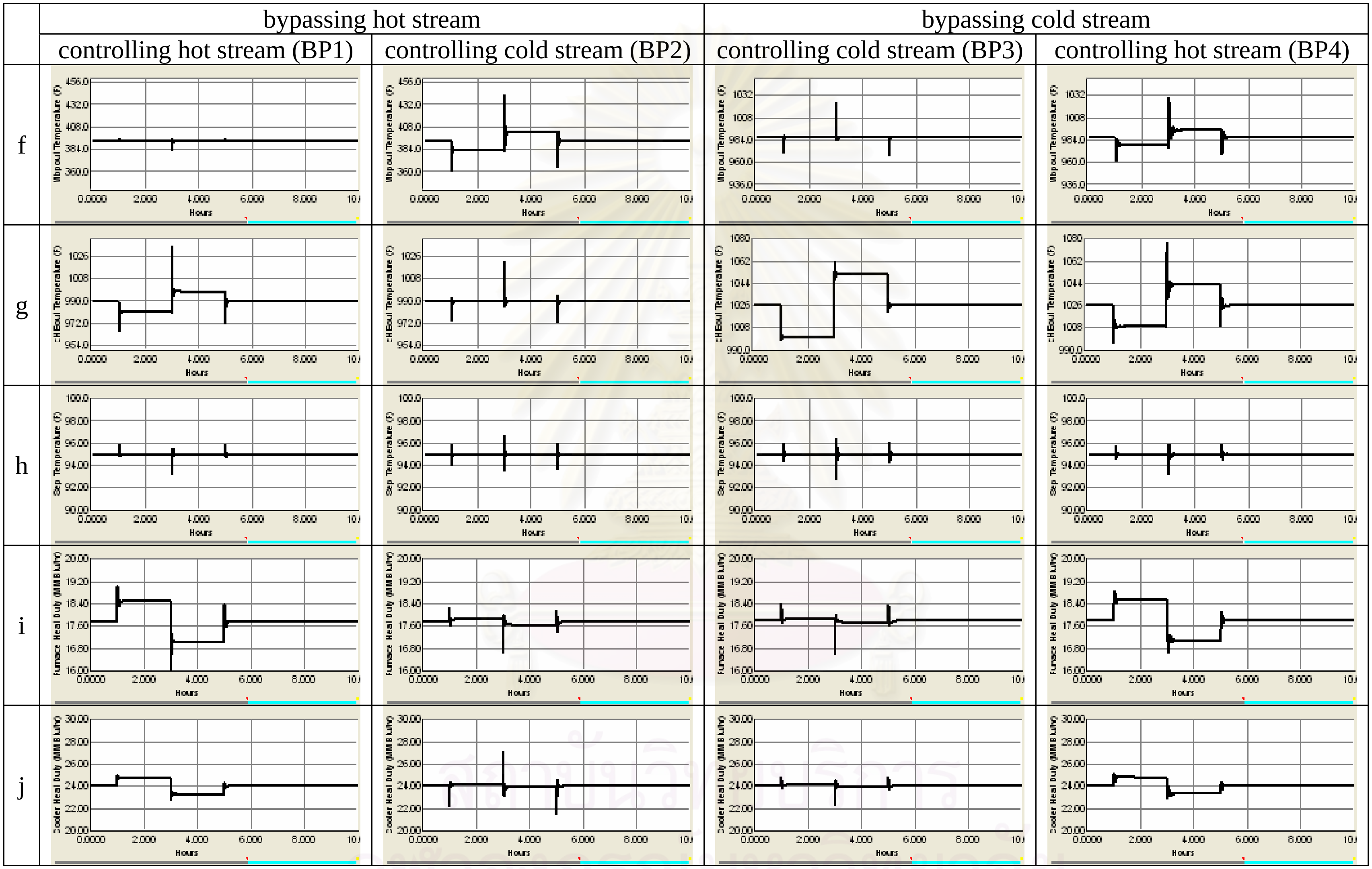


Figure 5.4 Dynamic responses of four alternative of bypass control to change in the disturbance load of hot stream.

5.2.3 Change in the Fresh Toluene Feed Flowrates

Figure5.5 shows the dynamic responses of four alternative of bypass control of the reference control structure1 to a change in the disturbance load of hot stream (Reactor product stream). In order to make this disturbance, first the hot inlet temperature of FEHE (i.e. stream hHEin in Figure 5.1) is decreased from 1150 to 1130 ∘F at time equals 60 minutes, and the temperature is increased from 1130 to 1170 ∘F at time equals 180 minutes, then its temperature is returned to its nominal value of 1150 ∘F at time equals 300 minutes.

As can be seen, when change in the fresh toluene feed, thus cold inlet temperature (Figure 5.5a), reactor inlet temperature (Figure 5.5b) and reactor outlet temperature (Figure 5.5c) more oscillated especially bypassing at cold stream and controlling at hot stream (BP4). Controlling hot stream (BP1 and BP4) more oscillate than other alternatives. Separator temperature (Figure 5.5h) of bypassing at cold stream (BP3 and BP4) more oscillate. All of alternatives more lost in furnace heat duty and in cooler heat duty. Bypassing at hot stream and controlling at cold stream (BP2) and bypassing and controlling at cold stream (BP3) nearly lost in furnace heat duty (Figure 5.5i) and cooler heat duty (Figure 5.5j).

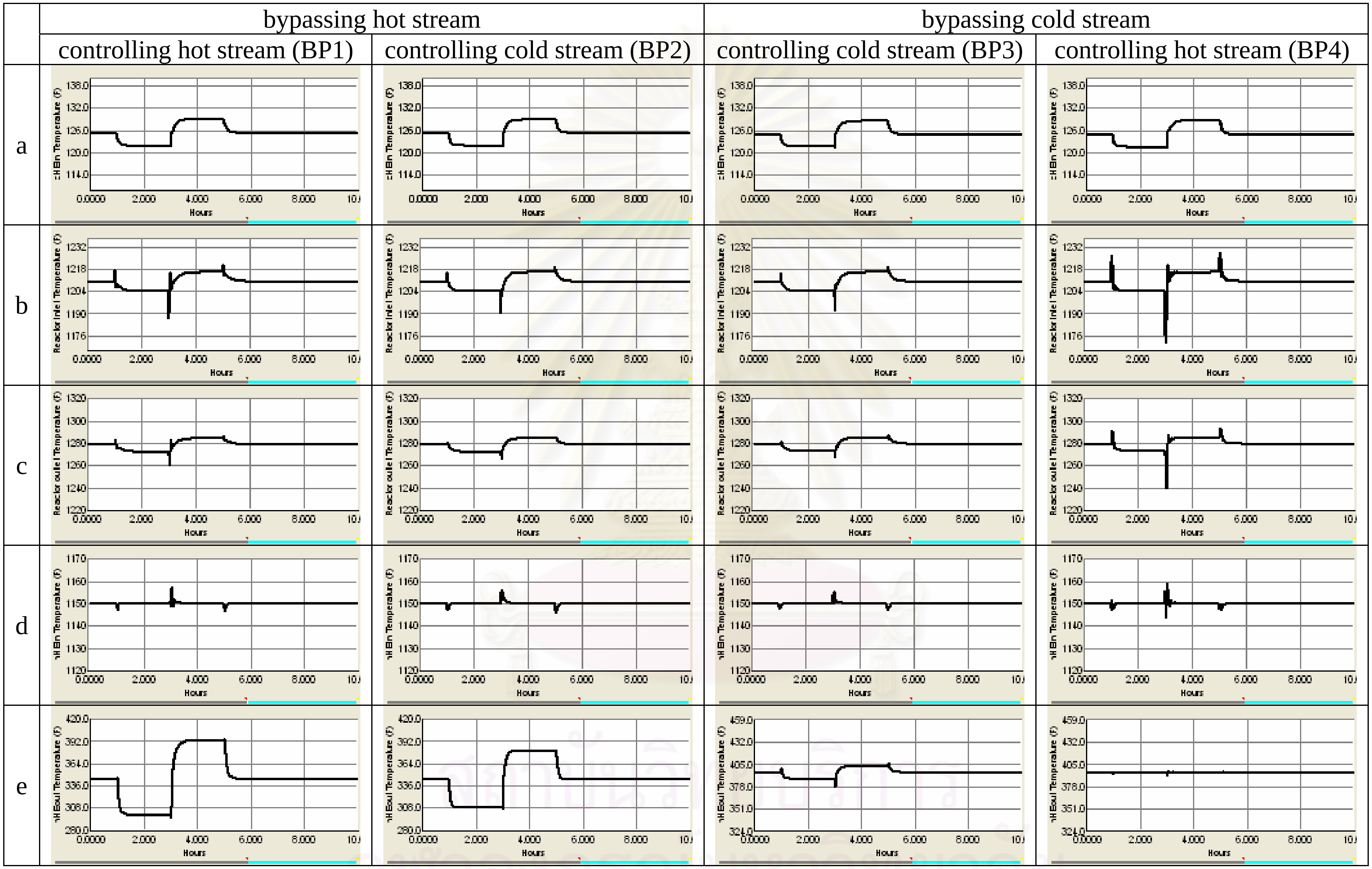


Figure 5.5 Dynamic responses of four alternative of bypass control to change in the fresh toluene flowrates.

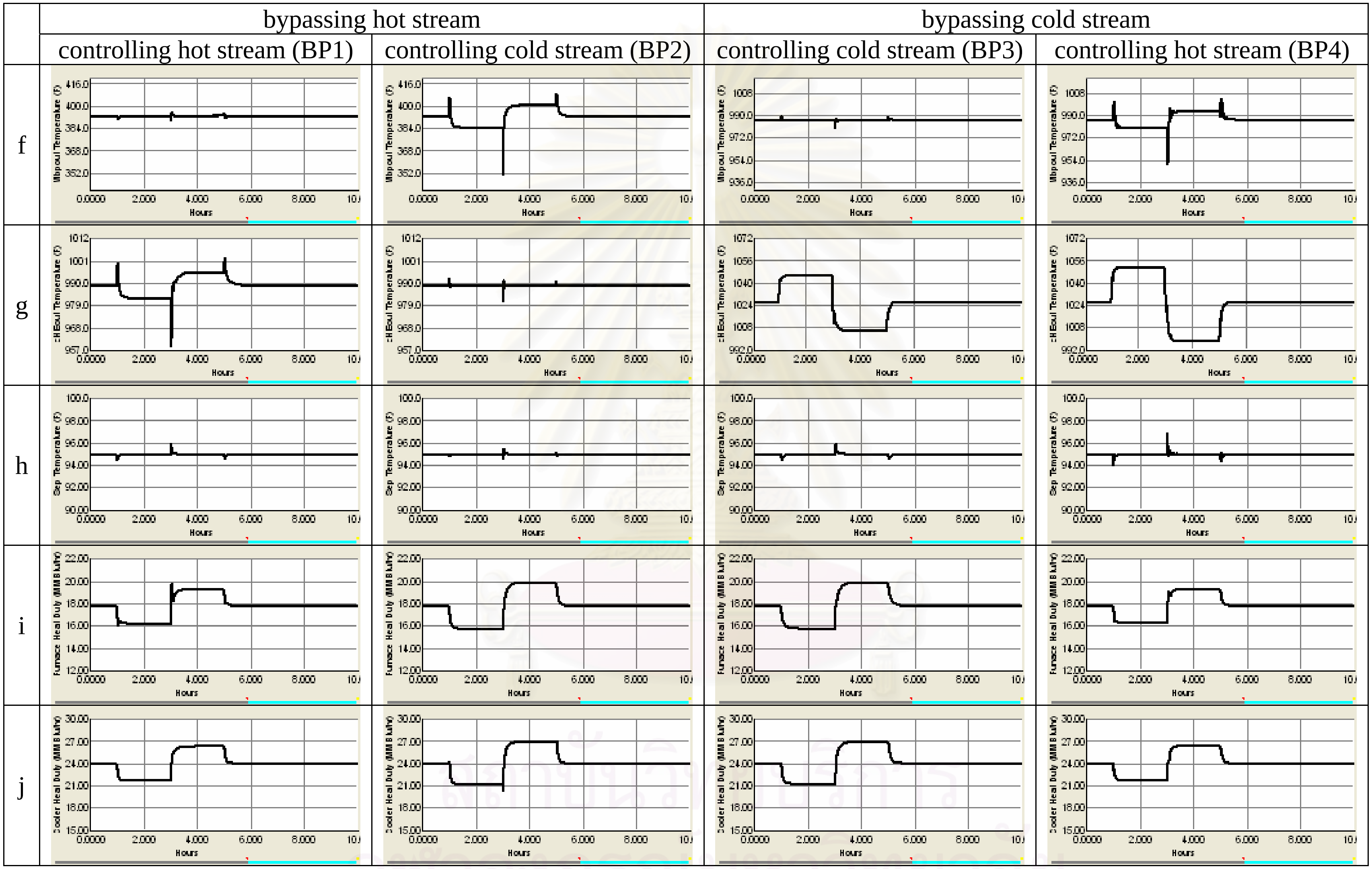


Figure 5.5 Dynamic responses of four alternative of bypass control to change in the fresh toluene flowrates.

5.3 Evaluation of the Dynamic Performance of Four Alternatives of the Bypass Location and the Control Point of the Reference Control Structure1.

In this section, IAE method is used to evaluate the dynamic performance of four alternative of bypass control. Table 5.1-5.4 shows the IAE results for the change in the dynamic disturbance in reaction section of HDA process with temperature control loops in different alternative control structure (BP1, BP2, BP3 and BP4) respectively.

Table 5.1-5.4 shows the IAE results of four alternative of bypass control to change in disturbance load cold stream, hot stream and toluene flowrates. When change in disturbance load hot stream and toluene flowrates, the bypassing and controlling at cold stream (BP3) has small the summation of IAE value more than others, as can see in Table5.3. This alternative good control in toluene flowrates disturbance because bypassing and controlling at cold stream help to reduce disturbance effect to temperature in process. The bypassing at hot stream and controlling at cold stream has small the summation of IAE value when change in disturbance load cold stream, as can see in Table5.2. However, the summation value of IAE value in bypassing and controlling at cold stream (BP3) smaller than other bypass control structure because bypassing and controlling at cold stream rescues disturbance effect in system.

Table 5.1 The IAE results of the bypassing and controlling hot stream (BP1) of the reference control structure 1 (REF1).

Bypassing hot stream-Controlling hot stream (BP1)			
	Cold stream	Hot Stream	Toluene flowrate
TCBP	4.2578	6.1947	60.359
TCQ	2.8075	79.009	54.212
TCR	7.595	44.994	63.364
TCS	0.33909	3.7984	5.9452
Reactor outlet Temp	13.708	302.4	1393.8
SUM	28.70739	436.3961	1577.68

Table 5.2 The IAE results of the bypassing hot stream controlling cold stream (BP2) of the reference control structure 1 (REF1).

Bypassing hot stream-Controlling cold stream (BP2)			
	Cold stream	Hot Stream	Toluene flowrate
TCBP	2.2493	42.047	16.79
TCQ	1.1925	72.563	80.589
TCR	1.7525	18.835	57.36
TCS	0.36825	4.0343	2.9971
Reactor outlet Temp	2.8792	277.64	1412.4
SUM	8.44175	415.1193	1570.136

Table 5.3 The IAE results of the bypassing cold stream controlling cold stream (BP3) of the reference control structure 1 (REF1).

<table>
<tr><th colspan="4">Bypassing cold stream-Controlling cold stream (BP3)</th></tr>
<tr><th></th><th>Cold stream</th><th>Hot Stream</th><th>Toluene flowrate</th></tr>
<tr><td>TCBP</td><td>2.607</td><td>46.58</td><td>29.806</td></tr>
<tr><td>TCQ</td><td>1.157</td><td>70.525</td><td>49.513</td></tr>
<tr><td>TCR</td><td>2.126</td><td>23.421</td><td>59.598</td></tr>
<tr><td>TCS</td><td>0.810</td><td>6.775</td><td>8.602</td></tr>
<tr><td>Reactor outlet Temp</td><td>3.188</td><td>265.53</td><td>1394.9</td></tr>
<tr><td>SUM</td><td>9.888</td><td>412.831</td><td>1542.424</td></tr>
</table>

Table 5.4 The IAE results of the bypassing cold stream controlling hot stream (BP4) of the reference control structure 1 (REF1).

<table>
<tr><th colspan="4">Bypassing cold stream-Controlling hot stream (BP4)</th></tr>
<tr><th></th><th>Cold stream</th><th>Hot Stream</th><th>Toluene flowrate</th></tr>
<tr><td>TCBP</td><td>6.2963</td><td>22.118</td><td>12.479</td></tr>
<tr><td>TCQ</td><td>12.914</td><td>100.86</td><td>60.16</td></tr>
<tr><td>TCR</td><td>53.786</td><td>169.51</td><td>285.4</td></tr>
<tr><td>TCS</td><td>1.4215</td><td>6.5776</td><td>7.3366</td></tr>
<tr><td>Reactor outlet Temp</td><td>75.64</td><td>445.79</td><td>1601</td></tr>
<tr><td>SUM</td><td>150.0578</td><td>744.8556</td><td>1966.376</td></tr>
</table>

5.4 Dynamic Simulation Results of Variation of Heat Exchanger Size for Four Controls Structure Alternatives (REF1, CS1, CS2, CS3).

From section 5.2 bypass locations and control points were scrutinized. The bypassing and controlling at cold stream was selected because the IAE result of this structure is smaller than others. The bypassing and controlling at cold stream help to reduce effect of disturbance to temperature in process. In this section, the bypassing and controlling at cold stream was simulated in the reference control structure1 (REF1) and our control structure (CS1, CS2 and CS3). The furnace heat duty was changed by the variation of heat exchanger duty. We separate the duty of heat exchanger into four sizes; the smallest duty is 4.59 MBtu/hr (HS1), next 5.32 MBtu/hr (HS2), 6.09 MBtu/hr (HS3) and the largest duty is 6.88 MBtu/hr (HS4) respectively.

The disturbance testing is used to compare the dynamic response of control structure alternative of variation of heat exchanger duty. By step change in the disturbance load of cold stream (Reactor feed stream), the disturbance load of hot stream (Reactor product stream) and change in the fresh toluene feed flowrates. Results for the disturbance load changes are as follows:

5.4.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Figure5.6-5.9 shows the dynamic responses of the variation of heat exchanger size (HS1, HS2, HS3 and HS4) of the reference control structure1 (REF1) and our control structure (CS1, CS2 and CS3) to a change in the disturbance load of cold stream (reactor feed stream). In order to make this disturbance, first the fresh feed toluene temperature is decreased from 100 to 80 $_{o}$F at time equals 60 minutes, and the temperature is increased from 80 to 120 $_{o}$F at time equals 180 minutes, then its temperature is returned to its nominal value of 100 $_{o}$F at time equals 300 minutes.

As can be seen, when change in disturbance cold stream (Figure 5.6-5.9a) effect to slightly swing in reactor inlet temperature (Figure 5.6-5.9c), reactor outlet temperature (Figure 5.6-5.9d), quench outlet temperature (Figure 5.6-5.9f) and separator temperature (Figure 5.6-5.9h). That response has much effect to cold stream outlet FEHE (Figure 5.6-5.9b) of the small size (HS1) because the small size has small area for receive the exchange energy. The change in cold stream inlet FEHE has direct effect to hot stream outlet FEHE (Figure 5.6-5.9g) because we do not control in hot stream. The hot stream outlet has more effect to separator temperature (Figure 5.6-5.9h) of large size heat exchanger (HS4) because the largest size heat exchanger has smallest cooler duty. Four control structures (REF1, CS1, CS2 and CS3) have the same response but what control structure is good dynamic performance we can see in section 5.5 describes about the IAE results of each control structure.

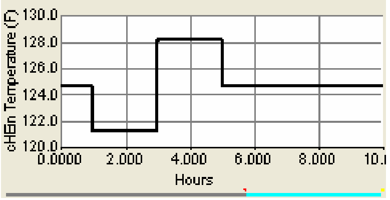
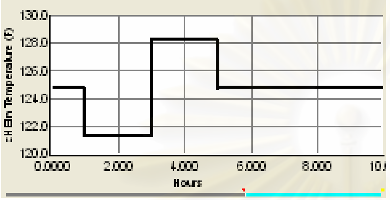
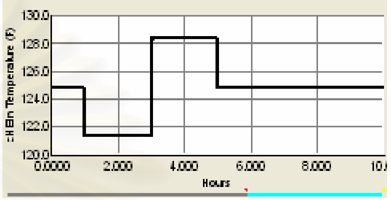
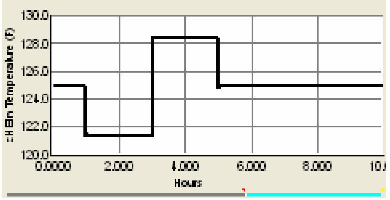
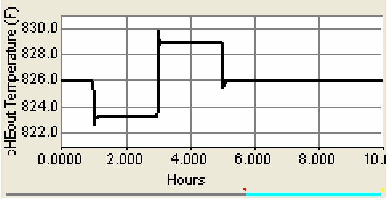
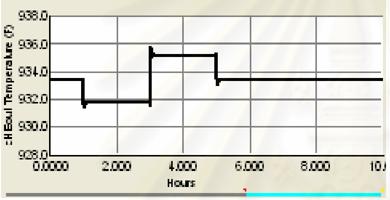
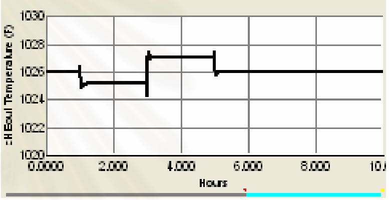
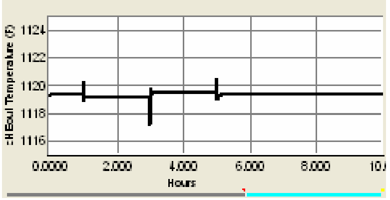
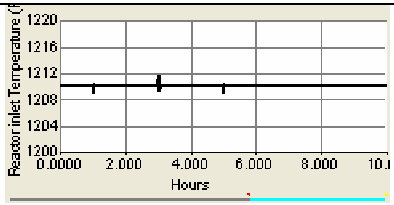
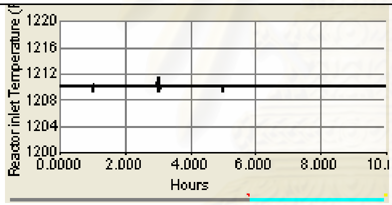
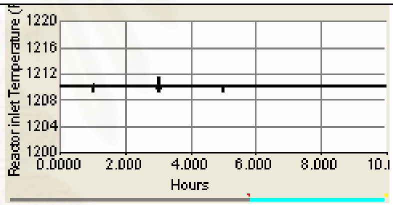
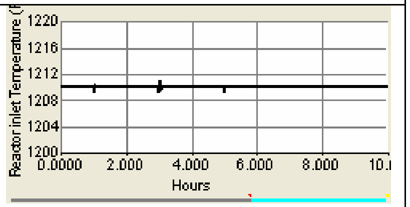
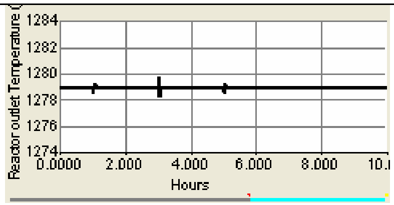
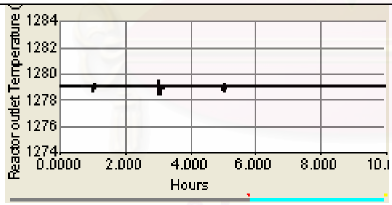
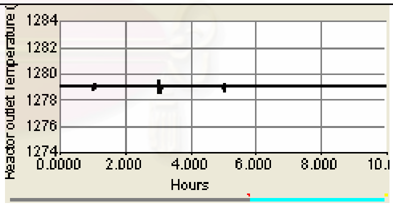
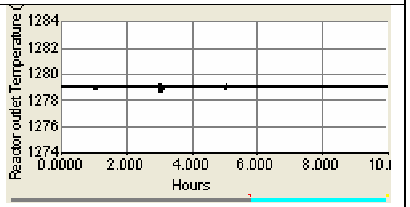
	HS1	HS2	HS3	HS4
a				
b				
c				
d				

