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การออกแบบโครงสร้างการควบคุมแบบแพลนท์ไวด์

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Abstract

Hydrodealkylation (HDA) plant with different energy integration schemes is a realistically complex chemical process, since three heat exchanger network alternative can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduced are the causes of a low level of control performance. Therefore, this work presents three plantwide control structures for three different energy integration schemes. In order to illustrate the dynamic behaviors of the control structures in HDA plant change in the heat load disturbance of cold stream and change in the recycle toluene flowrates were made. Three control structures have been tested and compared, the first control structure is a modification of Luyben control structure using valve position control concept to control temperature of a column. The second control structure was the modification of the first control structure by adding a cooling unit to control the outlet temperature from the reactor, instead of using internal process flow. In the third control structure, a ratio control was added to the second control structure for controlling the ratio of hydrogen and toluene within the process. The result shows the third control structure gives a smaller settling time and can reject disturbances better than other control structures. However, the utility consumption of the first control structure is less than thoses of the second and the third control structures. HDA process alternative 3 gives the slowest response compared with other alternatives indicated by the IAE values. It can be concluded from this research that the implementation of complex energy integration to the process deteriorates the dynamic performance of the process.

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บทคัดย่อ

โรงงานไฮโดรดิแอลคิลเลชันที่มีแผนเบ็ดเสร็จเชิงพลังงานแตกต่างกัน เป็นกระบวนการทางเคมีที่มีความซับซ้อน ด้วยเหตุที่ข่ายงานเครื่องแลกเปลี่ยนความร้อนสามรูปแบบสามารถปรับปรุงโดยนำสายป้อนกลับและเบ็ดเสร็จเชิงพลังงานสู่กระบวนการ แต่อย่างไรก็ตามการนำสายป้อนกลับและเบ็ดเสร็จเชิงพลังงานสู่กระบวนการเป็นสาเหตุให้สมรรถนะการควบคุมต่ำลง ดังนั้นในงานนี้จึงนำเสนอโครงสร้างการควบคุมแบบแบบแพลนไวด์สามโครงสร้าง สำหรับกระบวนการที่มีแผนเบ็ดเสร็จเชิงพลังงานแตกต่างกันสามรูปแบบ ในการแสดงพฤติกรรมเชิงพลวัตรของการออกแบบโครงสร้างควบคุมแบบแพลนท์ไวด์ในโรงงานไฮโดรดิแอลคิลเลชัน โดยสร้างการรบกวนภาระทางความร้อนของกระแสเย็นและเปลี่ยนอัตราการไหลของทอลูอีนแปรใช้ใหม่ โดยมีโครงสร้างการควบคุมสามโครงสร้างได้ถูกทดสอบและเปรียบเทียบ โครงสร้างการควบคุมที่ 1 ได้แก้ไขโครงสร้างการควบคุมของลูเบนโดยใช้การควบคุมโดยใช้ตำแหน่งของวาล์ว (Valve Position Control) ในการควบคุมอุณหภูมิในคอลัมน์โครงสร้างการควบคุมที่ 2 ได้แก้ไขโครงสร้างการควบคุมที่ 1 โดยใช้หน่วยหล่อเย็น (Cooling Unit) ในการควบคุมอุณหภูมิขาออกจากถังปฏิกรณ์แทนการใช้กระแสภายในกระบวนการ ส่วนโครงสร้างการควบคุมที่ 3 นำโครงสร้างการควบคุมที่ 2 มาเพิ่มวงควบคุมแบบสัดส่วน โดยควบคุมสัดส่วนสารไฮโดรเจนต่อทอลูอีนในกระบวนการให้มีค่าคงที่ ผลการศึกษาแสดงว่าโครงสร้างการควบคุมที่ 3 สามารถปฏิเสธตัวรบกวนได้มากกว่าและเร็วกว่าโครงสร้างการควบคุมอื่น แต่อย่างไรก็ตามโครงสร้างการควบคุมที่ 1 ใช้พลังงานน้อยกว่าโครงสร้างการควบคุมที่ 2 และโครงสร้างการควบคุมที่ 3 กระบวนการไฮโดรดิแอลคิลเลชันรูปแบบที่ 3 ให้การตอบสนองช้าที่สุดเมื่อเปรียบเทียบกับรูปแบบอื่นโดยบ่งชี้จากค่าความคลาดเคลื่อนสัมบูรณ์ ดังนั้นในงานวิจัยนี้สามารถสรุปได้ว่ารูปแบบพลังงานเบ็ดเสร็จที่ซับซ้อนทำให้สมรรถนะทางพลวัตรด้อยลง

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r_1	Reaction rate of hydrodealkylation of toluene reaction
r_2	Reaction rate of side reaction of hydrodealkylation of toluene reaction
p_T	The partial pressure of toluene, psia
p_H	The partial pressure of hydrogen, psia
p_B	The partial pressure of benzene, psia
p_D	The partial pressure of diphenyl, psia
V_R	Reactor volume
T	Temperature
P	Pressure
CS1	Design control structure I
CS2	Design control structure II
CS3	Design control structure III

CHAPTER I

INTRODUCTION

1.1 Background

Most industrial process contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. The economic can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduce a feedback of material and energy among unit upstream and downstream.

Many controls of heat-integrated systems have been studied by several workers. Terrill and Douglas (1987a, 1987b, 1987c) have proposed six HEN alternatives for the hydrodealkylation of toluene (HDA) process, in which their energy saving ranges between 29 % and 43 %. Further, study of plantwide process control has also been done by several authors. Luyben et al. (1997) presented a general heuristic presented a general heuristic design procedure for plantwide process control. Their nine steps of the proposed procedure center around the fundamental principles of plantwide control were energy management, production rate, product quality, operational, environmental and safety constraints, liquid-level and gas-pressure inventories, make-up of reactants, component balances, and economic or process optimization. In Luyben et al. (1999), the HDA process alternative 1 of Terrill and Douglas was used as one of four cases to apply their nine steps plantwide control design procedure. Wongsri and Kietawarin (2002) apply Luyben nine steps plantwide control design procedure to present and compare among 4 control structures designed for HDA process alternative 1 withstanding disturbances that cause production rate change, the control structures was compared with reference on Luyben (1998) plantwide process control book. In 2004, Wongsri and Thaicharoen presented the new control structures for the hydrodealkylation of toluene (HDA) process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben's structure. In the same year Wongsri and Hermawan Y.D. studied the control strategies for energy-integrated HDA plant (i.e. alternatives 1 and 6) based on the heat pathway heuristics (HPH). The study reveals that, by selecting an appropriate heat pathway through the network, the utility consumptions can be reduced according to the input heat load disturbances; hence the dynamic MER can be achieved.

Although several authors have studied the general design and control strategies for energy-integrated HDA plant but there is no report on study of the effect of energy integration on control performance for six HEN alternatives HDA plant, so in this research, it will focus on heuristic-based plantwide control procedure applied to HDA process for hydrodealkylation of toluene to form benzene that consists of a reactor, furnace, vapor-liquid separator, recycle compressor, heat exchangers and distillations. This plant is a realistically complex chemical process. It is considering that the energy integration for realistic and large processes is meaningful, useful and essential to design a control strategy for process associate with energy integration, so it can be operated well. So the main objective of this study is to evaluate performance of the control structures for the HDA process with energy integration schemes that are designed by Terrill and Douglas (i.e. alternative 1, 2, 3, 4, 5 and 6). In this work, the commercial software HYSYS is chosen to carry out both steady state and dynamic simulations.

1.2 Research Objectives

To develop the design of the plant wide control structure for hydrodealkylation (HDA) process both with and without heat integration.

1.3 Scope of research

1. Simulation of the hydrodealkylation (HDA) of toluene process is performed by using a commercial process simulator -HYSYS.
2. The heat integration for the hydrodealkylation (HDA) process is obtained from Terrill and Douglas 1987 (alternative 1, 2 and3).
3. The basic concepts and steps of plantwide process control, introduced by the pioneer researchers such as Buckley and Luyben, are applied to develop the design methods of this study.

CHAPTER II

SURVEY OF RELATED LITERATURE

2.1 Plantwide Control Fundamental

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 entire plant consisting of many interconnected unit operations.

2.1.1 Incentives for Chemical Process Control

A chemical plant is an arrangement of processing units (reactors, heat exchangers, pumps, distillation columns, absorbers, evaporators, tanks, etc.), integrated with one another in a systematic and rational manner. The plant's overall objective is to convert certain raw materials into desired products using available source of energy, in the most economical way.