Figure 5.6 Dynamic response of the variation of heat exchanger of reference control structure (REF1) to change in disturbance load cold stream

	HS1	HS2	HS3	HS4

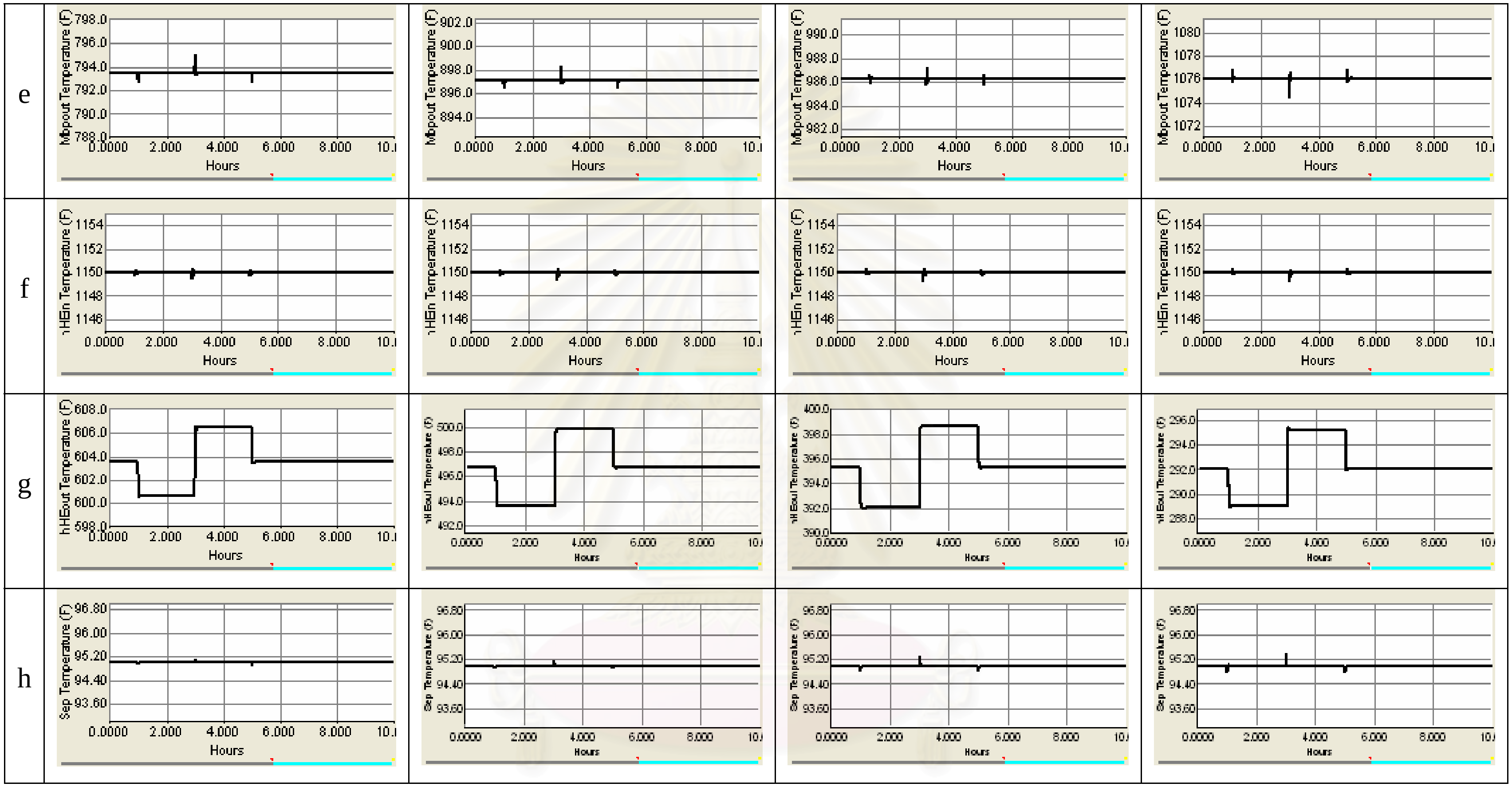


Figure 5.6 Dynamic response of the variation of heat exchanger of reference control structure (REF1) to change in disturbance load cold stream

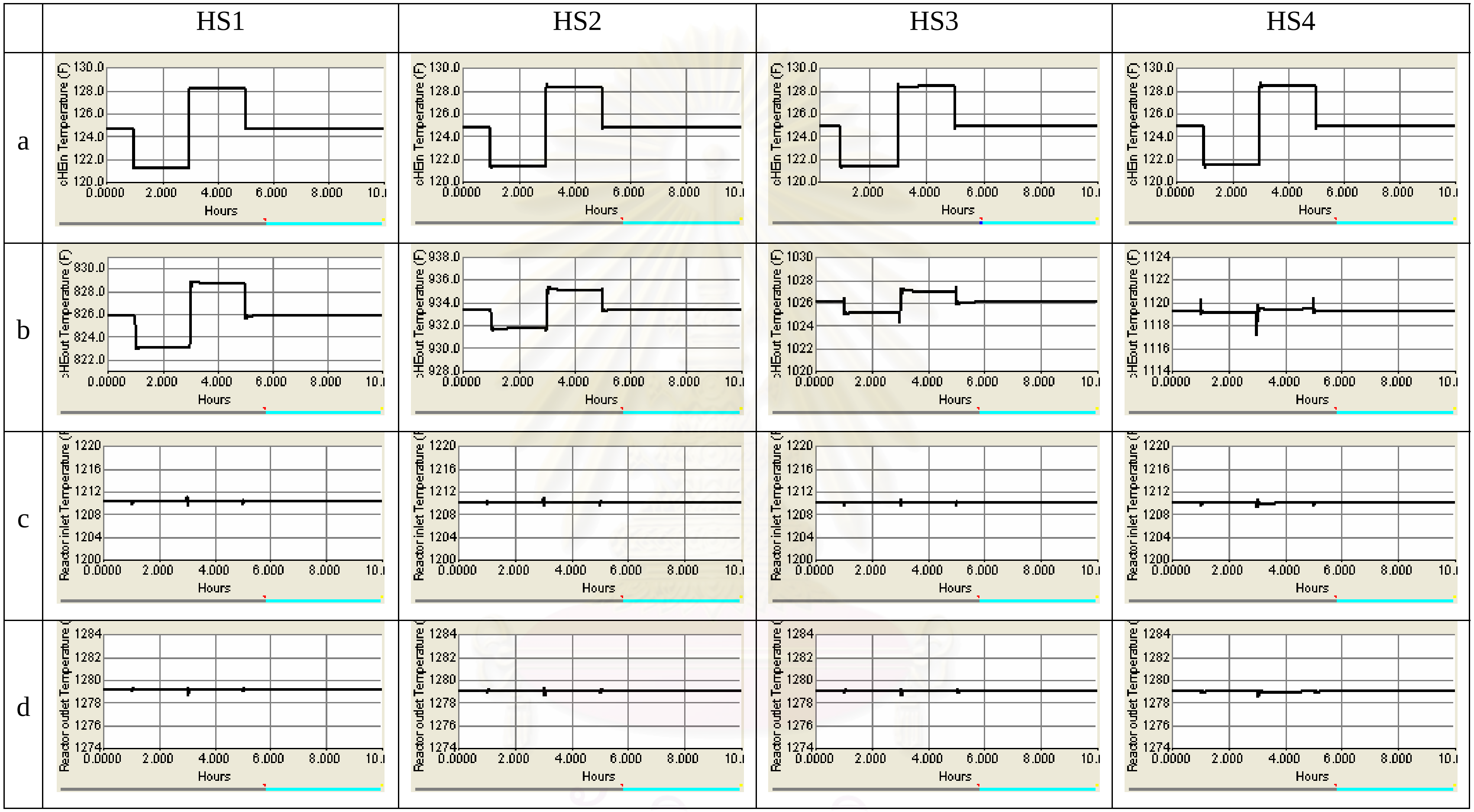


Figure 5.7 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance load cold stream

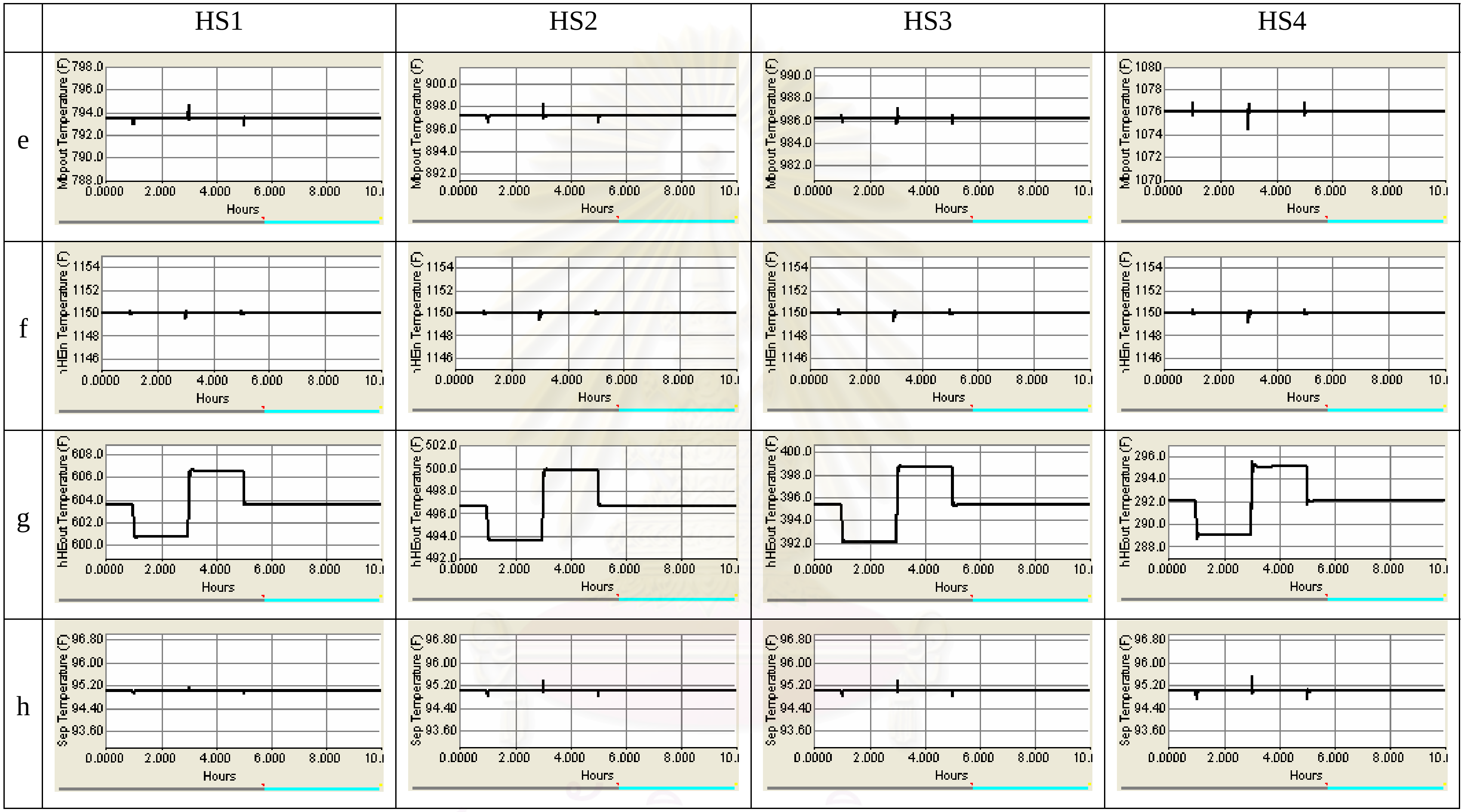


Figure 5.7 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance load cold stream

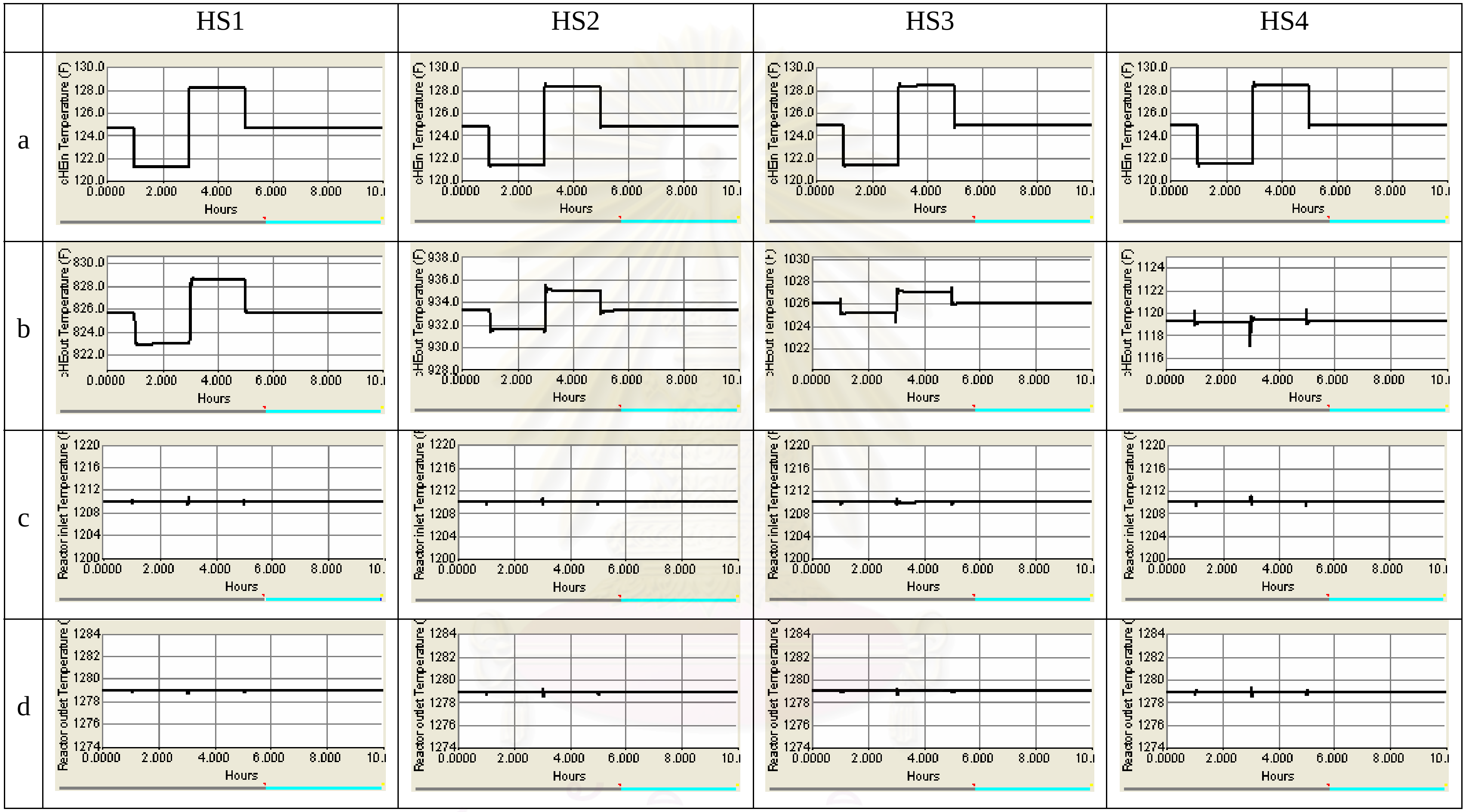


Figure 5.8 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance load cold stream

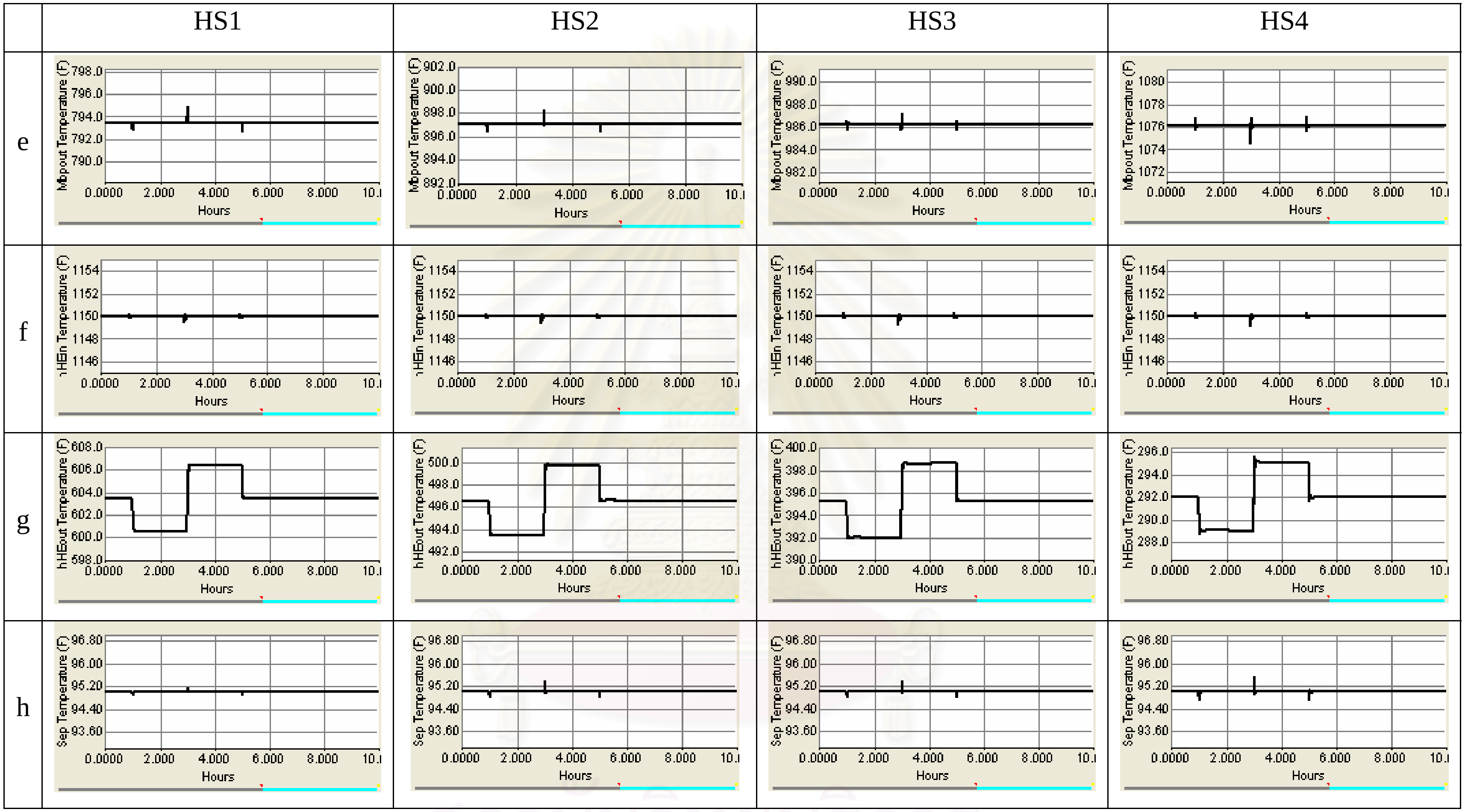


Figure 5.8 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance load cold stream

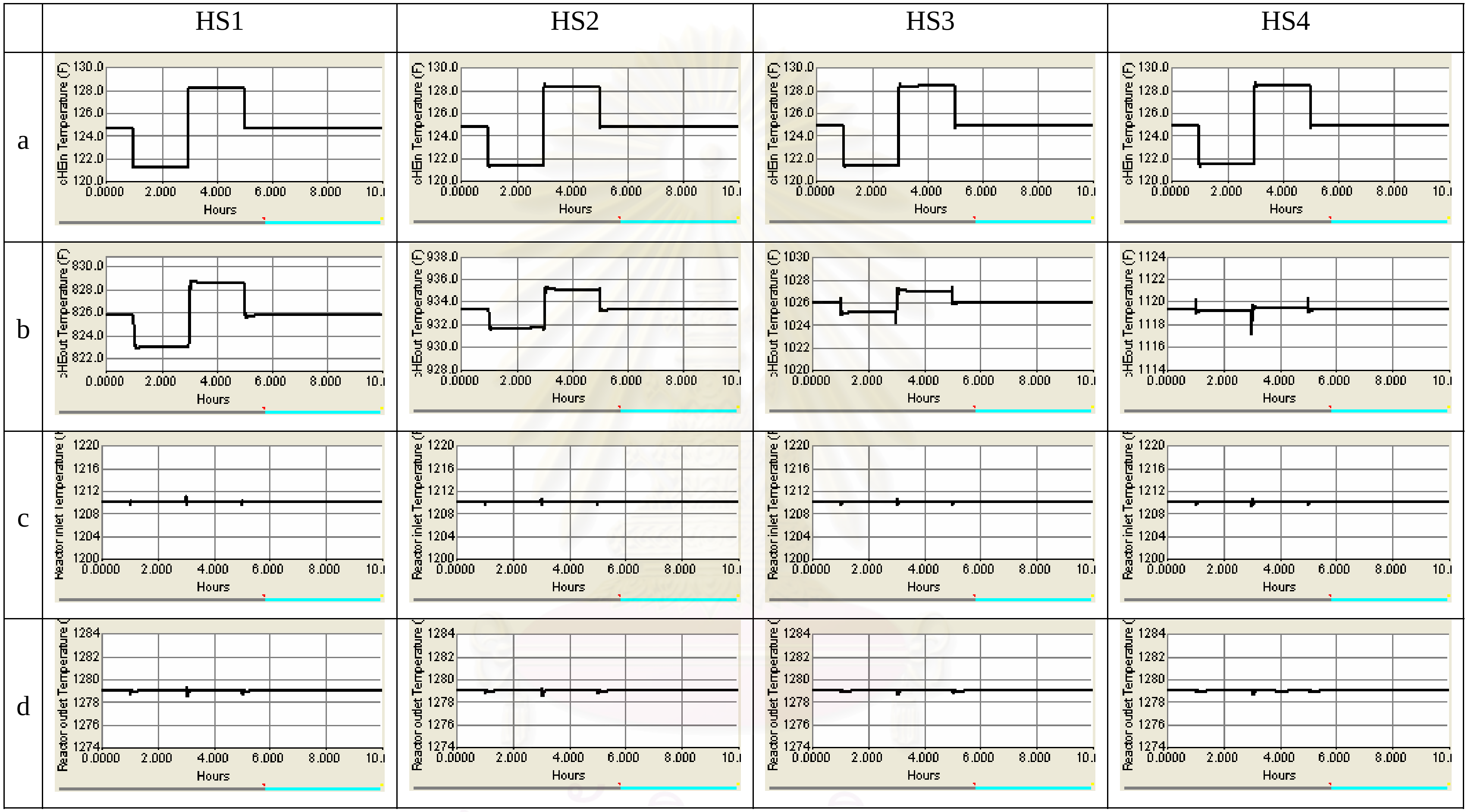


Figure 5.9 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance load cold stream