There are three general classes of needs that a control system is called on to satisfy: suppressing the influence of external disturbances, ensuring the stability of a chemical process, and optimizing the performance of a chemical process.

2.1.1.1 Suppressing the Influence of External Disturbances

Suppressing the influence of external disturbances on a process is the most common objective of a controller in a chemical plant. Such disturbances, which denote the effect that the surroundings (external world) have on a reactor, separator, heat exchanger, compressor and so on, are usually out of the reach of human operator. Consequently, a control mechanism that will make the proper change on the process must me introduced to cancel the negative impact that such disturbances may have on the desired operation of a chemical plant. In other words:' in order to face all disturbances entering the process, the strategies for control are very important.

2.1.1.2 Ensuring the Stability of a Chemical Process

The process is stable or self-regulating, if the process variable such as temperature, pressure, concentration, or flow rate stay at a certain point or at a desired steady state value as time progresses. Otherwise, the process is unstable and requires external control for the stabilization of their behavior.

2.1.1.3 Optimizing the Performance of a Chemical Process

Safety and the satisfaction of product specifications are the two principal operational objectives for a chemical plant. Once these are achieved, the next goal is how to make the operation of the plant more profitable. Given the fact that the conditions that affect the operation of the plant do not remain the same. It is clear that the operation of the plant can be changed (flow rates, pressures, concentrations, temperatures) in such a way that an economic objective (profit) is always maximized.

2.1.2 Integrated Processes

Three basic features of integrated chemical processes lie at the root of the need to consider the entire plant's control system, as follows: the effect of material recycle, the effect of energy integration, and the need to account for chemical component inventories. However, there are fundamental reasons why each of these exists in virtually all-real processes.

2.1.2.1 Material recycles

Material is recycled for six basic and important reasons

1. Increase conversion: For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.
2. Improve economics: In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than it is to reach the necessary conversion level in one reactor or several in series. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.
3. Improve yields: In reaction system such as, $A \rightarrow B \rightarrow C$, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much of the undesirable product C. Therefore the concentration of B is kept fairly low in the reactor and a large recycle of A is required.
4. Provide thermal sink: In adiabatic reactors and in reactors where cooling is difficult and exothermic heat effects are large, it is often necessary to feed excess material to the reactor (an excess of one reactant or a product) so that the reactor temperature increase will not be too large. High temperature can potentially create several unpleasant events: it can lead to thermal runaways, it can deactivate catalysts, it can cause undesirable side reactions, it can cause mechanical failure of equipment, etc. So the heat of reaction is absorbed by the sensible heat required to rise the temperature of the excess material in the stream flowing through the reactor.
5. Prevent side reactions: A large excess of one of the reactants is often used so that the concentration of the other reactant is kept low. If this limiting reactant is not kept in low concentration, it could react to produce undesirable products. Therefore the reactant that

is in excess must be separated from the product components in the reactor effluent stream and recycled back to the reactor.

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

2.1.2.2 Energy integration

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

2.1.2.3 Chemical component inventories

A plant’s chemical species can be characterized into three types: reactants, products, and inerts. A material balance for each of these components must be satisfied. This is typically not a problem for products and inerts. However, the real problem usually arises when reactants (because of recycle) are considered and accounted for their inventories within the entire process. Because of their value, it is necessary to minimize the loss of reactants exiting the process since this represents a yield penalty. So reactants from leaving are prevented. This means we must ensure that every mole of reactant fed to the process is consumed by reactions.

2.1.3 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex. Two basic effect of recycle is: Recycle has an impact on the dynamics of the process. The overall time constant can be much different than the sum of the time constants of the time constants of the individual units. Recycle leads to the snowball effect. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates.

2.2 Basic Concepts of Plantwide Control

2.2.1 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. He try to make these as small as possible so that good, tight control is achievable, but stability constraints impose limitations on the achievable performance.

2.2.2 Douglas doctrines

Because 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 the tight control of stream compositions exiting the process are needed 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.

2.2.3 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. All components (reactants, product, and inerts) have a way to leave or be consumed within the process. Most of the problems occur in the consideration of reactants, particularly when several chemical species are involved. Because raw material costs and maintain high-purity products usually must be minimized, 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.

2.2.4 Luyben laws

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

1. To prevent the snowball effect, all recycle loops should be flow controlled.
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 $A + B \rightarrow$ products. In system with consecutive reactions such as $A + B \rightarrow M + C$ and $M + B \rightarrow D + C$, 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.

2.2.5 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.

2.2.6 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.

2.2.7 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 (K_u) and ultimate period (P_u). Then either the Ziegler-Nichols setting or the Tyreus-Luyben (1992) settings can be used:

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

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

2.3 Step of Plantwide Process Control Design Procedure

The nine steps of the design procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental, and safety constraints; liquid level and gas pressure inventories; makeup of reactants; component balances; and economic or process optimization.

Step1: Establish control objectives

Assess steady-state design and dynamic control objectives for the process. This is probably the most important aspect of the problem because different criteria lead to different control structures. These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of operating conditions.

Step 2: Determine control degrees of freedom

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

Step 3: Establish energy management system

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

Heat removal in exothermic reactors is crucial because of the potential for thermal runaways. In endothermic reactions, failure to add enough heat simply results in the reaction slowing up. If the exothermic reactor is running adiabatically, the control system must prevent excessive temperature rise through the reactor (e.g., by setting the ratio of the flow rate of the limiting fresh reactant to the flow rate of a recycle stream acting as a thermal sink).

Increased use of heat integration can lead to complex dynamic behavior and poor performance due to recycling of disturbances. If not already in the design, trim heaters/coolers or heat exchanger bypass lines must be added to prevent this. Energy disturbances should be transferred to the plant utility system whenever possible to remove this source of variability from the process units.

Step 4: Set production rate

Establish the variable that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate. To obtain higher production rate, the overall reaction rates must be increased. This can be accomplished by raising temperature, increasing reactant concentrations, increasing reactor holdup, or increasing reactor pressure. The selected variable must be dominant for the reactor.

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

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

Select the best valves to control each of the product-quality, safety, and environmental variables. Tight controls of these quantities are required for economic and operational reasons. Hence manipulated variables should be selected such that the dynamic relationships between controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants, and the latter prevents problems with the range-ability of the manipulated variable (control-valve saturation)

Step 6: Fix a flow in every recycle loop and control inventories (pressure and level)

Determine the valve to control each inventory variable. These variables include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit.

Proportional-only control should be used in non-reactive control loops for cascade unit in series. Even in reactor-level control, proportional control should be considered to help filter flow-rate disturbances to the down stream separation system. There is nothing necessarily sacred about holding reactor level constant.

In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flows in recycle loops are controlled by levels. Two benefits result from this flow-control strategy. First, the plant's separation section is not subjected to large load disturbances. Second, consideration must be given to alternative fresh reactant makeup control strategies rather than flow control. In dynamic sense, level controlling all flows in recycle loop is a case of recycling of disturbances and should be avoided.

Step 7: Check component balances

Component balances are particularly important in process with recycle streams because of their integrating effect. The specific mechanism or control loop must me identified to guarantee that there will be no uncontrollable buildup of any chemical component within the process (Downs drill). In process, the reactant components aren't required to leave in the product streams because of the yield loss and the desired product purity specification. Hence the use of two methods is limited: consuming the reactants by reaction or adjusting their fresh feed flow. The purge rate is adjusted to control the inert composition in the recycle stream so that an economic balance is maintained between capital and operating costs.

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations. A tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor.

Step 9: Optimize economics or improve dynamic controllability

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

2.4 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.

2.4.1 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.

2.4.2 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, the heat pathways in the process can be separated to three different paths as illustrate in. Fig.2.1. 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.

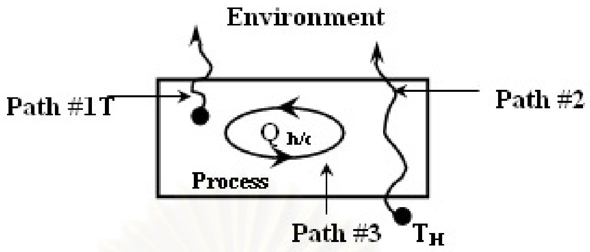

Figure 2.1: Heat pathways

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.

2.4.3 Heat recovery

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

2.5 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. The two exit temperatures can be controlled provided that the two inlet flowrates can be independently manipulated. However, these flowrates are normally unavailable to manipulate. Therefore two degrees of freedom for temperature control are neglected. One of these degrees of freedom can be restored fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Fig. 2.2a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig 2.2b.