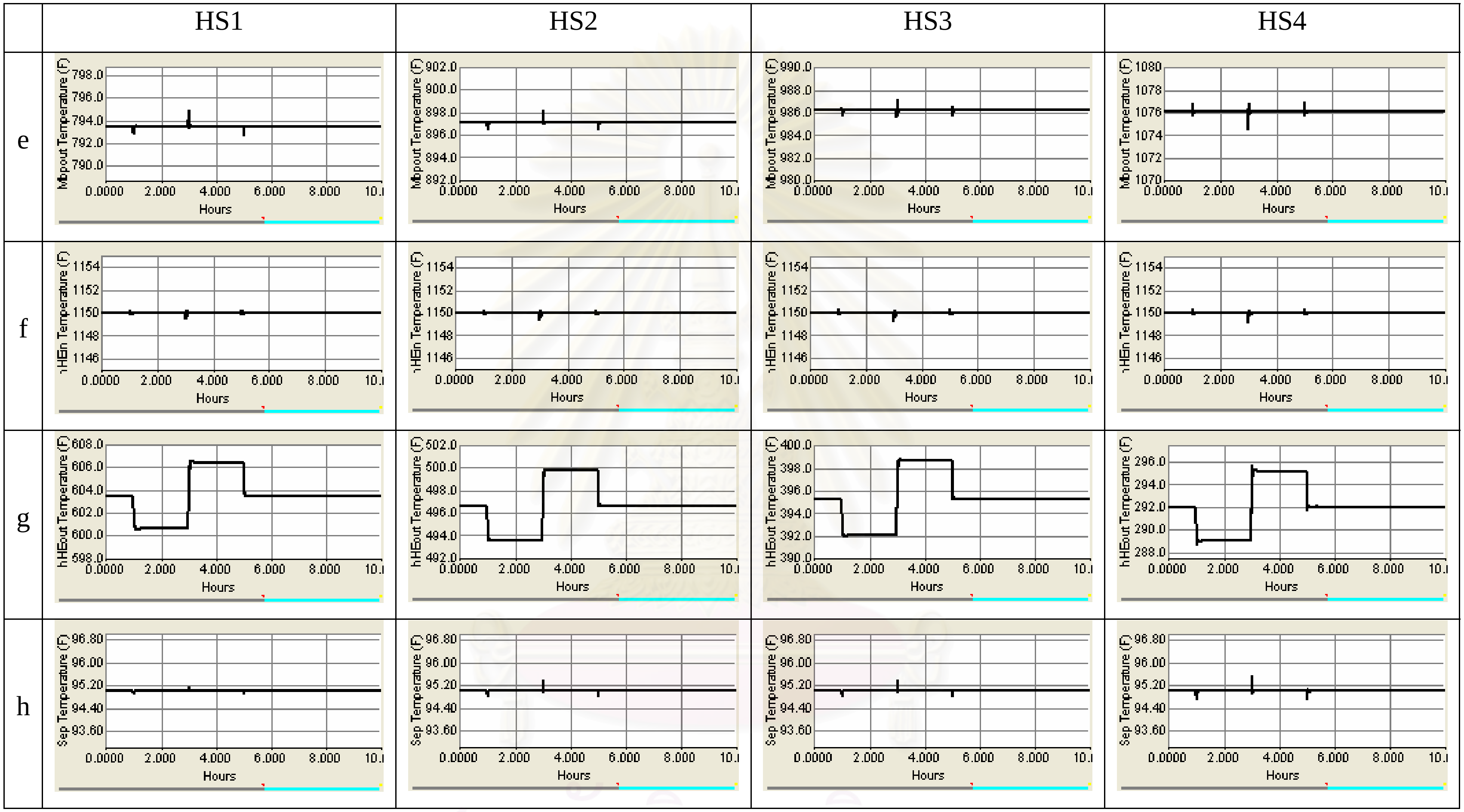


Figure 5.9 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance load cold stream

5.4.2 Change in the Disturbance Load of Hot Stream (Reactor Product Stream)

Figure5.10-5.13 shows the dynamic responses of the variation of heat exchanger size (HS1, HS2, HS3 and HS4) of the reference control structure1 (REF1) and our control structure (CS1, CS2 and CS3) to a change in the disturbance load of hot stream (Reactor product stream). In order to make this disturbance, first the hot inlet temperature of FEHE (i.e. stream hHEin in Figure 5.1) is decreased from 1150 to 1130 $_{\circ}$F at time equals 60 minutes, and the temperature is increased from 1130 to 1170 $_{\circ}$F at time equals 180 minutes, then its temperature is returned to its nominal value of 1150 $_{\circ}$F at time equals 300 minutes.

As can be seen, when change in disturbance load hot stream more oscillate in hot stream inlet FEHE (Figure 5.10-5.13f) effect to hot stream outlet FEHE (Figure 5.10-5.13g) and cold stream outlet FEHE (Figure 5.10-5.13b). This response has extreme effect to separator temperature (Figure 5.10-5.13h) and reactor inlet temperature (Figure 5.10-5.13c) of the largest size of heat exchanger because the large size of heat exchanger has the smallest duty of cooler and furnace to handle disturbance. Four control structures (REF1, CS1, CS2 and CS3) have the same response but what control structure is good dynamic performance we can see in section 5.5 describes about the IAE results of each control structure.

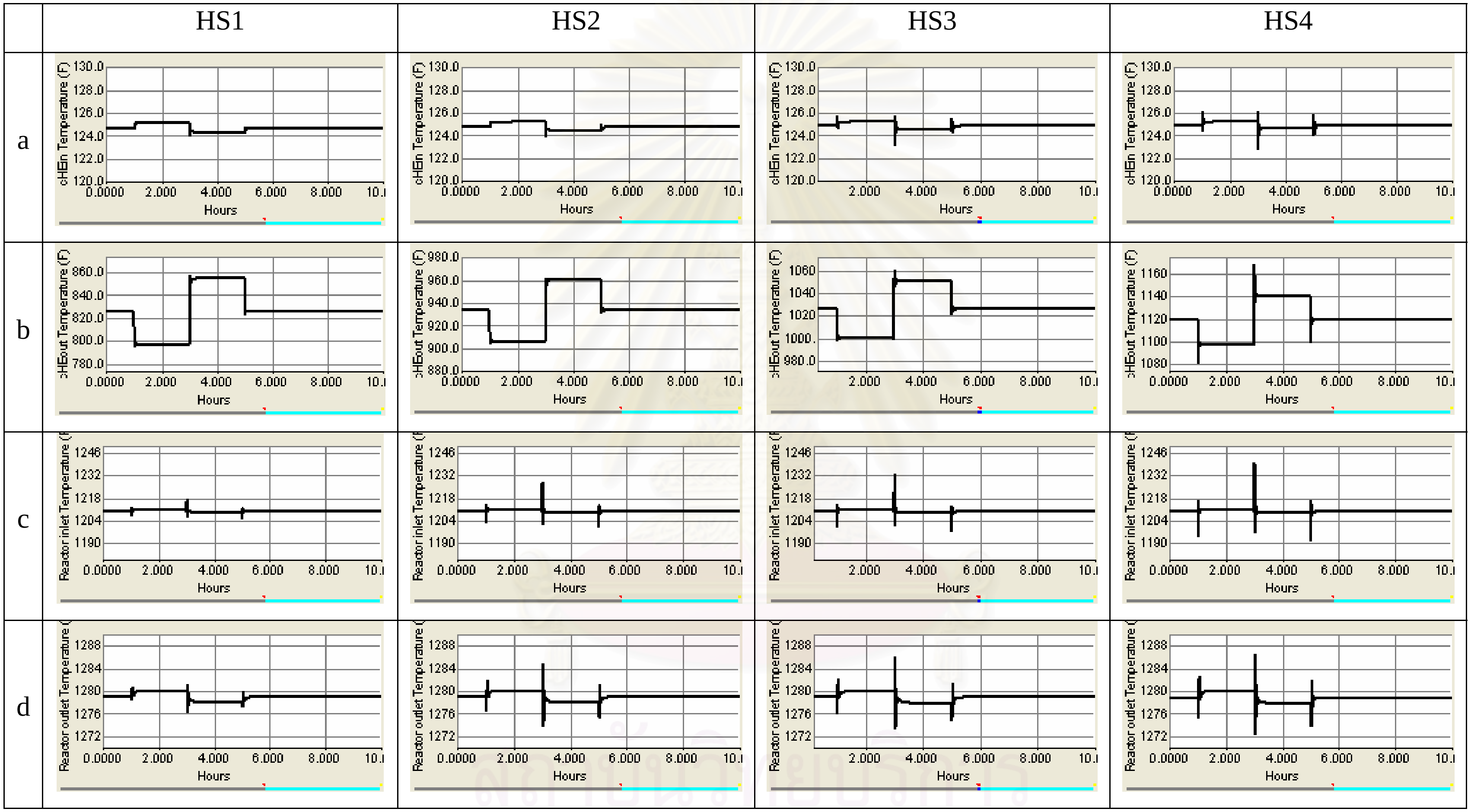


Figure 5.10 Dynamic response of the variation of heat exchanger of the reference control structure1 (REF1) to change in disturbance load hot stream

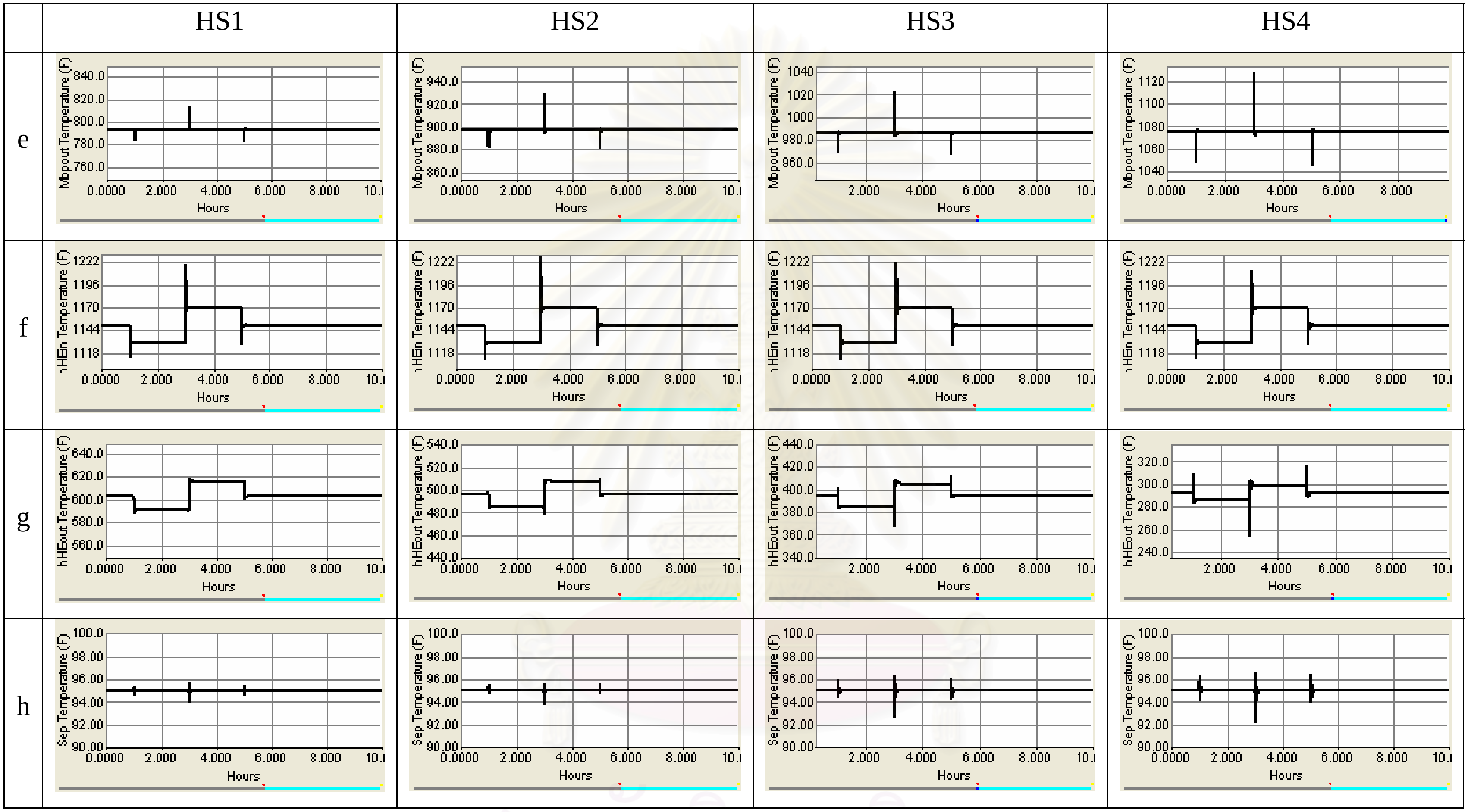


Figure 5.10 Dynamic response of the variation of heat exchanger of the reference control structure1 (REF1) to change in disturbance load hot stream

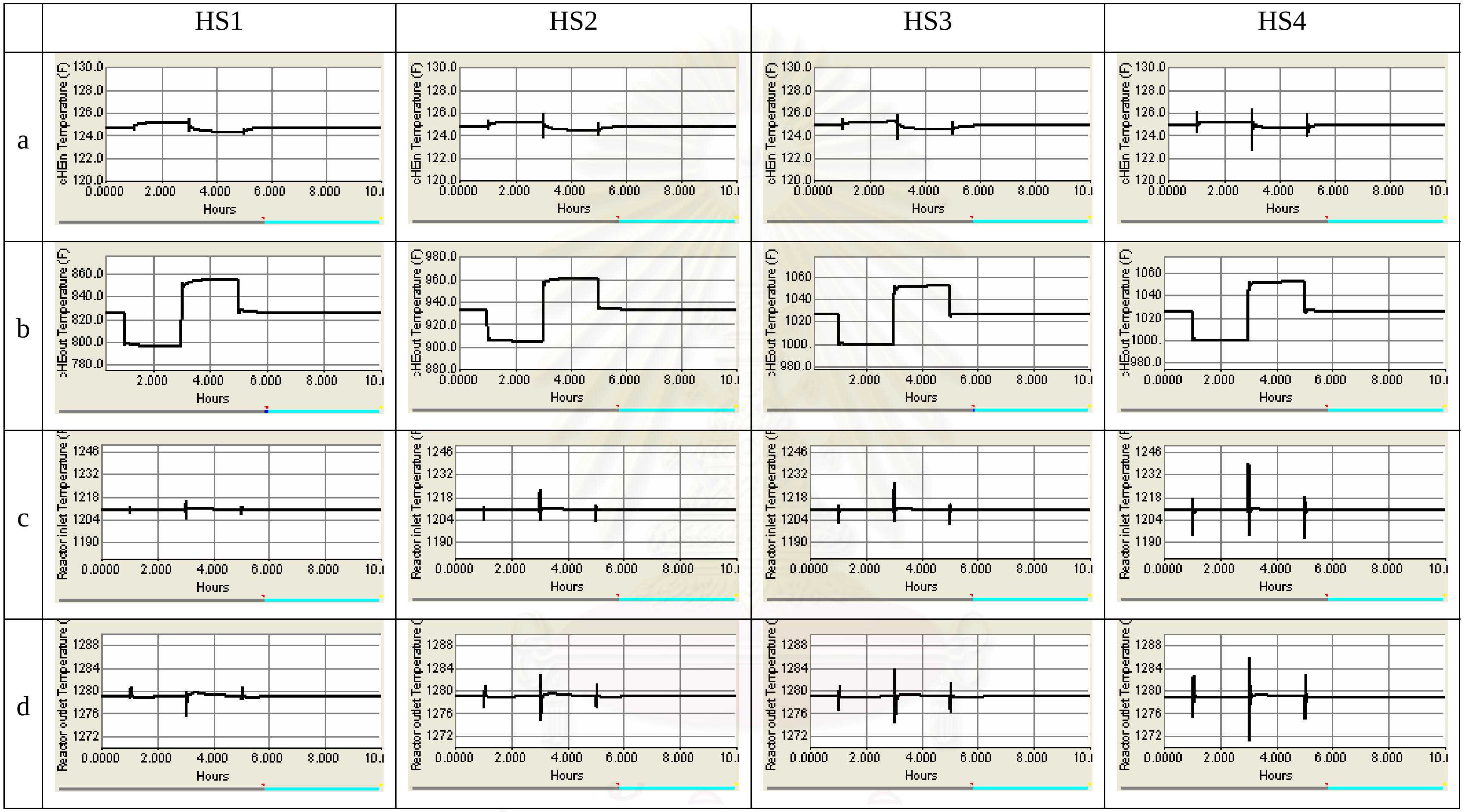


Figure 5.11 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance load hot stream

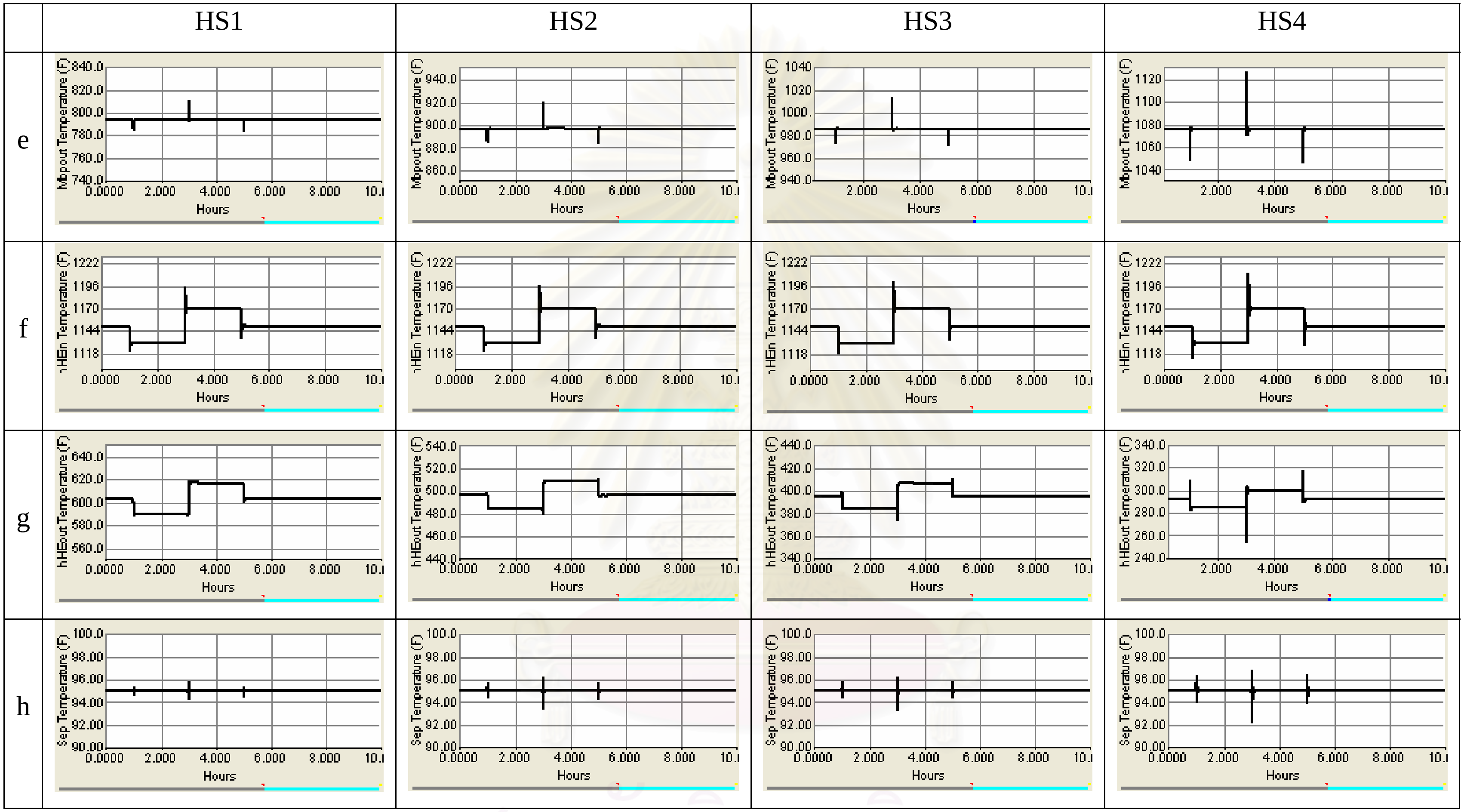


Figure 5.11 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance load hot stream

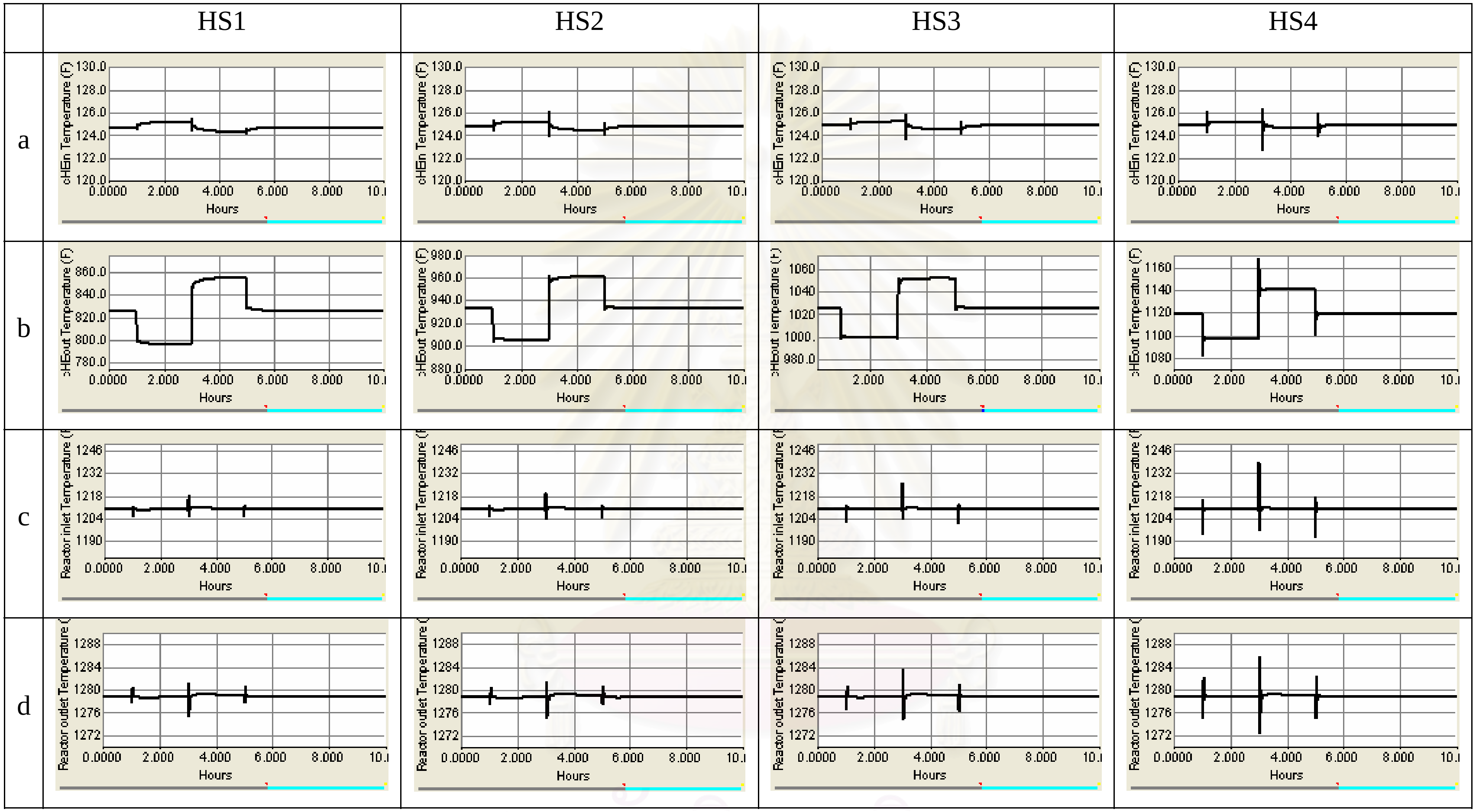


Figure 5.12 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance load hot stream