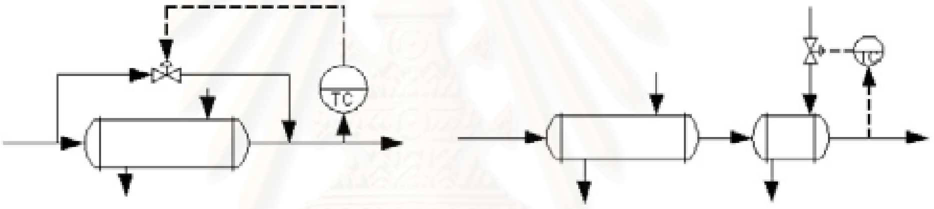

Figure 2.2: Control of P/P heat exchangers (a) Use of bypass; (b) use of auxiliary utility exchanger.

2.5.1 Use of auxiliary utility exchangers

When the P/P exchanger is combined with a utility exchanger, there are a few design decisions to make. The relative sizes between the recovery and the utility exchangers have to be established first. From a design standpoint making the recovery exchanger large and the utility exchanger small is required. This leads to 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, decision on how to combine the utility exchanger with the P/P exchanger must be made. This could be done either in a series or parallel arrangement. Physical implementation issues may dictate this choice but it could affect controllability. Finally, decision on how to control the utility exchanger for best overall control performance has to be made.

Consider a distillation column that uses a large amount of high-pressure stream in its thermo siphon reboiler. Heat-integrate this column with the reactor is applied to reduce operating costs. A practical way of doing this is to generate stream in a waste heat boiler connected to the reactor as suggested. Some or all of this steam is used 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.

2.5.2 Use of Bypass Control

When the bypass method is used for unit operation control, there are several choices about the bypass location and the control point. Figure 2.3 shows the most common alternatives. The question like ”Which option is the best?” may be raised. The best option depends on what definition of the ”best” is given. As with many other examples, it boils down to a trade-off between design and control. Design considerations might suggest that the cold side is measured and bypassed 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 the most important stream should be measured, regardless of temperature, and bypassed on the same side. This minimizes the effects of exchanger dynamics in the loop. A large fraction of the controlled stream needs to be bypassed since it improves the control range. This requires a large heat exchanger.

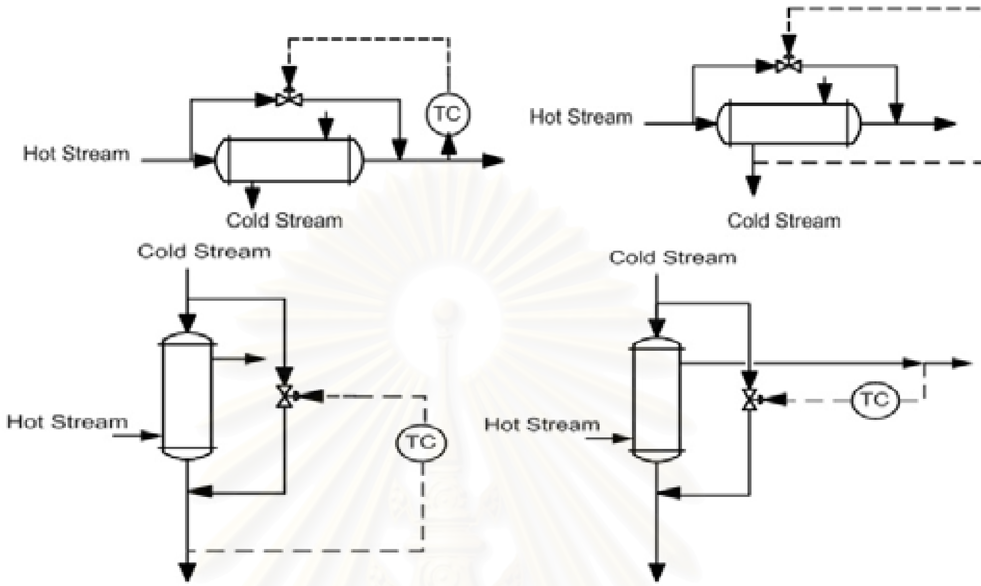

Figure 2.3: Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

2.6 Valve Position Control

Shinskey (1976) proposed the use of type of control configuration that he called valve position control. This strategy provides a very simple and effective method for achieving ”optimizing control”. The basic idea is illustrated by several important applications.

Since relative volatilities increase in most distillation systems as pressure decrease, the optimum operation would be to minimize the pressure at all times. One way to do this is to just completely open the control valve on the cooling water. The pressure would then float up and down as cooling water temperatures changed.

However, if there is a sudden drop in cooling water temperature (as can occur during a thunder shower or ”blue norther”), the pressure in the column can fall rapidly. This can cause flashing of the liquid on the tray, will upset the composition and level controls on the column, and could even cause the column to flood.

To prevent this rapid drop, Shinskey developed a ”floating-pressure” control system. A conventional PI pressure controller is used. The output of the pressure controller goes to the cooling water valve, which is AC so that it will fail open. The pressure controller output is also sent to another controller, the ”valve position controller” (VPC). This controller looks at the signal to the valve, compares it with the VPC setpoint signal, and sends out a signal which is the setpoint of the pressure controller. Since the valve is AC, the setpoint of VPC is about 5 percent of scale so as to keep the cooling water valve almost wide open.

The VPC scheme is a different type of cascade control system. The primary control is the position of the valve. The secondary control is the column pressure. The pressure controller is PI and tuned fairly tightly so that it can prevent the sudden drops in pressure. Its setpoint is slowly changed by the VPC to drive the cooling water valve nearly wide open. A slow-acting, integral-only controller should be used in the VPC.

Luyben show another of the application of VPC to optimize a process as figure 2.4. The temperature of a reactor must be controlled. The reactor is cooled by both cooling water flowing through a jacket surrounding the reactor and by condensing vapor that boil off the reactor in a heat exchanger that is cooled by a refrigerant. This form of cooling is called ”autorefrigeration”.

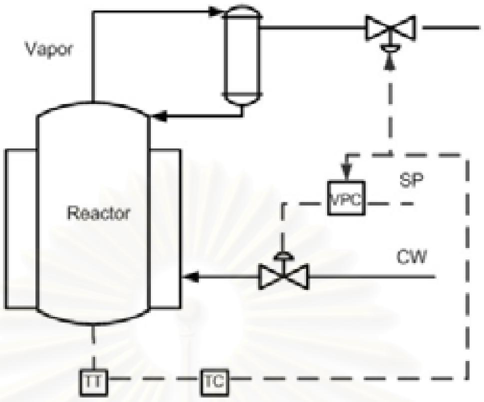

Figure 2.4: Use of VPC to minimize energy cost.

From an energy-cost perspective, cooling water and not refrigerant are suggested because water is much cheaper. However, the dynamic response of the temperature to a change in cooling water may be much slower than to a change in refrigerant flow. This is because the change in water flow must change the jacket temperature, which then changes the metal wall temperature, which then begins to change the reaction mass temperature. Changes in refrigerant flow quickly raise or lower the pressure in the condenser and change the amount of vaporization in the reactor, which is reflected in reactor temperature almost immediately.

So, from a control point of view, he would like to use refrigerant to control temperature. Much tighter control could be achieved as compared to using cooling water. The VPC approach handles this optimization problem very nicely. Simply control temperature with refrigerant, but send the signal that is going to controller which will slowly move the cooling water valve to keep the refrigerant valve nearly closed. Since the refrigerant valve is AC, the setpoint signal to the VPC will be about 5 to 10 percent of full scale.

2.7 Related Literature

2.7.1 A Hierarchical Approach to Conceptual Design

A synthesis/analysis procedure for developing first flowsheets and base-case designs had been established by J. M. Douglas (1985). The procedure was described in terms of a hierarchy of decision levels , as (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).

J. M. Douglas (1985) considered a continuous process for producing benzene by hydrodealkylation of toluene (HDA Process) to illustrate the procedure. The complete process was always considered at each decision level, but additional level terminates in an economic analysis. Experience indicated that less than one percent of the ideas for new designs were ever commercialized, and therefore it was highly desirable to discard poor projects quickly. Similarly, the later level decisions were guided by the economic analysis of the early level decisions.

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 flow rate 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 flow rate constant by adjusting fuel to the furnace, (6) Hold the temperature of the cooling water leaving the partial condenser constant.

In plantwide control systems and strategies papers, 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.