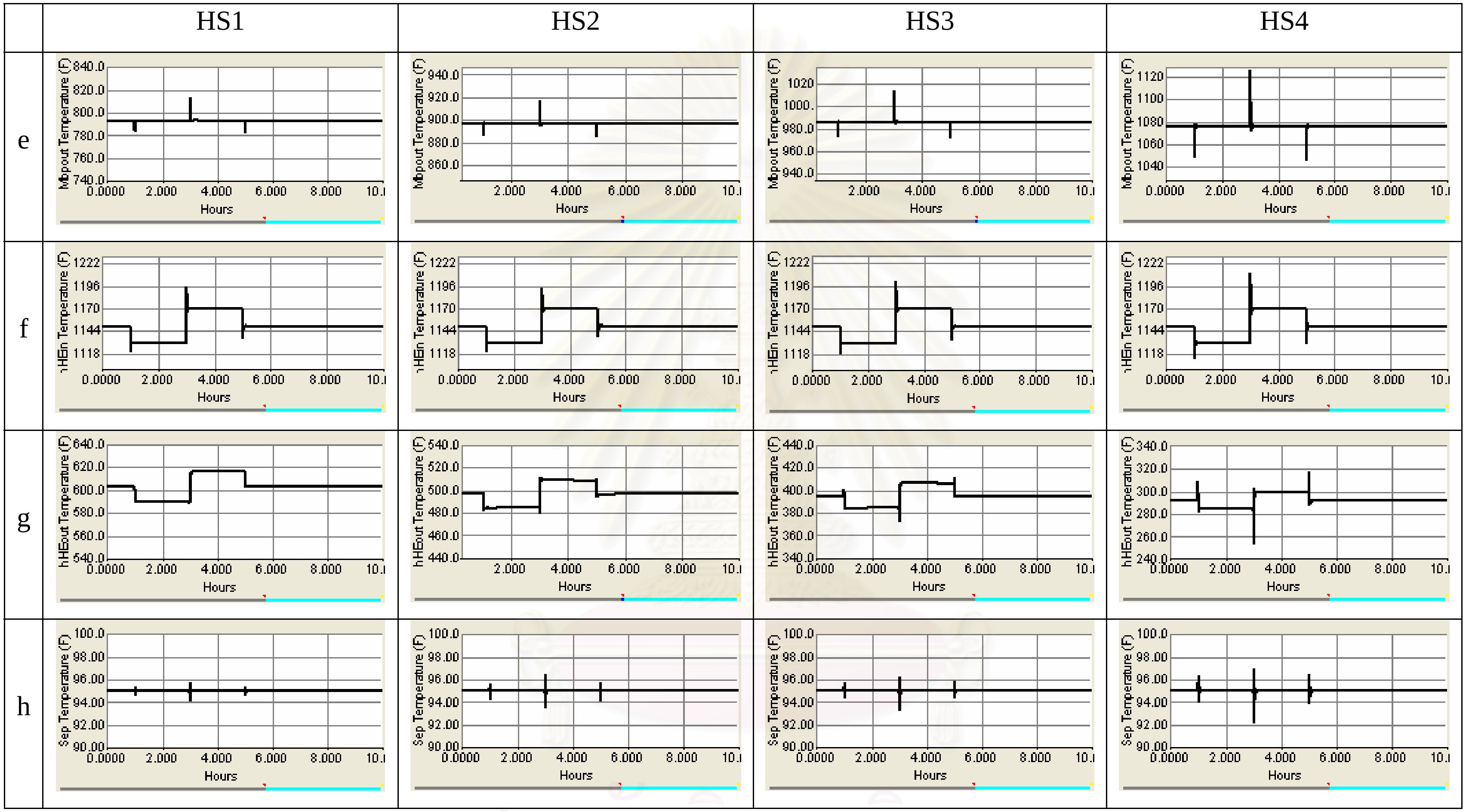


Figure 5.12 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance load hot stream

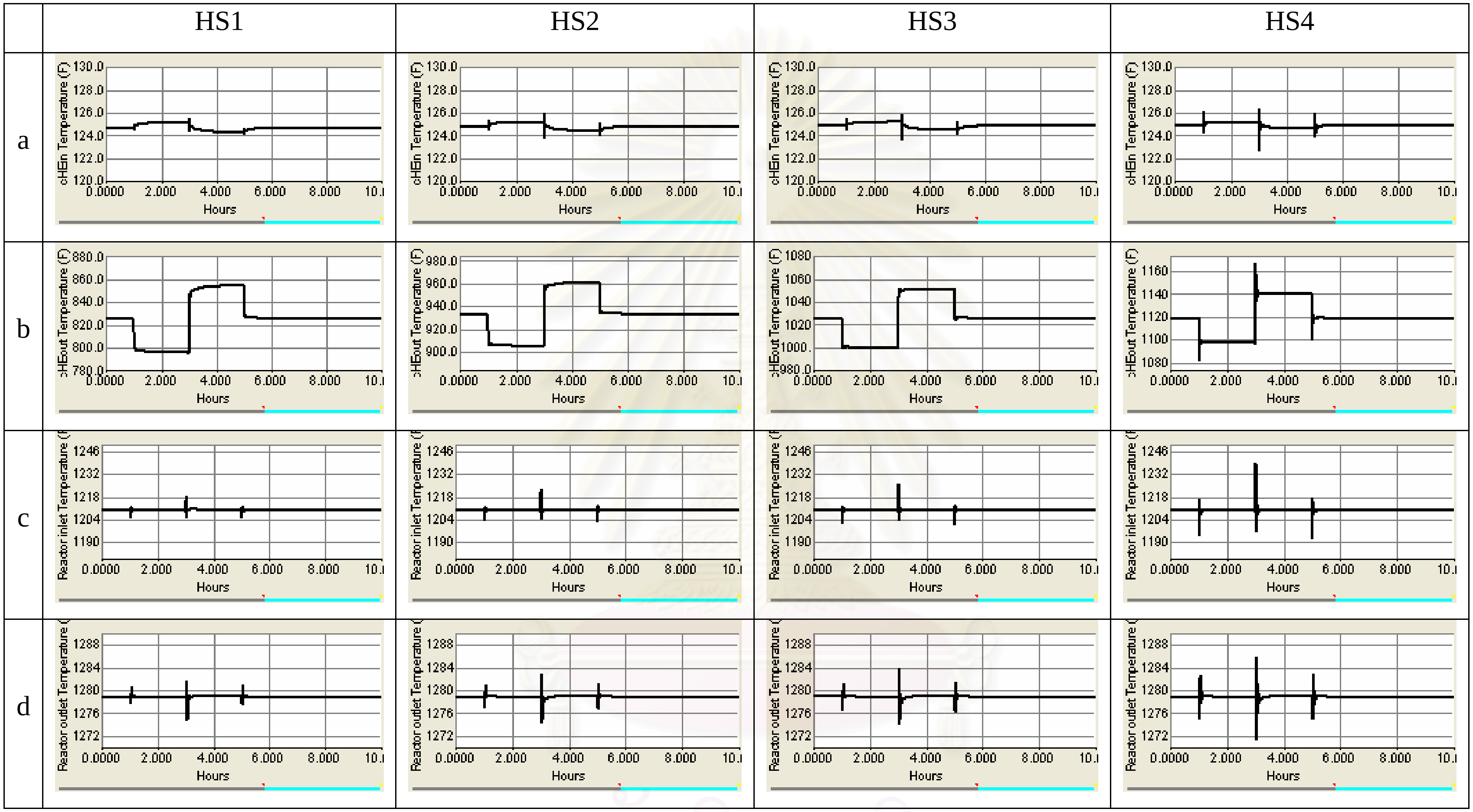


Figure 5.13 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance load hot stream

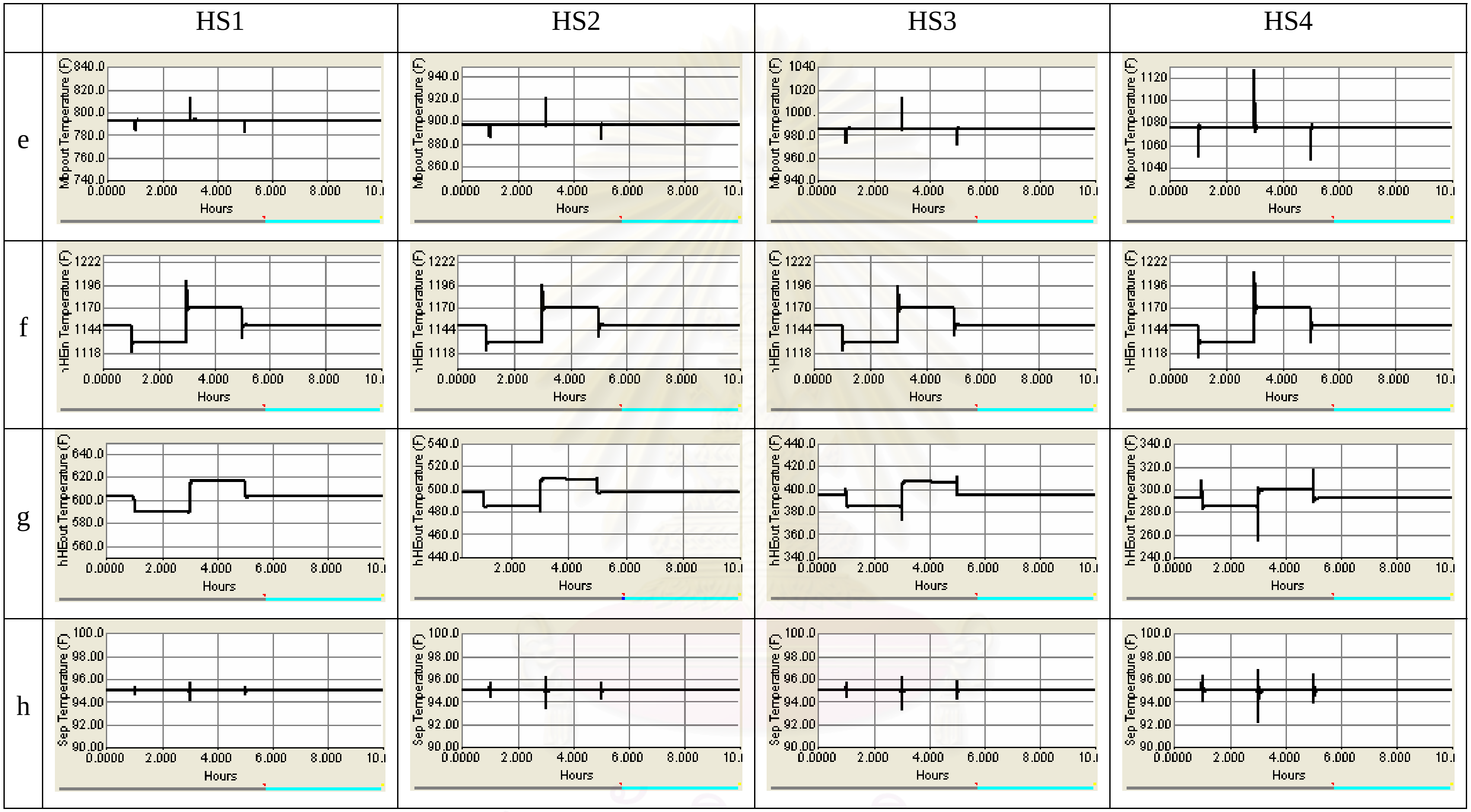


Figure 5.13 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance load hot stream

5.4.3 Change in the Fresh Toluene Feed Flowrates

Figure5.14-5.17 shows the dynamic responses of the variation of heat exchanger size (HS1, HS2, HS3 and HS4) of the reference control structure1 (REF1) and our control structure (CS1, CS2 and CS3) to a change in the disturbance load of hot stream (Reactor product stream). In order to make this disturbance, first the fresh toluene feed flowrate (i.e. stream FFTOL in Figure 5.1) is decreased from 300 to 270 lbmole/hr at time equals 60 minutes, and the fresh toluene feed flowrate is increased from 270 to 330 lbmole/hr at time equals 180 minutes, then its flowrate is returned to its nominal value of 300 lbmole/hr at time equals 300 minutes.

As can be seen, when change in fresh toluene feed flowrates effect to more step change in cold stream inlet FEHE (Figure 5.14-5.17a), reactor inlet temperature (Figure 5.14-5.17c) and reactor outlet temperature (Figure 5.14-5.17c) of the smallest heat exchanger size because the small size has small area to receive the exchange energy of increase in toluene flowrates. This disturbance has extreme effect to the outlet mixer temperature (Figure 5.14-5.17e) of the smallest heat exchanger size because bypass valve fully open or close can not control the outlet mixer temperature at its setpoint. This response has small effect to separator temperature (Figure 5.14-5.17h) and reactor inlet temperature (Figure 5.14-5.17c) of the smallest size of heat exchanger because the smallest size of heat exchanger has the largest duty of cooler and furnace to handle disturbance. Four control structures (REF1, CS1, CS2 and CS3) have the same response but what control structure is good dynamic performance we can see in section 5.5 describes about the IAE results of each control structure.

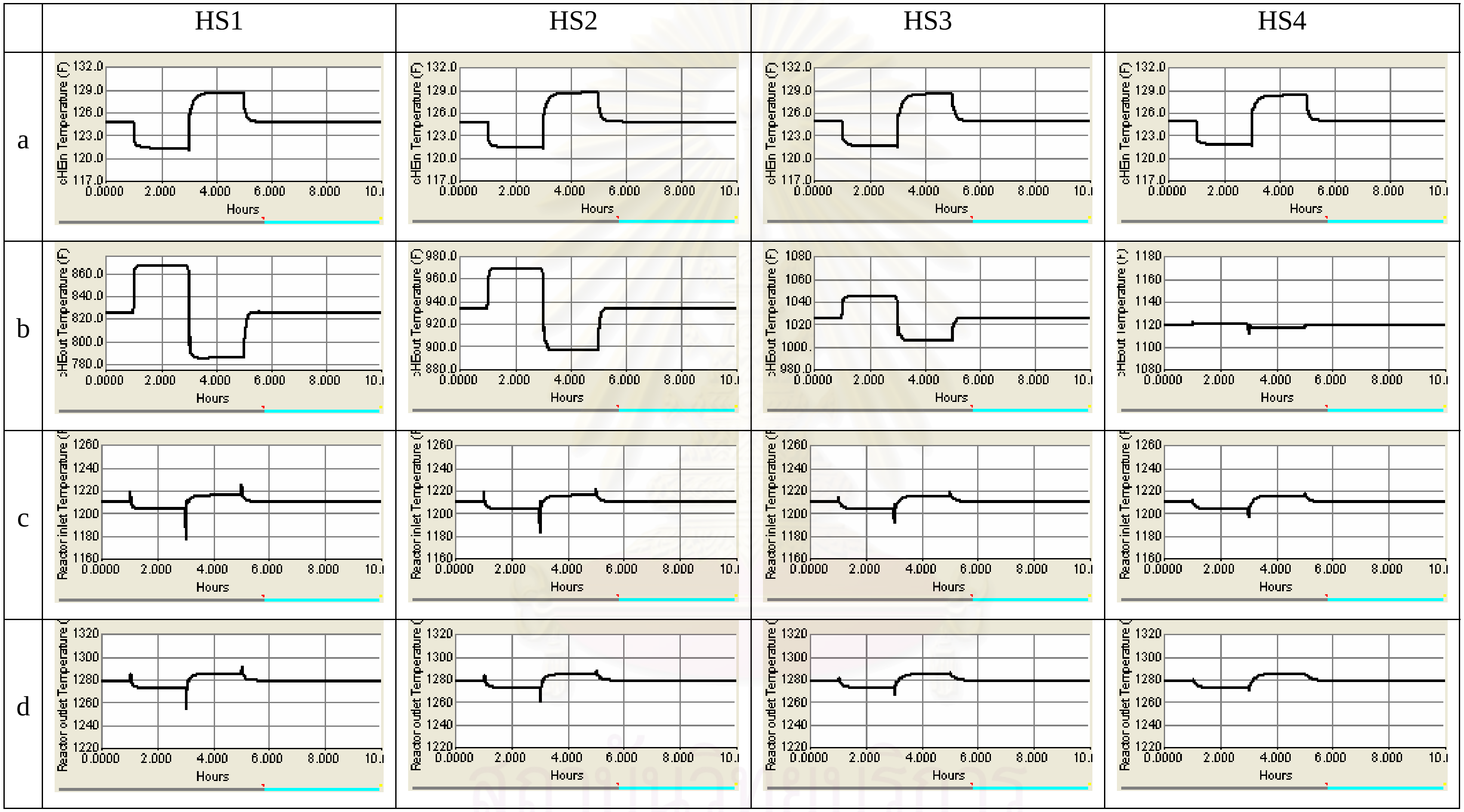


Figure 5.14 Dynamic response of the variation of heat exchanger of the reference control structure1 (REF1) to change in disturbance fresh toluene feed flowrate

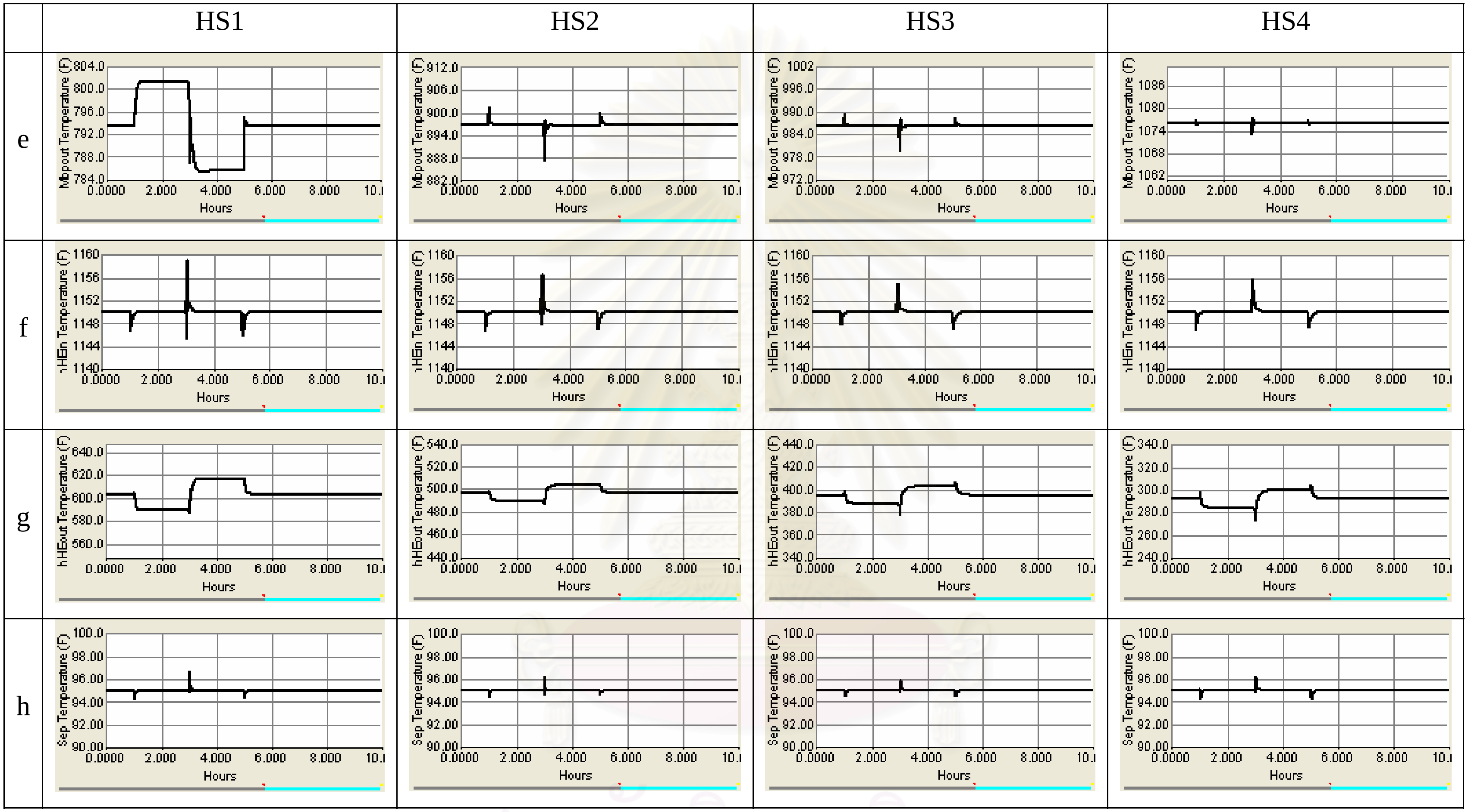


Figure 5.14 Dynamic response of the variation of heat exchanger of the reference control structure1 (REF1) to change in disturbance fresh toluene feed flowrate