Tyreus and W.L. Luyben (1993) considered second-order kinetics with two fresh feed makeup streams. Two cases are considered: (1) instantaneous and complete one pass conversion of one of the two components in the reactor so there is an excess of only one component that must be recycled and (2) incomplete conversion per pass so there are two recycle streams. It is shown that the generic liquid-recycle rule proposed by Luyben applies in both of these cases: ”snowballing” is prevented by fixing the flow rate somewhere in the recycle system. An additional generic rule is proposed: fresh feed makeup of any component cannot be fixed unless the component undergoes complete single-pass conversion. In the complete one-pass conversion case, throughput can be set by fixing the flow rate of the limiting reactant. The makeup of the other reactant should be set by level control in the reflux drum of the distillation column.

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.

2.7.2 Heat Exchanger Network (HEN)

Energy conservation has always been important in process design. Thus it was common practice to install feed-effluent exchangers around reactors and distillation columns. The starting point for an energy integration analysis is the calculation of the minimum heating and cooling requirements for heat exchanger network (HEN). The design of heat exchanger networks is based on analysis of the heat fluxes in the network as a work as a whole. One representative of such methods is the Linnhoff ”pinch” method. This technique uses the H/T diagram with cumulative curves for the quantities of heat dissipated and absorbed in various sections of the plant at defined temperatures. The method can be applied to utility systems and to the integration of thermal engines.

Linhoff, B. and Hindmarsh, E. (1983) presented a novel method for the design of HEN. The method is the first to combine sufficient simplicity to be used by hand with near certainty to identify ”best” designs, even for large problems. Best design feature the highest degree of energy recovery possible with a given number of capital items. Moreover, they feature network patterns required for good controllability, plant layout, intrinsic safety, ect. Typically, 20 -30 % energy savings, coupled with capital savings, can be realized in state-of-the art flowsheets by improved HEN design. The task involves the placement of process and utility heat exchangers to heat and cool process streams from specified supply to specified target temperatures.

Generally, minimum cost networks feature the correct degree of energy recovery and the correct number of units. This is achieved in two stages. First, the method aims for a minimum energy solution, corresponding to a specified , with no more units than is compatible with minimum energy. This task is achieved through understanding of the pinch phenomenon, hence the method is called the pinch design method. Second, the method involves a controlled reduction in number of units. This may require ”backingoff” from minimum utility usage.

Linhoff, B., Dunford, H., and Smith, R., (1983) studied heat integration of distillation column into overall process. The result show good integration between distillation and the overall process can result in column operating at effectively zero utility cost. Generally, the good integration is when the integration as column not crossing heat recovery pinch of the process and either the reboiler or the condenser being integrated with the process. If these criteria can be met, energy cost for distillation can effectively be zero.

In a series papers, studies of the sensitivity of the total processing cost to heat exchanger network alternatives and steady state operability evaluation were undertaken by D. L. Terrill and J. M. Douglas (1987a,b,c). They considered a heat exchanger network for HDA process. The T-H (temperature-enthalpy) diagram was considered and obtained six alternative heat exchanger networks, all of which had close to maximum energy recovery. Most of the alternatives include a pressure shifting of the recycle column, and the other distinguishing feature is the number of column reboilers that are driven by the hot reactor products. The benefit obtained from energy integration with the base-case flow rates for the six alternatives, the energy saving from the energy integration fall between 29 and 43% but cost savings were in the range from -1 to 5%. The cost savings were not as dramatic because the raw material costs dominate the process economics.

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

2.7.3 Design and Control of Energy-Integrated Plants

Renanto Handogo and W. L. Luyben (1987) studied the dynamics and control of heatintegrated reactor/column system. An exothermic reactor was the heat source, and a distillation column reboiler was the heat sink. Two types of heat-integration systems were examined: indirect and direct heat integration. Both indirect and direct heat integration systems are found in industry. In the indirect heat integration system, steam generation was used as the heating medium for the reboiler. The direct heat-integration system used the reactor fluid to directly heat the column. The indirect heat-integration system was found to have several advantages over the direct heat integration system in term of its dynamic performance. Both systems were operable for both large and small temperature differences between the reactor and column base.

M.L. Luyben, and W.L. Luyben (1995) examines the plantwide design and control of a complex process. The plant contains two reaction steps, three distillation columns, two recycle streams, and six chemical components. Two methods, a heuristic design procedure and a nonlinear optimization, have been used to determine an approximate economically optimal steady-state design. The designs differ substantially in terms of the purities and flow rates of the recycle streams. The total annual cost of the nonlinear optimization design is about 20 % less than the cost of the heuristic design. An analysis has also been done to examine the sensitivity to design parameters and specifications. Two effective control strategies have been developed using guidelines from previous plantwide control studies; both require reactor composition control as well as flow control of a stream somewhere in each recycle loop. Several alternative control strategies that might initially have seemed obvious do not work.