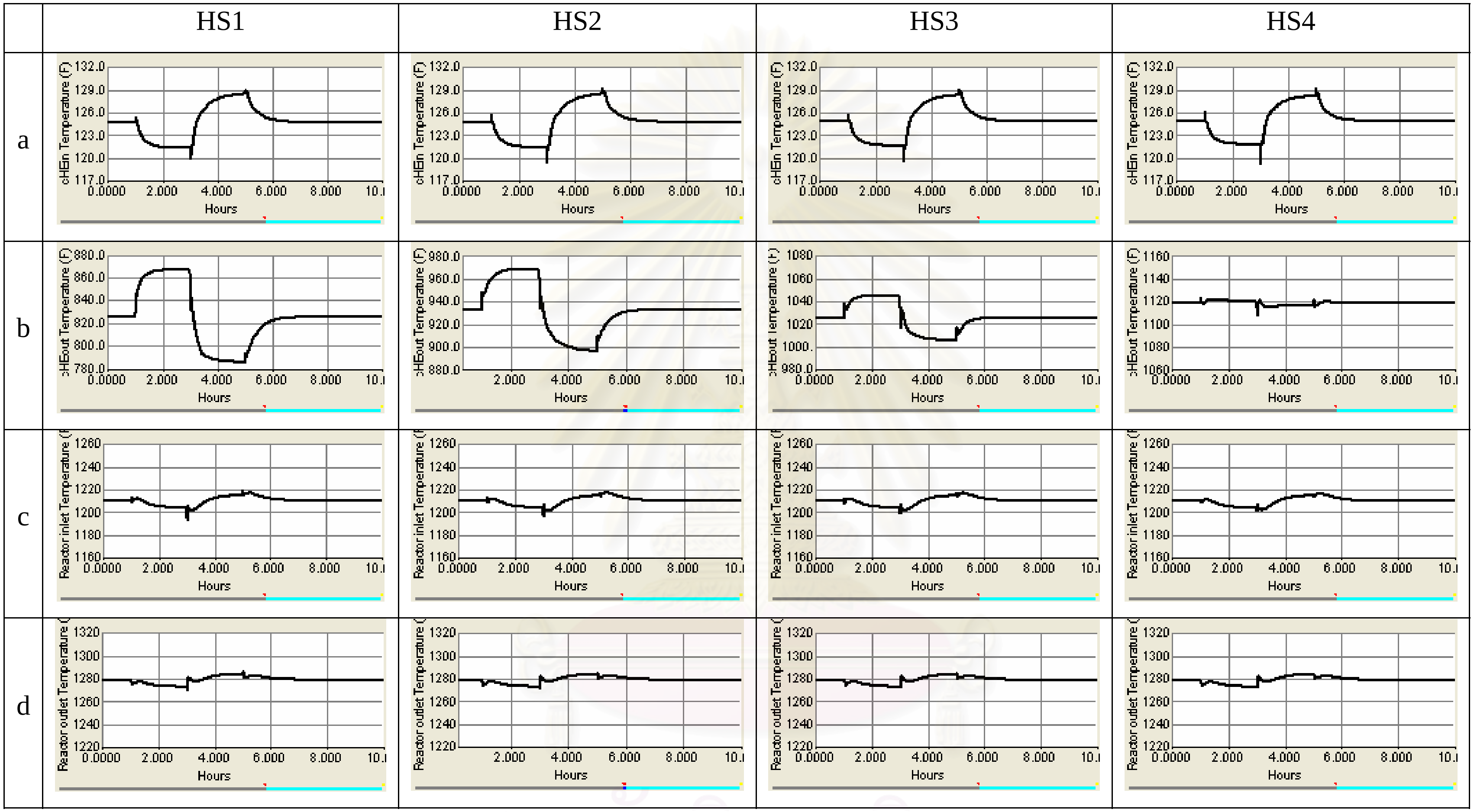


Figure 5.15 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance fresh toluene feed flowrate

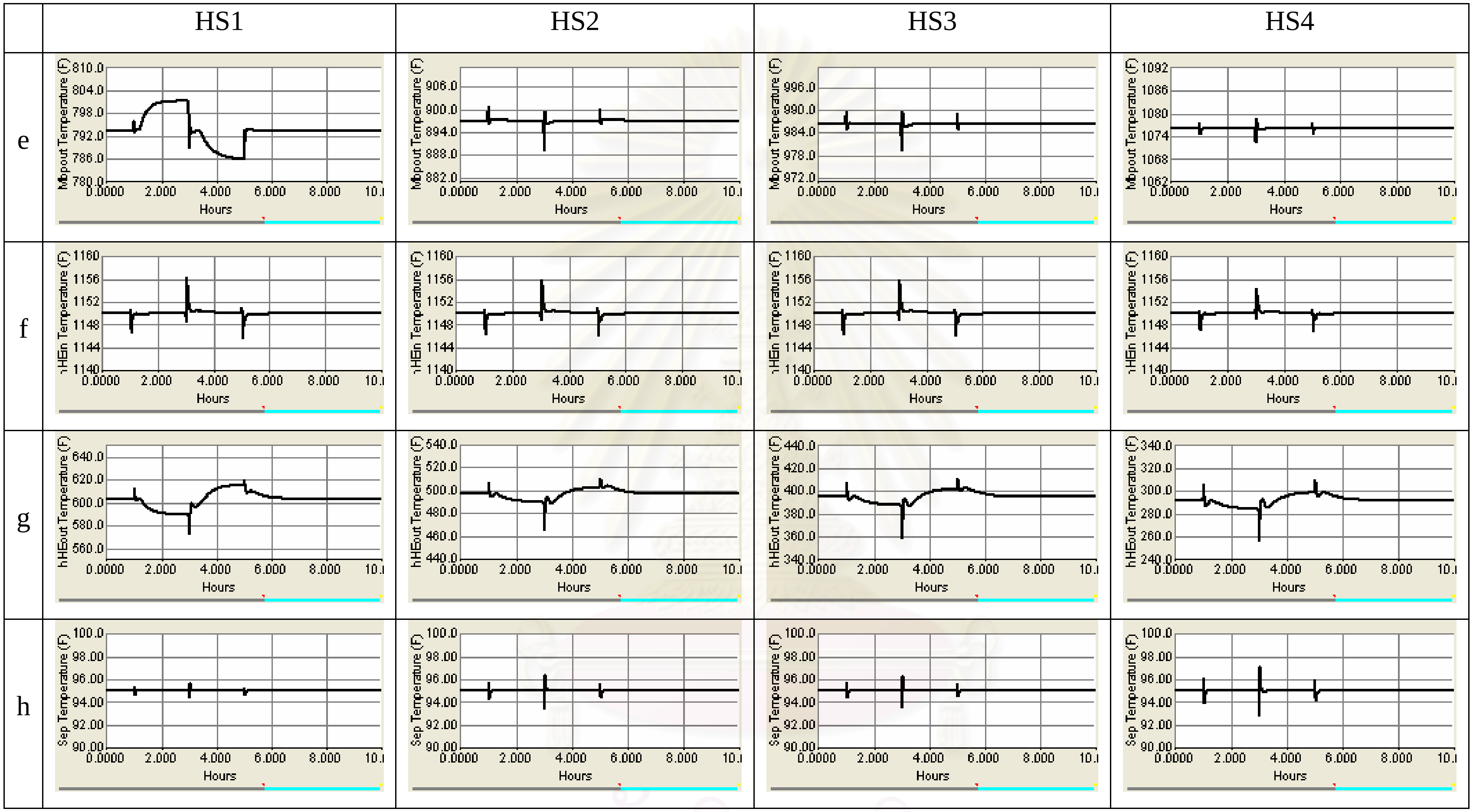


Figure 5.15 Dynamic response of the variation of heat exchanger of the control structure1 (CS1) to change in disturbance fresh toluene feed flowrate

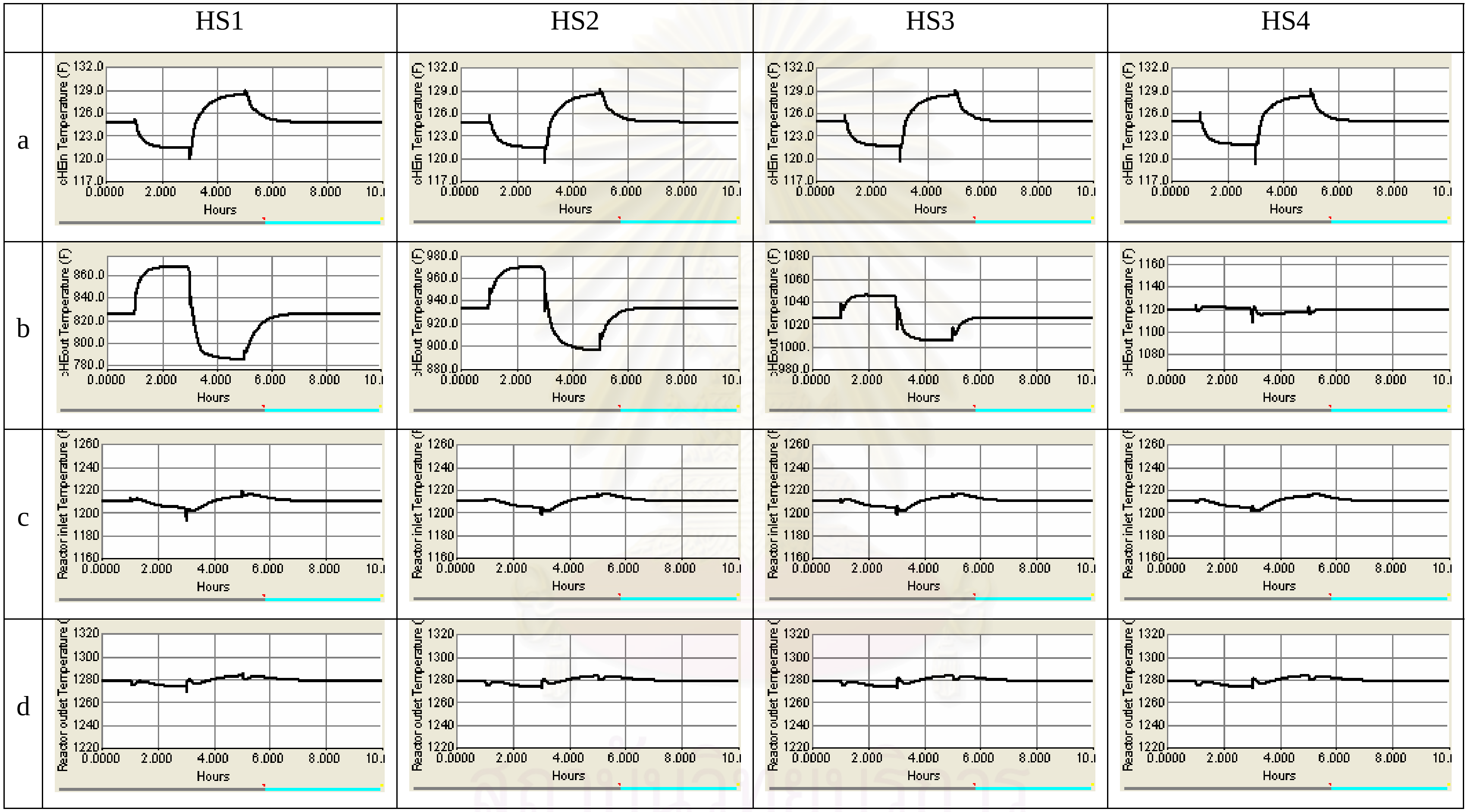


Figure 5.16 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance fresh toluene feed flowrate

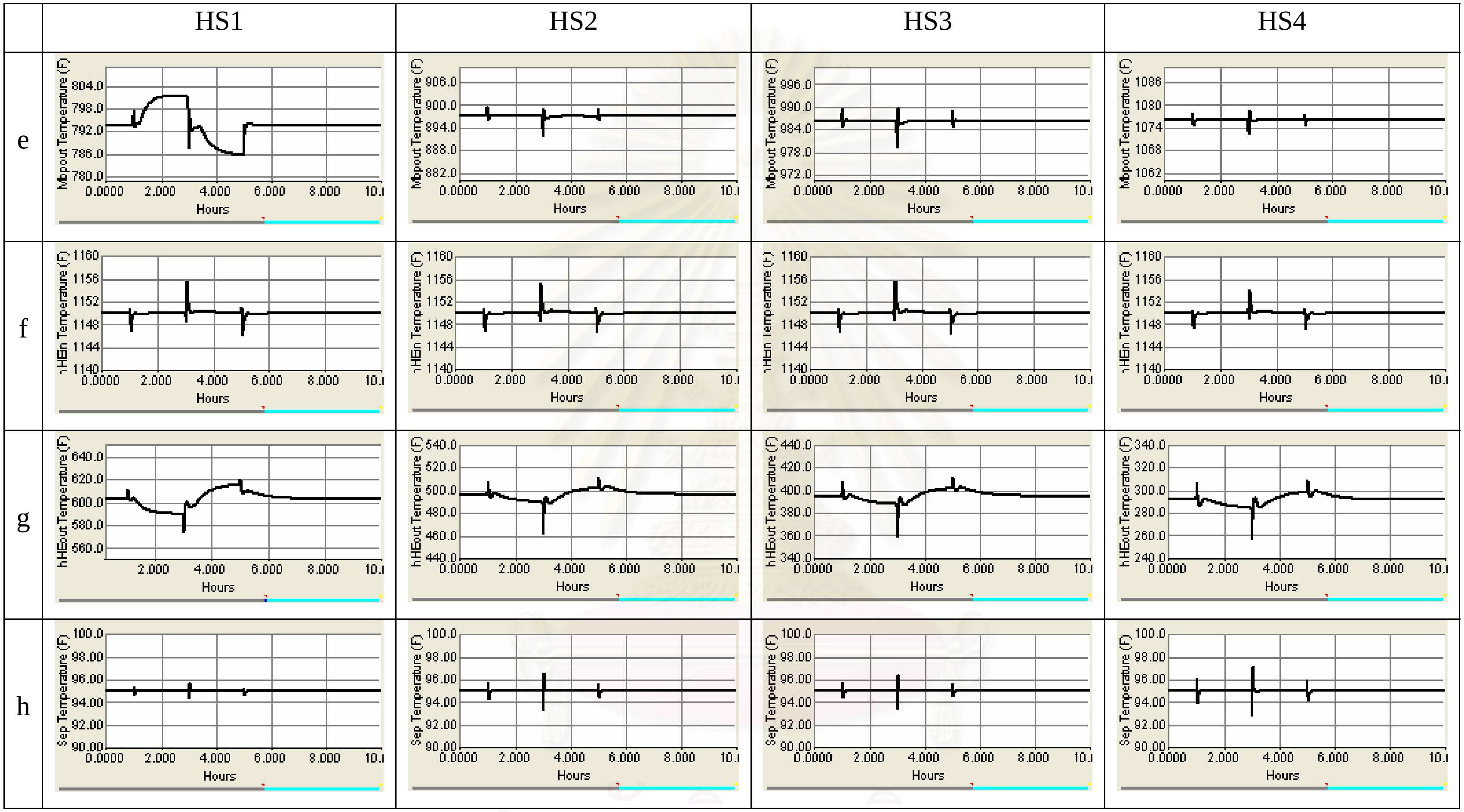


Figure 5.16 Dynamic response of the variation of heat exchanger of the control structure2 (CS2) to change in disturbance fresh toluene feed flowrate

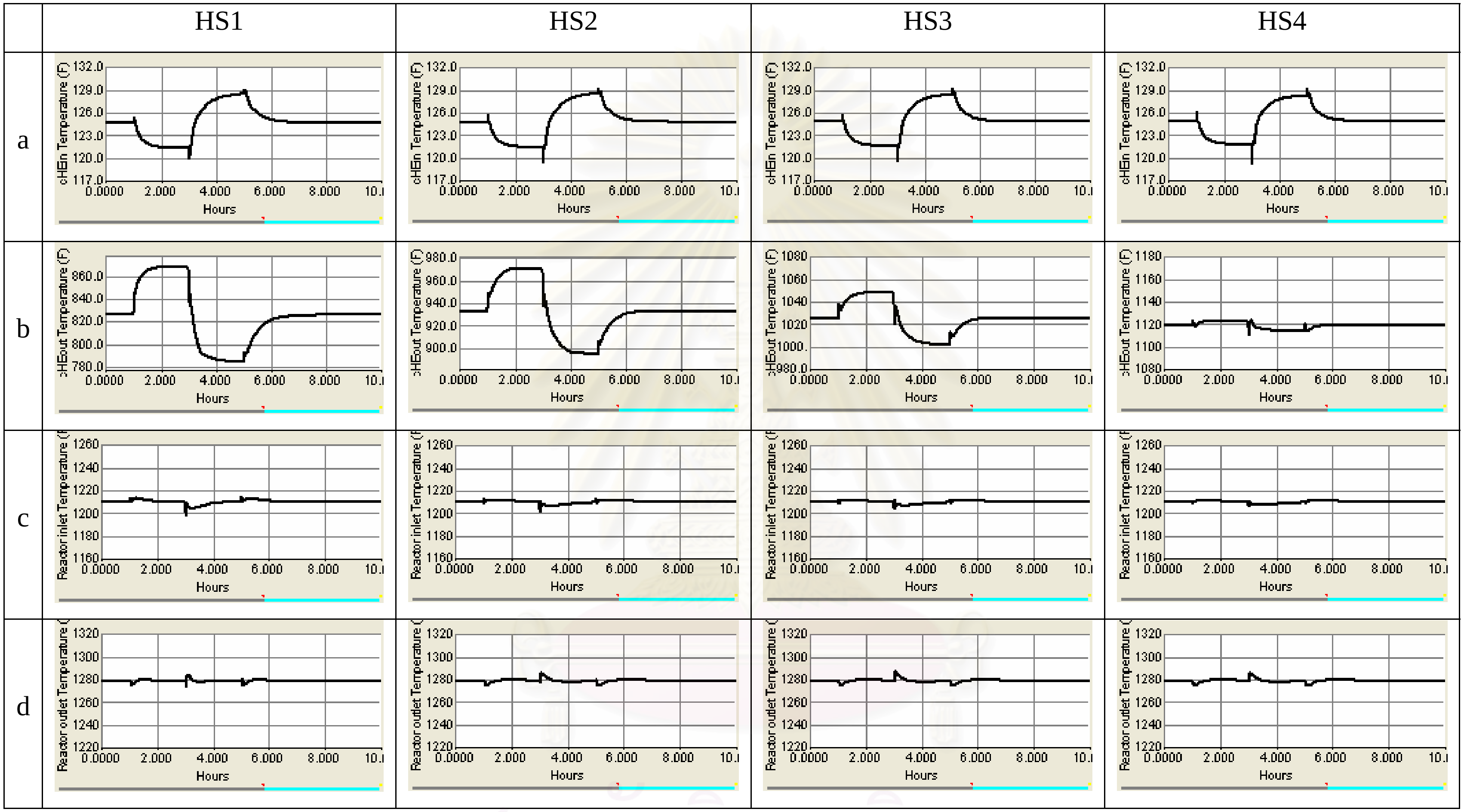


Figure 5.17 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance fresh toluene feed flowrate

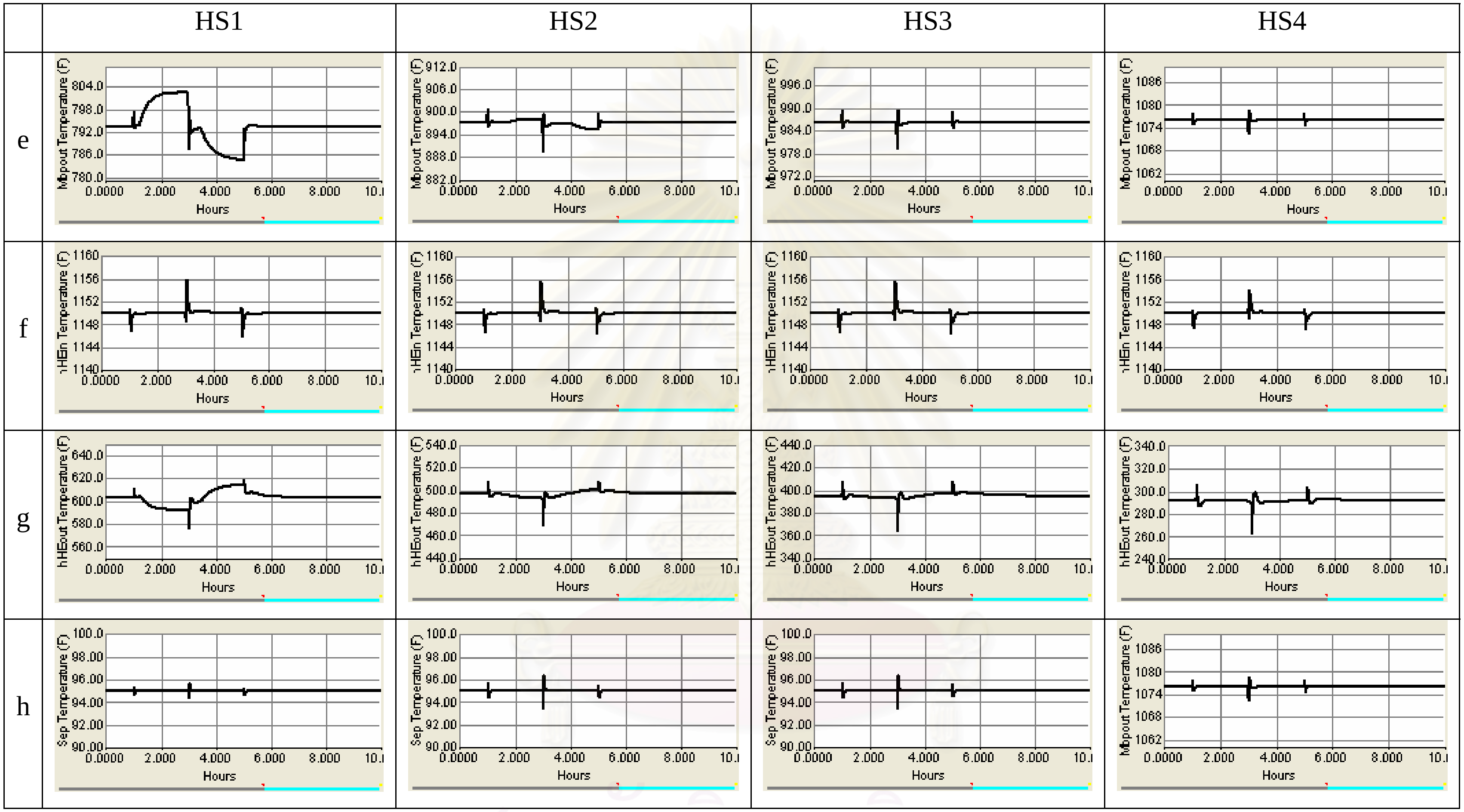


Figure 5.17 Dynamic response of the variation of heat exchanger of the control structure3 (CS3) to change in disturbance fresh toluene feed flowrate

5.5 Evaluation of the Dynamic Performance of Variation of Heat Exchanger Size for Four Controls Structure Alternatives (REF1, CS1, CS2, CS3).

In this section, IAE method is used to evaluate the dynamic performance of variation of heat exchanger size. Table 5.5-5.16 shows the IAE results for the change in the dynamic disturbance in reaction section of HDA process with different alternative control structure (REF1, CS1, CS2 and CS3) respectively.

5.5.1 Change in the Disturbance Load of Cold Stream (Reactor Feed Stream)

Table 5.5-5.8 shows the IAE results of the reference control structures and our control structure (REF1, CS1, CS2, and CS3) to change in disturbance load cold stream.

As can be seen in Table 5.5, control loop of bypass temperature, reactor temperature and quench outlet temperature of small size heat exchanger is more IAE value than large size of heat exchanger. In the reference control structure the large size heat exchanger has the smallest IAE result.

In Table 5.6-5.7, control loop of reactor temperature loop of large heat exchanger size is more IAE value than small size but bypass temperature, quench outlet temperature and hot stream outlet heat exchanger of small size heat exchanger is more IAE value than large size of heat exchanger. In the control structure1 and 2 (CS1 and CS2) the large size heat exchanger has the smallest IAE result.

In Table 5.8, control loop of bypass temperature and quench outlet temperature of small size heat exchanger is more IAE value than large size of heat exchanger. In the control structure3, the reactor outlet temperature was controlled. The large size heat exchanger has the smallest IAE result.

Table 5.5 The IAE results of the reference control structure 1 (REF1) for four size of heat exchanger

Reference control structure 1 (REF1)				
	HS1	HS2	HS3	HS4
TCBP	4.475	3.479	2.689	2.188
TCQ	1.456	1.405	1.135	0.953
TCS	0.313	0.296	0.868	1.352
Routlet Temp	4.150	3.957	3.184	2.767
Rinlet Temp	5.143	4.852	3.506	3.395
hHEout Temp	793.680	745.040	730.770	699.750
SUM	809.216	759.028	742.152	710.405

Table 5.6 The IAE results of the control structure 1 (CS1) for four size of heat exchanger

Control structure 1 (CS1)				
	HS1	HS2	HS3	HS4
TCBP	3.120	2.571	2.258	2.123
TCQ	1.023	1.124	1.023	0.903
TCS	0.336	0.816	0.838	1.563
Routlet Temp	3.438	4.085	4.323	4.790
Rinlet Temp	3.373	5.539	7.027	8.221
hHEout Temp	791.590	743.780	728.480	699.740
SUM	802.881	757.915	743.948	717.339

Table 5.7 The IAE results of the control structure 2 (CS2) for four size of heat exchanger

Control structure 2 (CS2)				
	HS1	HS2	HS3	HS4
TCBP	4.074	3.153	2.616	2.108
TCQ	1.321	1.049	1.048	0.858
TCS	0.313	0.860	0.830	1.563
Routlet Temp	2.628	3.717	4.698	5.994
Rinlet Temp	3.400	4.648	7.004	8.621
hHEout Temp	791.370	744.590	728.630	698.710
SUM	803.106	758.017	744.826	717.854

Table 5.8 The IAE results of the control structure 3 (CS3) for four size of heat exchanger

Control structure 3 (CS3)				
	HS1	HS2	HS3	HS4
TCBP	4.210	3.250	2.585	1.971
TCQ	1.423	1.188	1.078	0.926
TCS	0.324	0.817	0.837	1.454
Routlet Temp	2.891	2.625	3.071	3.102
Rinlet Temp	3.459	3.621	3.785	3.841
hHEout Temp	793.440	744.790	730.510	698.150
SUM	805.747	756.290	741.866	709.443

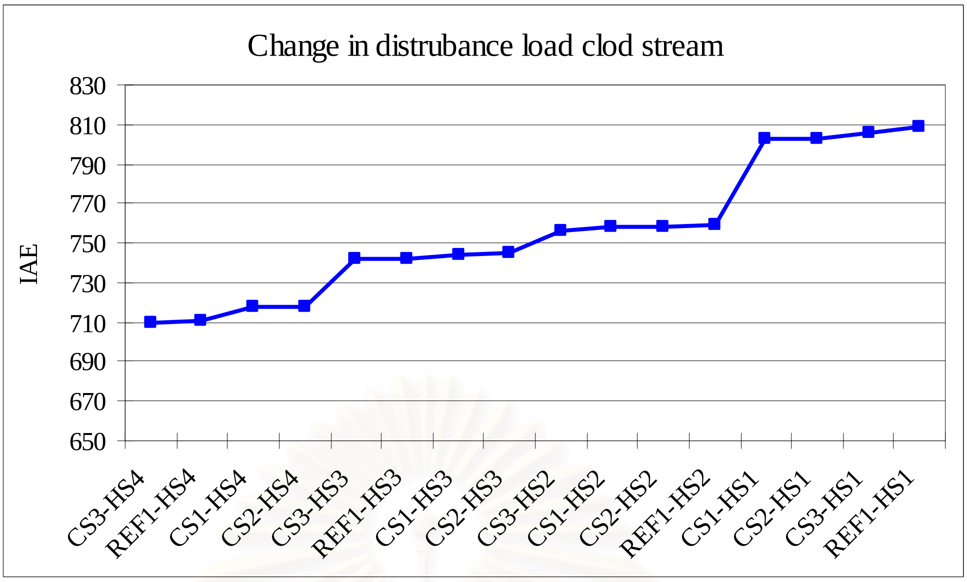


Figure 5.18 The IAE results of the variation of heat exchanger duty when change in disturbance load cold stream.

5.5.2 Change in the Disturbance Load of Hot Stream (Reactor Product Stream)

Table 5.9-5.12 shows the IAE results of the reference control structures and our control structure (REF1, CS1, CS2, and CS3) to change in disturbance load hot stream.

As can be seen, control loop of bypass temperature, reactor temperature and quench outlet temperature of small size heat exchanger is small IAE value than large size of heat exchanger because the small size heat exchanger has the large furnace heat duty and large cooler heat duty to receive disturbance load. However, hot stream outlet heat exchanger of the small size heat exchanger has more IAE value than large size heat exchanger because of the large heat transfer area of heat exchanger. In the reference control structure the large size heat exchanger has the smallest IAE result. The IAE result of other control structure is same as in the reference control structure. The control structure3 (CS3) is smallest summation of IAE result because the control structure3 control the reactor outlet temperature. The reference control structure1 (REF1) is the largest IAE result due to the IAE result of the reactor temperature loop.

Table 5.9 The IAE results of the reference control structure 1 (REF1) for four size of heat exchanger

Reference control structure 1 (REF1)				
	HS1	HS2	HS3	HS4
TCBP	22.347	44.621	46.580	46.658
TCQ	64.340	68.702	70.525	70.892
TCS	2.370	2.585	6.775	10.261
Routlet Temp	246.070	261.550	265.530	271.200
Rinlet Temp	251.800	272.830	280.010	293.120
hHEout Temp	2984.900	2651.600	2348.300	1459.000
SUM	3571.827	3301.888	3017.720	2151.131

Table 5.10 The IAE results of the control structure 1 (CS1) for four size of heat exchanger

Control structure 1 (CS1)				
	HS1	HS2	HS3	HS4
TCBP	20.795	40.169	40.245	48.188
TCQ	67.289	70.492	70.565	71.236
TCS	2.085	4.449	4.549	9.737
Routlet Temp	63.207	62.792	66.147	66.430
Rinlet Temp	104.860	104.600	97.816	106.590
hHEout Temp	3215.400	2913.800	2638.900	1785.800
SUM	3473.636	3196.302	2918.222	2087.981

Table 5.11 The IAE results of the control structure 2 (CS2) for four size of heat exchanger

Control structure 2 (CS2)				
	HS1	HS2	HS3	HS4
TCBP	35.501	38.733	40.507	47.044
TCQ	69.237	69.671	70.187	73.576
TCS	1.991	4.413	4.622	9.918
Routlet Temp	73.013	73.666	74.698	84.958
Rinlet Temp	101.750	108.290	109.960	121.660
hHEout Temp	3207.900	2931.200	2641.000	1795.400
SUM	3489.392	3225.973	2940.974	2132.556

Table 5.12 The IAE results of the control structure 3 (CS3) for four size of heat exchanger

Control structure 3 (CS3)				
	HS1	HS2	HS3	HS4
TCBP	39.406	41.528	42.413	50.878
TCQ	70.877	71.799	73.847	73.191
TCS	2.054	4.369	4.599	9.975
Routlet Temp	28.226	41.224	42.190	53.087
Rinlet Temp	61.605	62.460	67.174	83.155
hHEout Temp	3172.900	2876.800	2599.900	1749.100
SUM	3375.068	3098.180	2830.123	2019.386

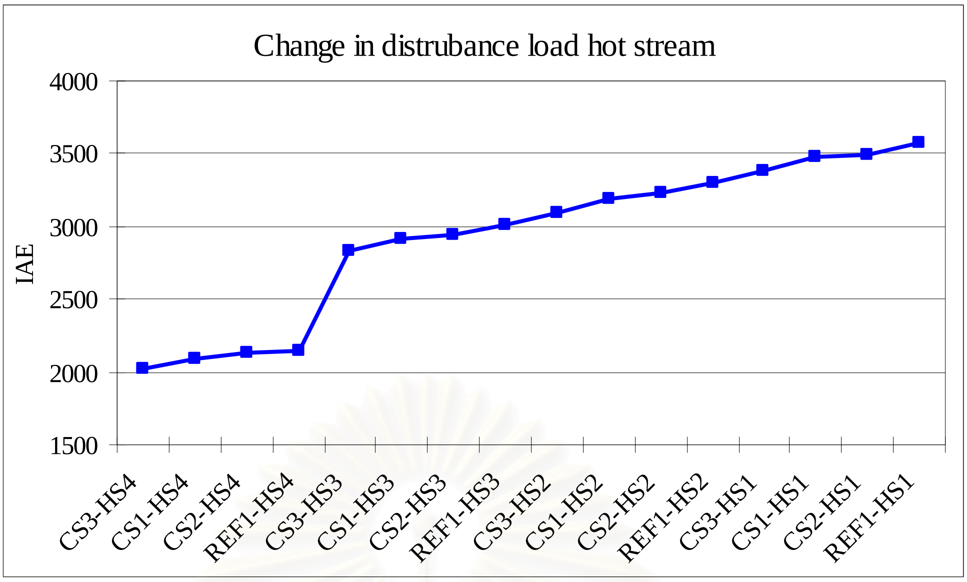


Figure 5.19 The IAE results of the variation of heat exchanger duty when change in disturbance load hot stream.

5.5.3 Change in the Fresh Toluene Feed Flowrates

Table 5.13-5.16 shows the IAE results of the reference control structures and our control structure (REF1, CS1, CS2, and CS3) to change in fresh toluene feed flowrates.

As can be seen, control loop of bypass temperature, reactor temperature and quench outlet temperature of small size heat exchanger is large IAE value than large size of heat exchanger because the large size heat exchanger has the large area to exchange energy. In smallest size heat exchanger, the bypass temperature loop is wrong IAE result because the bypass valve fully open or close can not control the bypass temperature at its setpoint. In the separator temperature loop, the small heat exchanger and the large cooler heat duty is smallest IAE result. In the reference control structure the large size heat exchanger has the smallest IAE result. The IAE result of other control structure is same as in the reference control structure. The control structure3 (CS3) is smallest summation of IAE result because the control structure3 control the reactor outlet temperature. The reference control structure1 (REF1) is the largest IAE result due to the IAE result of the reactor temperature loop.

Table 5.13 The IAE results of the reference control structure 1 (REF1) for four size of heat exchanger

Reference control structure 1 (REF1)				
	HS1	HS2	HS3	HS4
TCBP	1821.300	86.513	29.806	8.673
TCQ	58.012	47.644	49.513	54.106
TCS	5.973	4.129	8.602	11.011
Routlet Temp	1454.000	1424.200	1394.500	1391.900
Rinlet Temp	1458.700	1426.600	1400.300	1398.300
hHEout Temp	3236.800	1806.900	1870.000	1860.300
SUM	8034.785	4795.986	4752.721	4724.290

Table 5.14 The IAE results of the control structure 1 (CS1) for four size of heat exchangers.

Control structure 1 (CS1)				
	HS1	HS2	HS3	HS4
TCBP	1292.600	56.577	27.713	21.347
TCQ	77.337	80.894	75.797	55.789
TCS	7.021	14.930	13.747	20.627
Routlet Temp	1103.800	1082.000	1082.000	1082.700
Rinlet Temp	1304.900	1279.800	1270.500	1253.500
hHEout Temp	2577.500	1669.400	1587.000	1498.500
SUM	6363.158	4183.601	4056.757	3932.463

Table 5.15 The IAE results of the control structure 2 (CS2) for four size of heat exchangers.

Control structure 2 (CS2)				
	HS1	HS2	HS3	HS4
TCBP	1327.900	40.433	45.305	22.708
TCQ	79.201	78.073	75.430	55.143
TCS	6.971	15.585	14.849	21.150
Routlet Temp	972.780	965.640	984.700	986.990
Rinlet Temp	1250.000	1225.100	1212.100	1200.600
hHEout Temp	2484.500	1581.900	1500.300	1456.300
SUM	6121.352	3906.731	3832.684	3742.891

Table 5.16 The IAE results of the control structure 3 (CS3) for four size of heat exchangers

Control structure 3 (CS3)				
	HS1	HS2	HS3	HS4
TCBP	1499.800	188.840	47.616	21.455
TCQ	64.439	63.714	64.477	45.492
TCS	6.611	13.760	12.392	18.663
Routlet Temp	202.000	354.410	362.390	370.340
Rinlet Temp	510.580	471.030	436.480	410.260
hHEout Temp	2058.100	760.330	609.830	463.440
SUM	4341.530	1852.084	1533.185	1329.650

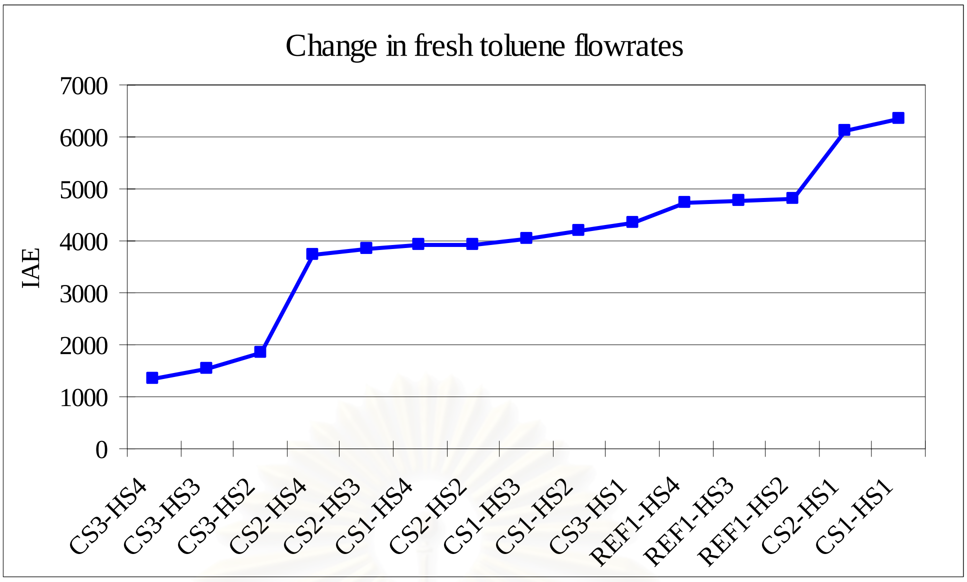


Figure 5.20 The IAE results of the variation of heat exchanger duty when change in fresh toluene feed flowrates.

5.6 Evaluation Economic Analysis and Trade off with Control Performance of Heat Exchanger Size for Four Controls Structure Alternatives (REF1, CS1, CS2, CS3).

A first study of the total processing costs to heat-exchanger network was undertaken by Terrill and Douglas (1987). They developed a Heat exchanger network for a base-case design for the HDA process.

From steady state pointview, on the evaluation of the economics of a HDA process. The term economics refers to the evaluation of capital costs and operating costs associated with the construction and operation of a HDA process. The methods by which the one-time costs associated with the construction of the plant and the continuing costs associated with the daily operation of the process are combined into meaningful economic criteria are provided.

Table 5.17 Results of cost estimation for HDA process with different heat exchanger cases.

Size	Heat Exchanger Cost ($)	Furnace Cost ($)	Grass Roots Cost ($)	Utility Cost ($/yr)			TAC ($/yr)
				Furnace	Cooler	Sum	
HS1	508000	1710000	2450000	1027480	72068	1099548	1344550
HS2	635000	1360000	2000000	787183	58007	845190	1045190
HS3	940000	977000	1920000	537950	43415	581365	773365
HS4	2970000	557000	3530000	279578	28287	307865	660865

The grass roots cost of heat exchanger and furnace is estimate cost of delivered equipment costs and installed equipment costs in all working time about 10 years. Total annual cost is the grass roots cost per year plus the summation of utility cost per year.

The capital cost of smallest heat exchanger duty (HS1) is smallest in all of heat exchanger but very expensive in capital cost of furnace and utility cost. The total annual cost of HS1 is so highly about 1,344,550 $/year. The capital cost of largest heat exchanger (HS4) is highest but the capital cost of furnace and utility cost are inexpensive. The total annual cost of HS4 is low-price about 660,865 $/year.

The utility cost of furnace and cooler of each control structure when disturbance load of cold stream were shown in table 5.18. The large heat exchanger is so low in furnace duty and cooler duty cost more than the small heat exchanger. Figure 5.20 show that the control structure 2 of largest size of heat exchanger (CS2-HS4) is lowest utility cost. The utility cost of largest size of each control structure difference about 100$/yr. The utility cost of the smallest size of heat exchanger of the control structure1 (CS1-HS1) is highly.

Table 5.18 The utility cost of each control structure that used when change in disturbance load of cold stream.

	Size	Furnace Heat Duty ($/yr)	Cooler Heat Duty ($/yr)
REF1	HS1	1046707.0	73191.6
	HS2	799728.0	58733.4
	HS3	579605.3	45846.5
	HS4	351382.4	32483.9
CS1	HS1	1047097.7	73217.8
	HS2	799987.2	58750.6
	HS3	579527.3	45841.3
	HS4	351239.9	32474.4
CS2	HS1	1046865.0	73199.9
	HS2	799531.4	58720.8
	HS3	579466.2	45837.4
	HS4	351174.1	32470.0
CS3	HS1	1046224.2	73160.9
	HS2	799606.3	58725.1
	HS3	579605.6	45845.4
	HS4	351240.1	32474.4

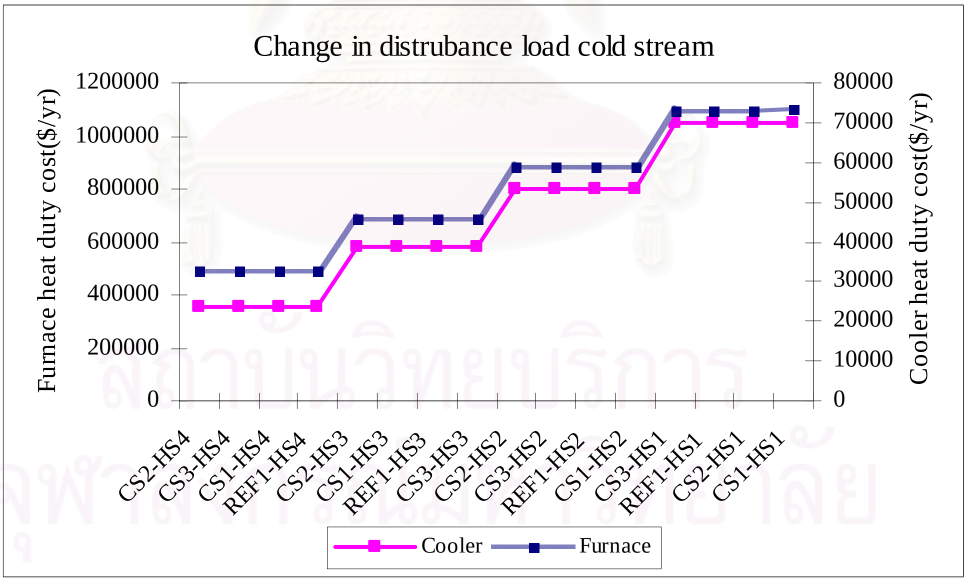


Figure 5.21 The utility cost of the variation of heat exchanger duty when change in disturbance load cold stream.

The utility cost of furnace and cooler of each control structure when disturbance load of hot stream were shown in table 5.19. The large heat exchanger is so low in furnace duty and cooler duty cost more than the small heat exchanger. Figure 5.21 show that the control structure 2 of largest size of heat exchanger (CS2-HS4) and control structure3 (CS3-HS4) are lowest utility cost. The utility cost of largest size of each control structure slightly difference about 30$/yr. The utility cost of the smallest size of heat exchanger of the control structure1 (CS1-HS1) and control structure3 are highly.

The utility cost of furnace and cooler of each control structure when change in fresh toluene feed flowrates were shown in table 5.20. Figure 5.22 show that the control structure 3 of largest size of heat exchanger (CS3-HS4) and control structure1 (CS1-HS4) are lowest utility cost. The utility cost of largest size of each control structure difference about 100$/yr. The utility cost of the smallest size of heat exchanger of the reference control structure1 (REF1-HS1) and control structure1 are highly.

Table 5.19 The utility cost of each control structure that used when change in disturbance load of hot stream.

	Size	Utility Duty ($/yr)	TAC ($/yr)
REF1	HS1	1046606.0	73184.5
	HS2	799737.3	58732.2
	HS3	579487.4	45836.5
	HS4	351241.0	32472.1
CS1	HS1	1047087.3	73215.5
	HS2	799981.7	58748.5
	HS3	579739.3	45852.3
	HS4	351252.9	32472.9
CS2	HS1	1046546.6	73179.1
	HS2	799606.7	58723.3
	HS3	579531.4	45839.6
	HS4	351193.2	32468.9
CS3	HS1	1046696.1	73189.2
	HS2	799722.3	58731.1
	HS3	579602.7	45843.2
	HS4	351222.5	32470.5

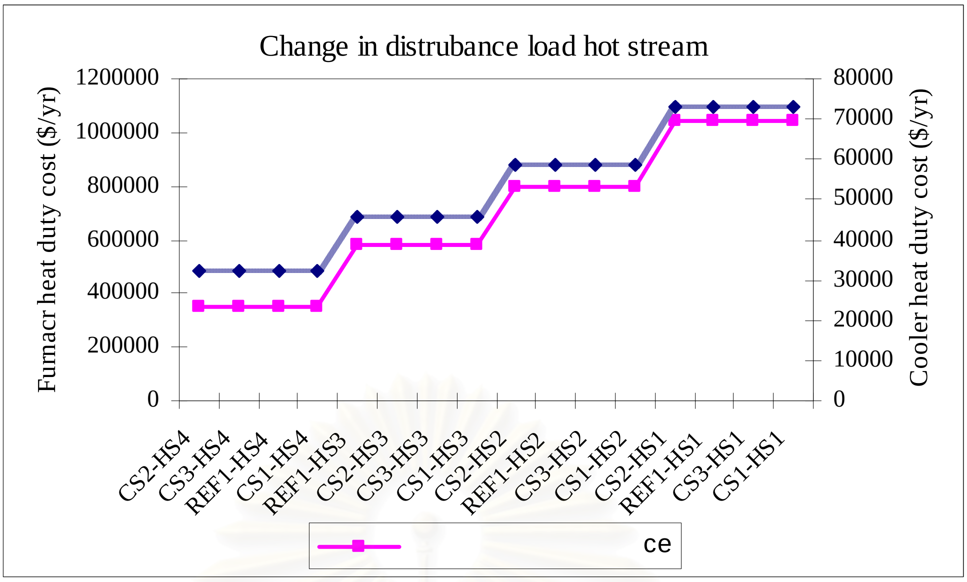


Figure 5.22 The utility cost of the variation of heat exchanger duty when change in disturbance load hot stream.

Table 5.20 The utility cost of each control structure that used when change in fresh toluene feed flowrates.

	Size	Furnace Heat Duty (Btu)	Cooler Heat Duty (Btu)
REF1	HS1	1047345.2	73247.2
	HS2	800151.5	58775.5
	HS3	579738.7	45868.1
	HS4	351404.8	32493.4
CS1	HS1	1046766.1	73211.9
	HS2	800008.8	58763.8
	HS3	579834.9	45870.2
	HS4	351403.7	32493.8
CS2	HS1	1046315.1	73180.1
	HS2	799720.1	58743.5
	HS3	579675.8	45859.3
	HS4	351404.8	32493.4
CS3	HS1	1046372.7	73180.0
	HS2	799825.9	58745.1
	HS3	579650.5	45852.5
	HS4	351318.9	32482.6

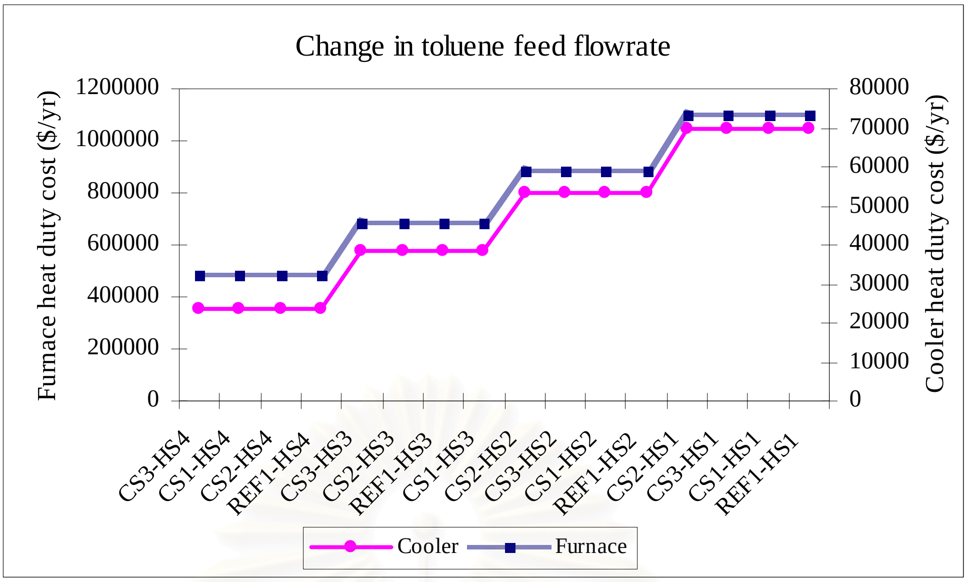


Figure 5.23 The utility cost of the variation of heat exchanger duty when change in fresh toluene feed flowrates.

CHAPTER VI

CONCLUSION

6.1 Introduction

This work has presented an approach to design of plantwide control system. The approach is base on basic idea of self-optimizing control to select control variables that to select controlled variables which when kept constant lead to minimum economic loss to design control structure of Hydrodealkylation process. The maximum scaled gain is used to selecting and pairing controlled variables with manipulated variables. This presented-method is elementary and effective. Dynamic simulations of Hydrodealkylation process can be presented in two points.

1. The effect of economic disturbance such as toluene feed flowrates, methane composition in the fresh gas feed and quench outlet temperature.
2. The effect of variation of heat exchanger duty to dynamic performance and utility cost.

The economic loss of process depends on selecting controlled variables which when kept constant lead to minimum economic loss when disturbance occur. This work, the control structure is tested by changing the fresh toluene feed flowrates, methane composition in the fresh gas feed and quench outlet temperature. For the results, the designed control structure has small loss when disturbance occurs because controlled variables small sensitive with disturbance and more sensitive with manipulated variables lead to minimum economic loss.

6.2 Control Structures Comparison

6.2.1 Comparison three Designed Control Structures Compare with Reference Structure that Presented by Skogestad.

This work has presented three designed control structures to compare with reference structure that presented by Skogestad. The dynamic simulation of this process reacts to various disturbances and changes in operating conditions.

6.2.1.1 Decrease fresh toluene feed flowrates

The designed control structures and reference structure result are similar. Decrease toluene feed flowrates direct effect to fresh gas feed flow of designed control structures because we use fresh gas feed flow to control hydrogen-to-aromatic ratio. The reactor inlet temperature and reactor outlet temperature in control structure1 (CS1) and CS2 are small oscillatory and slowly decrease. In the control structure 3 (CS3), the reactor inlet and outlet temperature are so small oscillatory and return to old setpoint because this structure control the reactor inlet temperature with setpoint from reactor outlet temperature. The control structure3 (CS3) is minimizing the deviation of benzene product from steady state about 6.59%. The reference control structure is maximizing the deviation of benzene product from steady state about 6.94%.

6.2.1.2 Increase fresh toluene feed flowrates

The increase in fresh toluene feed flowrates increases the production rate and fresh gas feed because of high reaction rate. Although, the responses of the increase fresh gas feed rate are more oscillatory than reference structure but the reactor inlet and outlet temperature are small oscillatory, in control structure3 (CS3) the reactor inlet and outlet temperature are so small oscillatory and return to setpoint because this structure control the reactor inlet temperature with setpoint from reactor outlet temperature. The control structure3 (CS3) is minimizing the deviation of benzene product from steady state about 6.25%. The reference control structure is maximizing the deviation of benzene product from steady state about 6.87%.

6.2.1.3 Increase Methane mole fraction in fresh gas feed.

The designed control structures slightly oscillate and rapidly return to setpoint faster than reference structure. The furnace heat duty and cooler heat duty are rarely oscillatory but the compressor power slow decrease to new point because of increasing in methane mole fraction. The deviation of benzene product from steady state of each control structure is slightly decreased about 0.08%.

6.2.1.4 Increase quenches outlet temperature

The control structure1 (CS1) is faster dynamic response than other structures in reactor inlet temperature than other structure, because they are controlled the setpoint of reactor temperature with toluene conversion at reactor. The reference structure is more swing in reactor temperature and furnace heat duty. The deviation of benzene product from steady state of reference control structure is decreased about 0.08%. The deviation of benzene product from steady state of designed control structures are increased about 0.02-0.03%.

All of control structures can operate to achieve the objective and within process constraints. The performance of all control structures can present in IAE value and can compared their performance with IAE value in chapter 4. The design control structures are smaller average cost in furnace duty, cooler duty and compressor work than reference structure. The control structure3 (CS3) is minimizing the deviation of benzene product from steady state.

6.2.2 Comparison between variation of heat exchanger duty and dynamic control performance

This work has presented four variation of heat exchanger duty of each control structures to compare about dynamic performance and utility cost. The dynamic simulation of this process reacts to various disturbances.

6.2.2.1 Disturbance load cold stream

The large size of heat exchanger is good performance to reduce disturbance effect to reactor inlet temperature but poor performance to control separator temperature because of small cooler duty. All of structure of large size heat exchanger is smaller IAE value in reactor inlet temperature loops than small size.

6.2.2.2 Disturbance load hot stream

The large sizes of heat exchanger have poor performance to control reactor inlet temperature and separator temperature. The largest size of heat exchanger has the smallest duty of cooler and furnace to handle disturbance. The small heat exchanger duty is good performance to control because of large furnace and cooler duty but utility cost of this size is high-flown. The hot stream outlet heat exchanger of large size is small IAE value because of large area. That mean, the large area of heat exchanger can handle disturbance before disturbance effect to separation section.

6.2.2.3 Fresh toluene feed flowrates

The large sizes of heat exchangers have good performance to control reactor inlet temperature because the large size heat exchanger has large area for exchange energy from increasing in toluene flowrates. The smallest size of heat exchanger can not control bypass outlet temperature (furnace inlet temperature) because this size has small area but can control reactor inlet temperature with largest furnace duty. We should not use smallest heat exchanger area for handle flow disturbance.

In Table 6.1 show result of comparison between total annual cost of HDA and IAE value with different heat exchanger cases of designed control structure. The smallest furnace duty HS4 is the most inexpensive and the smallest IAE value when disturbance occur. This experiment contradicts with the idea of Luyben, 1998 that the tolerance to such disturbances improves as the size of the furnace increase and as they introduce more flexibility in term of additional manipulated variables like bypasses and quench loops. However, these extra manipulate variables can never remove the existence of the unstable operating point like a large furnace can.

Table 6.1 Results of comparison between total annual cost of HDA process and IAE value with different heat exchanger cases of designed control structure.

Control Structure 1							
Size	TAC ($/yr)	IAE(SUM)			IAE(Separator)		
		Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate	Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate
HS1	1344550	802.881	3473.636	6363.158	0.336	2.085	7.021
HS2	1045190	757.915	3196.302	4183.601	0.816	4.449	14.930
HS3	773365	743.948	2918.222	4056.757	0.838	4.549	13.747
HS4	660865	717.339	2087.981	3932.463	1.563	9.737	20.627

Control Structure 2							
Size	TAC ($/yr)	IAE(SUM)			IAE(Separator)		
		Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate	Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate
HS1	1344550	803.106	3489.392	6121.352	0.313	1.991	6.971
HS2	1045190	758.017	3225.973	3906.731	0.860	4.413	15.585
HS3	773365	744.826	2940.974	3832.684	0.830	4.622	14.849
HS4	660865	717.854	2132.556	3742.891	1.563	9.918	21.150

Control Structure 3							
Size	TAC ($/yr)	IAE(SUM)			IAE(Separator)		
		Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate	Disturbance load cold stream	Disturbance load hot stream	Fresh toluene feed flowrate
HS1	1344550	805.747	3375.068	4341.530	0.324	2.054	6.611
HS2	1045190	756.290	3098.180	1852.084	0.817	4.369	13.760
HS3	773365	741.866	2830.123	1533.185	0.837	4.599	12.392
HS4	660865	709.443	2019.386	1329.650	1.454	9.975	18.663

6.3 Recommendations

The maximum scaled gain method is the elementary and effective tool to select controlled variables. However the maximum scaled gain method is effective with large scaled plant do not have the heat integrated in process. Maybe in case heats integrated are presented in process this method is not sufficient.

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APPENDICES

APPENDIX A

COST EQUATIONS AND CURVES FOR THE CAPCOST PROGRAM

The purpose of this appendix is to present the equations and figures that describe the relationships used in the capital equipment-costing program CAPCOST. The program is based on the module factor approach to costing that was originally introduced by Guthrie and modified by Ulrich.

A.1 Purchased Equipment Costs

All the data for the purchased cost of equipment were obtained from a survey of equipment manufactures during the period May to September of 2001, so an average value of the CEPCI of 397 over this period should be used when accounting for inflation. The data for the purchased cost of the equipment, at ambient operating pressure and using carbon steel construction, C_p^0, was fitted to the following equation:

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 \left[\log_{10}(A)\right]^2 \qquad \text{(A.1)}$$

where A is the capacity or size parameter for the equipment. The data for K_1, K_2 and K_3, along with the maximum and minimum values used in the correlation are given in the Table A.1.

A.2 Pressure Factors

A.2.1 Pressure Factors for Process Vessels

The pressure factor for horizontal and vertical process vessels of diameter *D* meters and operating at a pressure of *P* barg is based on the ASME code for pressure vessel design. At base material conditions using a maximum allowable stress for carbon steel, *S*, of 944 bar, a weld efficiency, *E*, of 0.9, a minimum allowable vessel thickness of 0.0063 m (1/4 inch), and a corrosion allowance, *CA*, of 0.00315 m (1/8 inch) gives the following expression:

$$F_{p,vessel} = \frac{\dfrac{(P+1)D}{2[850-0.6(P+1)]}+0.00315}{0.0063} \qquad (A.2)$$

If $F_{p,vessel}$ is less than 1, then $F_{p,vessel} = 1.$ for pressures below -0.5 barg, $F_{p,vessel} = 1.25.$

A.2.2 Pressure Factors for Other Process Equipment

The pressure factors, F_p, for the remaining process equipment are given by The following general form:

$$\log_{10} F_p = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \qquad (A.3)$$

The units of pressure, *P*, are bar gauge or barg unless stated otherwise. The pressure factors are always greater than unity; the values of constants in equation A.3 for different equipment are given in Table A.2. The values for the constants given in Table A.2 were regressed from data in Guthrie and Ulrich.

A.3 Material Factors and Bare Module Factors

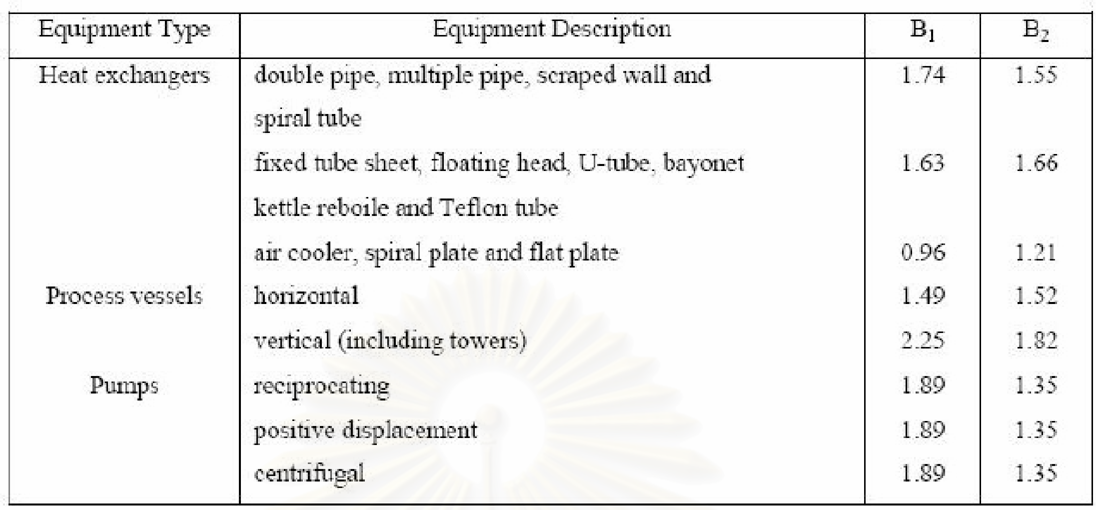
A.3.1 Bare Module and Material Factors for Heat Exchangers, Process Vessel, and Pumps

The bare module factors for this equipment are given by the following equation:

$$C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P) \qquad (A.4)$$

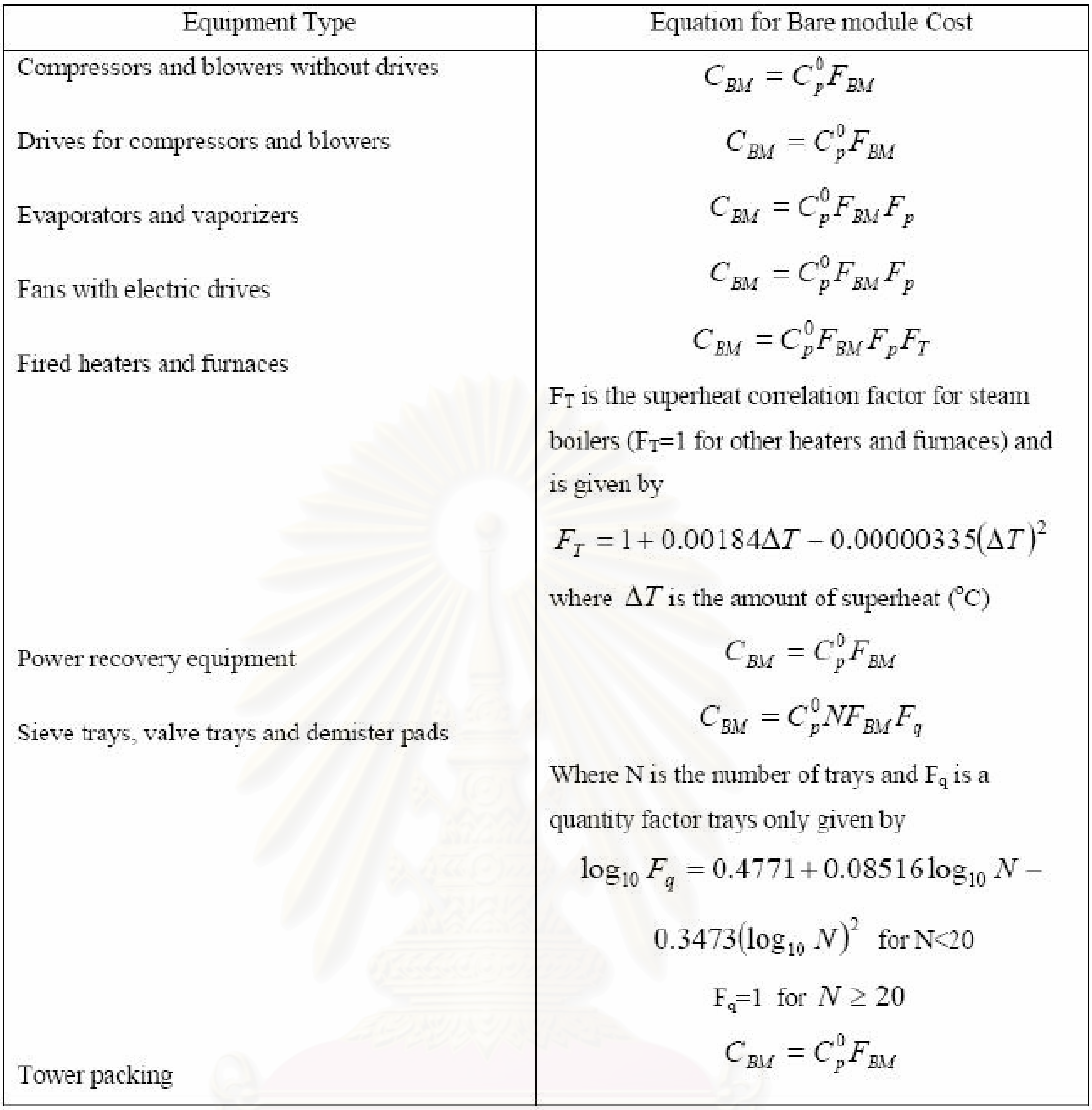
The values of the constants B_1 and B_2 are given in Table A.1. The bare module cost for ambient pressure and carbon steel construction, C_{BM}^0 and the bare module factor for the equipment at these conditions, F_{BM}^0 are found by setting F_M and F_P equal to unity.

Table A.1 Constant for Bare Module Factor to be used in Equation A.4



Equipment Type	Equipment Description	B_1	B_2
Heat exchangers	double pipe, multiple pipe, scraped wall and spiral tube	1.74	1.55
	fixed tube sheet, floating head, U-tube, bayonet kettle reboile and Teflon tube	1.63	1.66
	air cooler, spiral plate and flat plate	0.96	1.21
Process vessels	horizontal	1.49	1.52
	vertical (including towers)	2.25	1.82
Pumps	reciprocating	1.89	1.35
	positive displacement	1.89	1.35
	centrifugal	1.89	1.35

Table A.2 Equations for Bare Module Cost



Equipment Type	Equation for Bare module Cost
Compressors and blowers without drives	$C_{BM} = C_p^0 F_{BM}$
Drives for compressors and blowers	$C_{BM} = C_p^0 F_{BM}$
Evaporators and vaporizers	$C_{BM} = C_p^0 F_{BM} F_p$
Fans with electric drives	$C_{BM} = C_p^0 F_{BM} F_p$
Fired heaters and furnaces	$C_{BM} = C_p^0 F_{BM} F_p F_T$ F_T is the superheat correlation factor for steam boilers (F_T=1 for other heaters and furnaces) and is given by $F_T = 1 + 0.00184\Delta T - 0.00000335(\Delta T)^2$ where ΔT is the amount of superheat (°C)
Power recovery equipment	$C_{BM} = C_p^0 F_{BM}$
Sieve trays, valve trays and demister pads	$C_{BM} = C_p^0 N F_{BM} F_q$ Where N is the number of trays and F_q is a quantity factor trays only given by $\log_{10} F_q = 0.4771 + 0.08516 \log_{10} N - 0.3473(\log_{10} N)^2$ for N<20 F_q=1 for $N \geq 20$
Tower packing	$C_{BM} = C_p^0 F_{BM}$

A.3.2 Bare Module and Material Factors for the Remaining Process Equipment

For the remaining equipment, the bare modules costs are related to the material and pressure factors by equations different from Equation A.4. The form of these equations is given in Table A.2

APPENDIX B

TUNING OF CONTROL STRUCTURES

B.1 Tuning Controllers

Notice throughout this work uses several types of controllers such as P, PI, and PID controllers. They depend on the control loop. In theory, control performance can be improved by the use of derivative action but in practice the use of derivative has some significant drawbacks:

1. Three tuning constants must be specified.
2. Signal noise is amplified.
3. Several types of PID control algorithms are used, so important to careful that the right algorithm is used with its matching tuning method.
4. The simulation is an approximation of the real plant. If high performance controllers are required to get good dynamics from the simulation, the real plant may not work well.

B.2 Tuning Flow, Level and Pressure Loops

The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be turned with a small integral or reset time constant. A value of τ_I = 0.3 minutes work in most controllers. The value of controller gain should be kept modest because flow measurement signal are sometime noisy due to the turbulent flow through the orifice plate. A value of controller gain of K_C = 0.5 is often used. Derivative action should not be used.

Most level controllers should use proportional-only action with a gain of 1 to 2. This provides the maximum amount of flow smoothing. Proportional control means there will be steady state offset (the level will not be returned to its setpoint value). However, maintaining a liquid level at a certain value is often not necessary when the liquid capacity is simply being used as surge volume. So the recommended tuning of a level controller is K_C = 2.

Most pressure controllers can be fairly easily tuned. The process time constant is estimated by dividing the gas volume of the system by the volumetric flowrate of gas flowing through the system. Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Typical pressure controller tuning constants for columns and tanks are K_C = 2 and τ_I = 10 minutes.

B.3 Relay- Feedback Testing

The relay-feedback test is a tool that serves a quick and simple method for identifying the dynamic parameters that are important for to design a feedback controller. 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 merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the height of the relay, h. This height is typically 5 to 10 % of the controller output scale. The loop starts to oscillate around the setpoint with the controller output switching every time the process variable (PV) signal crosses the setpoint. Figure B.1 shows the PV and OP signals from a typical relay-feedback test.

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

$$K_U = \frac{4h}{a\pi} \qquad \text{(B.1)}$$

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

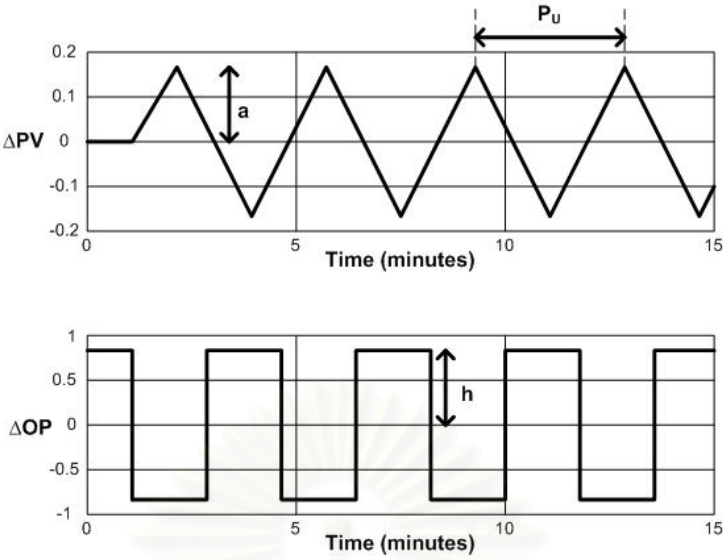


Figure B.1 Input and Output from Relay-Feedback Test

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

1. Only one parameter has to be specified (relay height).
2. The time it takes to run the test is short, particularly compared to the extended periods required for methods like PRBS.
3. The test is closedloop, so the process is not driven away from the setpoint.
4. The information obtained is very accurate in the frequency range that is important for the design of a feedback controller.
5. The impact of load changes that occur during the test can be detected by a change to asymmetric pulses in the manipulated variable.

These entire features make relay-feedback testing a useful identification tool. Knowing the ultimate gain, K_U and the ultimate period, P_U permits us to calculate controller settings. There are several methods that require only these two parameters. The Ziegler-Nichols tuning equations for a PI controller are:

$$\begin{aligned} K_C &= K_U / 2.2 \\ \tau_I &= P_U / 1.2 \end{aligned} \tag{B.2}$$

These tuning constants are frequently too aggressive for many chemical engineering applications. The Tyreus-Luyben tuning method provides more conservative settings with increased robustness. The TL equations for a PI controller are:

$$\begin{aligned} K_C &= K_U / 3.2 \\ \tau_I &= 2.2 P_U \end{aligned} \tag{B.3}$$

B.4 Inclusion of Lags

Any real physical system has many lags. Measurement and actuator lags always exist. In simulations, however, these lags are not part of the unit models. Much more aggressive tuning is often possible on the simulation than is possible in the real plant. Thus the predictions of dynamic performance can be overly optimistic. This is poor engineering. A conservative design is needed.

Realistic dynamic simulations require that we explicitly include lags and/or dead times in all the important loops. Usually this means controllers that affect Product quality or process constraint.

Table B.1 summarizes some recommended lags to include in several different types of control loops.

Table B.1 Typical measurement lags

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

APPENDIX C
Parameter Tuning

Table C.1 parameter tuning of the Base Case of HDA process

Controller	Controlled variable	Manipulated variable	Tuning parameter			Control action	PV range
			Kc	τI	τD		
FCTOL	Fresh toluene flowrate	fresh feed toluene valve: V2	0.5	0.3	-	reverse	0-600 lbmole/hr
FCH	Fresh gas flowrate	fresh gas feed valve : V1	0.5	0.3	-	reverse	0-900 lbmole/hr
rH2	Hydrogen in reactor inlet	compressor power: wcomp	0.99	0.813	-	reverse	0.2-0.5
PCR	Reactor inlet pressure	purge valve: V4	2	10	-	reverse	400-600 psi
TCR	reactor inlet temperature	furnace duty: qfur	0.83	1.12	0.248	reverse	1100-1310 oF
TCQ	quenched temperature	quench valve: V11	2.23	1.02	0.228	direct	1000-1300 oF
TCS	separator temperature	cooler duty: qcooler	0.90	0.276	0.061	direct	40-150 oF
LCS	Separator liquid level	Col.1 feed valve: V5	2	-	-	direct	0-100 %
CCH2	Methane in mixer outlet	setpoint of fresh gas feed : FCH	0.52	0.057	-	direct	0.5-0.64
CCR2	Toluene in quenches	setpoint of reactor temperature: TCR	0.056	2.84	-	direct	0-0.01

Table C.2 parameter tuning of the CS1 of HDA process

Controller	Controlled variable	Manipulated variable	Tuning parameter			Control action	PV range
			Kc	τI	τD		
FCTOL	Fresh toluene flowrate	fresh feed toluene valve: V2	0.5	0.3	-	reverse	0-600 lbmole/hr
rH2	Hydrogen in reactor inlet	fresh gas feed valve : V1	3.92	0.385	-	reverse	0.2-0.5
PCR	Reactor inlet pressure	purge valve: V4	2	10	-	reverse	400-600 psi
TCR	reactor inlet temperature	furnace duty: qfur	0.819	1.12	0.249	reverse	1100-1310 oF
TCQ	quenched temperature	quench valve: V11	2.20	1.03	0.229	direct	1000-1300 oF
TCS	separator temperature	cooler duty: qcooler	0.66	0.384	0.085	direct	40-150 oF
LCS	Separator liquid level	Col.1 feed valve: V5	2	-	-	direct	0-100 %
CCW	Methane in gas	compressor power: wcomp	0.306	4.19	-	reverse	0.57-0.77
%TCR2	Toluene conversion	setpoint of reactor temperature: TCR	0.208	2.01	0.446	reverse	0-100 %

Table C.3 parameter tuning of the CS2 of HDA process

Controller	Controlled variable	Manipulated variable	Tuning parameter			Control action	PV range
			Kc	τI	τD		
FCTOL	Fresh toluene flowrate	fresh feed toluene valve: V2	0.5	0.3	-	reverse	0-600 lbmole/hr
rH2	Hydrogen in reactor inlet	fresh gas feed valve : V1	3.92	0.385	-	reverse	0.2-0.5
PCR	Reactor inlet pressure	purge valve: V4	2	10	-	reverse	400-600 psi
TCR	reactor inlet temperature	furnace duty: qfur	0.825	1.11	0.246	reverse	1100-1310 oF
TCQ	quenched temperature	quench valve: V11	2.21	1.03	0.228	direct	1000-1300 oF
TCS	separator temperature	cooler duty: qcooler	0.66	0.384	0.085	direct	40-150 oF
LCS	Separator liquid level	Col.1 feed valve: V5	2	-	-	direct	0-100 %
CCW	Methane in gas	compressor power: wcomp	0.32	4.14	-	reverse	0.57-0.77
CCR2	Benzene in liquid	setpoint of reactor temperature : TCR	0.191	7.39	-	reverse	0.75-0.95

Table C.4 parameter tuning of the CS3 of HDA process

Controller	Controlled variable	Manipulated variable	Tuning parameter			Control action	PV range
			Kc	τI	τD		
FCTOL	Fresh toluene flowrate	fresh feed toluene valve: V2	0.5	0.3	-	reverse	0-600 lbmole/hr
rH2	Hydrogen in reactor inlet	fresh gas feed valve : V1	3.92	0.385	-	reverse	0.2-0.5
PCR	Reactor inlet pressure	purge valve: V4	2	10	-	reverse	400-600 psi
TCR	reactor inlet temperature	furnace duty: qfur	0.826	1.11	0.246	reverse	1100-1310 oF
TCQ	quenched temperature	quench valve: V11	2.22	1.03	0.228	direct	1000-1300 oF
TCS	separator temperature	cooler duty: qcooler	0.66	0.384	0.085	direct	40-150 oF
LCS	Separator liquid level	Col.1 feed valve: V5	2	-	-	direct	0-100 %
CCW	Methane in gas	compressor power: wcomp	0.32	4.14	-	reverse	0.57-0.77
TCR2	Reactor outlet temperature	setpoint of reactor temperature : TCR	0.112	5.59	1.24	reverse	1178-1378 oF

APPENDIX D

MAXIMUM SCALED GAIN METHOD

In the study of interaction of controlled variable it is common to use matrix notation. The use of matrix notation allow the compact representation of a system compose of many variables.

The scaled gain matrices are two dimensional arrays that contain scalar elements. In this module most of matrices involve real matrices. Consider the following matrix, which consist of n rows and m columns.

D.1 Rule of Selection Element in Maximum Scaled Gain

1. Select element that maximize the scaled gain value in both of row and column. After selecting maximum element, eliminate both of column and row (i and j)

   $$g_{ij} > g_{im} \text{ and } g_{ij} > g_{nj}$$

   when g_{ij} represents the element in the ith row and jth column of gain matrices

   n number of row
   m number of column

2. In case gain number of two control variables are equivalent, we chose controlled variable which is smallest sensitivity with other manipulated variables for reduce effect of interaction between loops.

   Example 2

   $$G = \begin{bmatrix} 5 & 5 & 2 \\ 1 & 3 & 4 \end{bmatrix}$$

   Combination 1: MV1-CV1, MV2-CV3

3. In case gain numbers of two controlled variables are small difference, we chose both of controlled variables for two combinations.

Example 3

$$G = \begin{bmatrix} 5 & 4 & 2 \\ 4 & 4 & 3 \end{bmatrix}$$

Combination 1: MV1-CV1, MV2-CV2

Combination 2: MV1-CV2, MV2-CV1

Example 4

$$G = \begin{bmatrix} 5 & 5 & 2 \\ 2 & 3 & 4 \end{bmatrix} \text{ MV1= [5 5 2], MV2 = [2 3 4]}$$

Combination 1: MV1-CV1, MV2-CV3

Combination 2: MV1-CV2, MV2-CV3

4. The maximum scale gains of variable indicate that controlled variable has a large and direct effect on manipulated variable. Besides, we should consider about distances between controlled variable and manipulated variable. The controlled variable should be located close to the manipulated variable, because for good controllability we want a small effective delay.

D.2 Comparison Step between Reference and This Work

Table D.1 on the left side show the plantwide control design procedure of the reference paper (Skogestad and Atonio, 2006) and procedure of this work was shown on the right side of Table D1. The reference paper divides procedure into two sections consists of top-down analysis and bottom-up design. The first step to the third step of this work is similar with the reference paper. In the fourth step and the fifth step, this work differ from the reference paper in that the former use maximum scaled gain to selecting and pairing, while the latter use a branch-and-bound algorithm (Cao et al., 1998a) for maximizing the minimum singular value to select controlled variables. The reference paper selects controlled variables in top-down analysis. Then, pair controlled variable with manipulated variable in bottom-up design step.

Table D.1 Comparison Step between Reference and This work

<table>
<tr><th>Step of Reference Paper</th><th>Step of This Work</th></tr>
<tr><td>(I) Top-down analysis</td><td></td></tr>
<tr><td>1. Definition of Operational Objectives

Step1 Definition of optimal operation
- cost
- Constraints</td><td>1. Definition of Operational Objectives

Step1 Definition of optimal operation
- cost
- Constraints</td></tr>
<tr><td>2. Manipulated variables and Degree of Freedom

Step 2 Determine degree of freedom</td><td>2. Manipulated variables and Degree of Freedom

Step 2 Determine degree of freedom</td></tr>
<tr><td>3. Primary Controlled Variables

Step 3 Identification of important disturbances
<table>
<tr><th></th><th>Disturbance Variables</th><th>Type</th><th>Magnitude</th></tr>
<tr><td>D1.</td><td>Fresh feed Toluene flow rate</td><td>Step</td><td>-15</td></tr>
<tr><td>D2.</td><td>Fresh feed Toluene flow rate</td><td>Step</td><td>+15</td></tr>
<tr><td>D3.</td><td>Fresh gas feed rate methane mole fraction</td><td>Step</td><td>+0.05</td></tr>
<tr><td>D4.</td><td>Hydrogen aromatic ratio in reactor inlet</td><td>Step</td><td>+0.5</td></tr>
<tr><td>D5.</td><td>Reactor-inlet pressure</td><td>Step</td><td>+20</td></tr>
<tr><td>D6.</td><td>Quench outlet temperature</td><td>step</td><td>+20</td></tr>
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</table>
</td></tr>
</table>

Step 4 Optimization
1. Quencher outlet temperature Tquencher = 1150 oF (upper bound).
2. Separator temperature Tsep = 95 oF (lower bound).
3. Fresh toluene feed rate Ftol = 300 lbmol/h (upper bound).
4. Reactor inlet pressure Prin = 500 psi (upper bound).
5. Hydrogen to aromatic ratio in reactor inlet rH2 = 5 (lower bound).

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5. Hydrogen to aromatic ratio in reactor inlet rH2 = 5 (lower bound).

Close loops active constraint with appropriate manipulated variable by using the maximum scaled gain method to pairing and selecting variables.

Table 3 The maximum scaled gain between five active constraints and six manipulated variables.

	Y1	Y18	Y20	Y31	Y45
U1	**0.0112**	-0.0441	0.0010	0.0312	0.0010
U2	-0.0054	**0.0412**	0.0014	-0.0147	-0.0005
U4	0.0083	0.0307	-0.0033	**-0.1375**	0.0006
U5	-0.0064	0.0043	0.0000	0.0308	0.0001
U6	0.0100	-0.0134	**-0.0021**	0.0067	0.0008
U7	-0.0018	-0.0060	0.0007	0.0256	**-0.0017**

CV	MV
fresh feed toluene (U1)	fresh feed toluene flow rate (Y1)
fresh gas feed (U2)	hydrogen aromatic ratio in reactor inlet(Y18)
purge flow (U6)	reactor pressure (Y20)
cooler heat duty (U4)	separator temperature (Y31)
quench flow (U7)	quench outlet temperature (Y45)

Step 5 Identification of candidate controlled variables

A branch-and-bound algorithm (Cao et al., 1998a) for maximizing the minimum singular value of $S_1GJ_{uu}^{-1/2}$ and S_1G was used to obtain the candidate sets of controlled variables

Table 1 Candidate controlled variable with small losses in local analysis

	Name	Nominal optimal	Optimal variation	Implementation error	Total Span
1	Furnace outlet temp	1210	5.25	60.5	65.8
2	Purge flow rate	443.70	22.185	58.28	80.464
3	mixer outlet methane mole fraction	0.5707	0.0310	0.0001	0.0311
4	mixer outlet benzene mole fraction	0.0083	0.0002	0.0001	0.0003
5	Quench outlet benzene mole fration	0.0922	0.0049	0.0001	0.0050
6	Quench outlet toluene mole fration	0.0047	0.0008	0.0001	0.0009
7	Quench outlet diphen mole fraction	0.0042	0.0004	0.0001	0.0005
8	Sep overhead bezene mole fraction	0.0087	0.0002	0.0001	0.0003
9	Sep liquid bezene mole fraction	0.8556	0.0106	0.0001	0.0107
10	Sep liquid toluene mole fraction	0.0462	0.0082	0.0001	0.0083
11	Sep liquid diphenyl mole fraction	0.0427	0.0026	0.0001	0.0027
12	Gas recycle (methane) mole fration	0.6695	0.0335	0.0001	0.0336
13	Gasrecycle benzene mole fration	0.0087	0.0002	0.0001	0.0003
14	Compressor power	470.01	109	4.7	113.7
15	Toluene conversion at the reactor	92.206	0.9319	0.9319	1.864

Step 5 Identification of candidate controlled variables

The maximum scaled gain method between candidate control variable and disturbance use to pre-screen the candidate variables which have many effect to disturbance. And then, the maximum scaled gain method between remained controlled variable and manipulated variable use to select controlled variables which have many effect to manipulated variables.

Table 4 The maximum scaled gain between candidates controlled variables and disturbances

	Y8	Y21	Y23	Y24	Y25	Y26	Y27	Y28
D1-D2	-0.571	0.049	0.709	-0.416	0.809	**-2.595**	**2.015**	0.182
D3	0.002	-0.001	-0.002	0.001	-0.002	0.013	-0.007	-0.001
D4	-0.548	0.013	**1.060**	-0.497	-0.001	**-1.778**	-0.271	0.088
D5	0.555	-0.101	-0.733	0.432	-0.753	-0.425	-0.867	-0.017
D6	0.065	-0.095	-0.081	0.047	-0.100	0.611	-0.337	-0.036

	Y29	Y34	Y35	Y41	Y42	Y43	Y47	Y48
D1-D2	**2.423**	0.762	-0.366	0.141	**-3.347**	**1.223**	0.693	-0.430
D3	-0.003	-0.002	0.001	-0.001	0.015	-0.005	-0.002	0.001
D4	-0.215	**1.051**	-0.504	0.125	**-1.676**	-0.153	**1.063**	-0.495
D5	0.097	-0.780	0.381	-0.091	0.270	-0.159	-0.720	0.447
D6	-0.295	-0.086	0.042	-0.031	0.686	-0.260	0.278	0.380

	Y49	Y50	Y51	Y60
D1-D2	0.708	**-2.729**	**1.859**	0.014
D3	-0.002	0.013	-0.007	0.000
D4	0.020	**-1.760**	-0.250	-0.012
D5	-0.632	-0.287	-0.718	0.899
D6	**-3.083**	**-2.600**	**-3.613**	0.048

Table 2 local analysis: Minimum singular values for candidate sets

	Var1	Var2	SVD
1	3	6	0.0078
2	3	10	0.0073
3	3	15	0.0066
4	3	9	0.0066
5	3	8	0.0045
6	3	13	0.0045
7	3	5	0.003
8	3	4	0.003
9	3	7	0.0053
10	1	2	0.0013
11	1	12	0.0013
12	2	12	0.0013
13	1	14	0.0013
14	2	14	0.0017
15	12	14	0.0003

CV
1. mixer outlet methane mole fraction (3)
2. Quench outlet toluene mole fration (6)

Table 5 The maximum scaled gain between candidates controlled variables and remained manipulated variables

	Y8	Y21	Y24	Y25	Y28	Y35	Y41	Y48	Y60
U3-SP	-0.246	**0.776**	0.007	0.623	**2.239**	-0.028	**1.307**	-0.268	-0.003
U5	0.195	-0.033	0.107	-0.320	-0.144	**0.121**	-0.110	0.142	0.076

	CV	MV
CS1	Toluene conversion in reactor	Setpoint of reactor inlet temperature loop
	Methane composition in gas	Compressor power
CS2	Benzene composition in liquid	Setpoint of reactor inlet temperature loop
	Methane composition in gas	Compressor power
CS3	Reactor outlet temperature	Setpoint of reactor inlet temperature loop
	Methane composition in gas	Compressor power

4. Production Rate

The decision on where to place the production rate manipulator is closely related to where in the process there are bottlenecks that limit the flow of mass and energy. In addition, the decision directly affects the way total inventory (liquid or gas) of individual units are controlled across the process

4. Production Rate and Process Constraint

The goal of the operation is to produce benzene at 256 lbmole/hr with 0.9997 purity. The operational and safety constraints are the following in Step1 Definition of optimal operation.

(II) Bottom-up design

5. Regulatory Control Layer

The main objective of this layer is to provide sufficient quality of control to enable a trained operator to keep the plant running safely without the use of the higher layers in the control system.

- Stabilization of unstable modes (including liquid levels)

CV	MV
Rin Temperature	Furnace heat duty
Separator level	liquid flow out of the separator

- Avoiding drift I: Pressure control

CV	MV
Reactor inlet pressure	purge flow rate

- Avoiding drift II: Temperature loops

CV	MV
quencher outlet temperature	flow rate of the cold liquid stream from the separator
Separator Temperature	Cooler heat duty

Use maximum scaled gain method to pairing controlled variables with manipulated variables
(In step 5)

<table>
<tr>
<td>

- Avoiding drift III: Flow control

<table>
<tr><th>CV</th><th>MV</th></tr>
<tr><td>toluene feed rate</td><td>Flow control</td></tr>
<tr><td>hydrogen feed rate</td><td>Flow control</td></tr>
</table>

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<td>

6. Supervisory Control Layer

The aim of the supervisory control layer is to keep the active constraints and unconstrained (self-optimizing) controlled variables at constant set points.

We will proceed with a more detailed analysis based on RGA methods which requires a linear model of the process and for this we use the linearization capabilities of Aspen DynamicsTM.

<table>
<tr><th></th><th>Ws</th><th>H2</th><th>RT</th></tr>
<tr><td>cHEinMe</td><td>-0.000009095</td><td>-0.036961484</td><td>0.000000244</td></tr>
<tr><td>quench tol</td><td>0.000014729</td><td>-0.077501225</td><td>-0.000001312</td></tr>
<tr><td>rH2</td><td>-0.617469880</td><td>0.000757987</td><td>-0.000063755</td></tr>
</table>

<table>
<tr><th>RGA</th><th>Ws</th><th>H2</th><th>RT</th></tr>
<tr><td>cHEinMe</td><td>0.001079</td><td>0.71923</td><td>0.2797</td></tr>
<tr><td>quench tol</td><td>0.000833</td><td>0.28077</td><td>0.71839</td></tr>
<tr><td>rH2</td><td>0.99809</td><td>1.52E-07</td><td>0.001912</td></tr>
</table>

</td>
<td>Use maximum scaled gain method to pairing controlled variables with manipulated variables
(In step 5)</td>
</tr>
<tr>
<td>7. Optimization layer</td>
<td>-</td>
</tr>
<tr>
<td>8. Validation</td>
<td>-</td>
</tr>
</table>

D.3 Pairing of Active Constraint and Controlled variables

In this work, we close loop of five active constraints before selecting other controlled variables. Normally, we should control dominate variable which effect to production rate or quality of product. Once we identify the dominant variables, we must also identify the manipulators (control valves) that are most suitable to control them. In this section, we explain reasoning why we close loop five active constraints before. The reasons were indicated with exemplary test.

D.3.1 Select Manipulated Variables for Active Constraint and other Controlled variables simultaneously.

We can select manipulated variables for five active constraints and other controlled variables simultaneously. The problems of this way consist of: the large dimension of problem and erroneous controlled variables were selected. The large dimension of problem because many candidate controlled variables were scrutinized at the same time while the erroneous controlled variables were selected because selected variables are more sensitive with manipulated variable but do not necessary to control them. Table D.2 show the scaled gain of manipulated variables with five active constraints and other candidate controlled variables. The reasons were shown in Table D.3. The erroneous controlled variables were selected such as composition of toluene and biphenyl in reactor outlet stream and quenches because those variables have large scaled gain more than five active constraints. The reactor pressure is importance active constraint that should control but scaled gain of reactor pressure is smaller than other variable. Therefore, we should close loop of five active constraints before other variables.

Table D.2 The scaled gain of manipulated variables with five active constraints and other candidate controlled variables.

	Y1*	Y2	Y7	Y8	Y18*	Y20*	Y21	Y24	Y25	Y26	Y27	Y28	Y29
U1	1.0000	-0.5964	-2.1668	1.1331	-3.9196	0.0889	-0.0016	1.1513	1.4973	3.2656	4.7947	-0.0952	0.3341
U2	-0.3600	1.0000	1.8676	-1.0652	2.7749	0.0960	0.0113	-1.0196	-0.6253	-3.6616	-2.0993	0.1541	-0.3875
U3-SP	-1.5393	-1.3215	-1.6575	0.7374	-3.8841	0.3566	0.6980	0.7967	2.3204	-34.169	24.5643	1.7686	2.1316
U4	0.4211	0.3576	0.0694	0.1356	1.5510	-0.1645	0.0266	0.0968	-1.3932	1.6546	-3.6420	-0.0969	8.7664
U5	-0.3316	-0.2826	0.0904	-0.0402	0.2243	0.0021	-0.0285	-0.0953	-0.1414	1.2893	-0.8593	-0.0983	-3.5564
U6	1.0733	0.9110	-0.1456	-0.0723	-1.4409	-0.2256	0.0436	0.0663	1.2268	-0.2838	3.1802	0.0818	2.0950
U7	-0.1234	-0.1050	-0.0147	-0.0413	-0.4163	0.0497	-0.0083	-0.0315	0.3894	-0.4395	1.0344	0.0245	-1.9360

Y31*	Y32	Y35	Y36	Y42	Y43	Y44	Y45*	Y48	Y49	Y50	Y51	Y52	Y61
2.772	0.0856	-2.716	1.2300	-0.3097	1.7540	3.550	0.0897	-2.7865	1.1568	0.815	2.650	4.2573	0.1126
-0.988	0.1067	2.269	-1.0631	0.2676	-2.9185	-1.433	-0.0316	2.3196	-1.0160	-0.344	-3.418	-1.8771	0.0579
10.489	0.3851	-2.137	0.6931	0.5390	-34.132	27.446	0.6089	-2.0462	0.7626	1.951	-34.10	26.080	0.244
-6.942	-0.1962	0.122	0.1041	-0.0015	2.1545	-3.851	0.0320	0.1168	0.1135	-1.027	1.711	-3.8356	-0.0684
1.593	-0.0169	0.183	-0.1305	-0.0520	1.6722	-0.274	0.0032	0.2345	-0.0859	-0.205	1.325	-0.7434	0.0534
0.722	-0.2411	-0.340	0.1427	-0.0024	-1.4766	1.976	0.0897	-0.4113	0.0738	0.727	-0.799	2.6408	-0.1745
1.775	0.0505	-0.026	-0.0347	-0.0061	-0.5714	1.113	-0.1167	-0.0624	-0.0715	0.606	-0.115	1.4604	0.0199

*active constraint variables

Table D.3 The pairing of controlled variables and manipulated variables

	Manipulated Variables	Controlled Variables (set1)	Controlled Variables (set2)
1	Fresh feed Toluene	Biphenyl composition at reactor outlet(Y27)	Biphenyl composition at reactor outlet(Y27)
2	Fresh feed Hydrogen	Toluene composition at quenches(Y51)	Hydrogen to aromatic ratio(Y18)
3	Setpoint of reactor temperature	Toluene composition at reactor outlet(Y26)	Toluene composition at reactor outlet(Y26)
4	Cooler cooling water valve	Benzene conversion at reactor(Y29)	Separator temperature(Y31)
5	Compressor power	Toluene composition at liquid stream(Y43)	Hydrogen composition at quenches(Y48)
6	Purge flow	Biphenyl composition at quenches(Y52)	Fresh toluene feed flowrate(Y1)
7	Quench flow	Separator temperature(Y31)	benzene composition at quenches(Y50)

VITA

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