M.L. Luyben, B.D. Tyreus, and W.L. Luyben (1997) presented A general heuristic design procedure is presented that generates an effective plantwide control structure for an entire complex process flowsheet and not simply individual units. The nine steps of the proposed procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental and safety constraints; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization. Application of the procedure is illustrated with three industrial examples: the vinyl acetate monomer process, the Eastman plantwide-control process, and the HDA process. The procedure produced a workable plantwide control strategy for a given process design. The control system was tested on a dynamic model built with TMODS, Dupont's in-house simulator. From the W.L. Luyben (2000) studied the process had the exothermic, irreversible, gas-phase reaction $A + B \longrightarrow C$ occurring in an adiabatic tubular reactor. A gas recycle returns unconverted reactants from the separation section. Four alternative plantwide control structures for achieving reactor exit temperature control were explored. The reactor exit temperature controller changed different manipulated variables in three of the four control schemes: (1) CS1, the set point of the reactor inlet temperature controller was changed; (2) CS2, the recycle flow rate was changed; and (3) CS3, the flow rate of one of the reactant fresh feeds was changed. The fourth control scheme, CS4, uses an "on-demand" structure. Looking at the dynamics of the reactor in isolation would lead one to select CS2 because CS1 had a very large deadtime (due to the dynamics of the reactor) and CS3 had a very small gain. Dynamic simulations demonstrated that in the plantwide environment, with the reactor and separation operating together, the CS3 structure gave effective control and offered an attractive alternative in those cases where manipulation of recycle flow rate was undesirable because of compressor limitations. The on-demand CS4 structure was the best for handling feed composition disturbances.

Wongsri and Kietawarin (2002) presented a comparison among 4 control structures designed for withstanding disturbances that cause production rate change of HDA process. The changes had been introduced to the amount of toluene and feed temperature before entering the reactor. Compared with the reference control structure using a level control to control toluene quantity in the system, the first control scheme measured toluene flow rate in the process and adjusted the fresh toluene feed rate. This structure resulted in faster dynamic response than the reference structure. The second control scheme was modified from the first scheme by adding a cooling unit to control the outlet temperature from the reactor, instead of using internal process flow. The result was to reduce material and separation ratio fluctuations within the process. The product purity was also quite steadily. In the third control scheme, a ratio control was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process. This scheme showed that it could withstand large disturbances. Dynamic study showed that the control structure had significant effect on process behavior. A good system control should quickly respond to disturbances and adjust itself to steady state while minimizing the deviation of the product quality. The control structures were compared with reference on plantwide process control book, Luyben 1998, the result was performance of these structures higher than reference.

Wongsri and Thaicharoen (2004) presented the new control structures for the hydrodealkylation of toluene (HDA) process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben’s structure (CS1). The result shows that hydrodealkylation of toluene process with heat integration can reduce energy cost. Furthermore, this process can be operated well by using plantwide methodology to design the control structure. The dynamic responses of the designed control structures and the reference structure are similar. The CS2 has been limited in bypass, so it is able to handle in small disturbance. CS3 has been designed to improve CS2 in order to handle more disturbances by using auxiliary heater instead of bypass valve to control temperature of stabilizer column. The recycle column temperature control response of the CS4 is faster than that of the previous control structures, because reboiler duty of column can control the column temperature more effective than bottom flow. CS5 on-demand structure has an advantage when downstream customer desires immediate responses in the availability of the product stream from this process. The energy used in CS6 control structure is less than CS1 and CS4.

Wongsri and Hermawan Y.D. (2004) studied the control strategies for energy integrated HDA plant (i.e. alternatives 1 and 6) based on the heat pathway heuristics (HPH), i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the dynamic MER can be achieved with some trade-off. In they work, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network. The new control structure with the LSS has been applied in the HDA plant alternatives 1 and 6. The designed control structure is evaluated based on the rigorous dynamic simulation using the commercial software HYSYS. The study reveals that, by selecting an appropriate heat pathway through the network, the utility consumptions can be reduced according to the input heat load disturbances; hence the dynamic MER can be achieved.

CHAPTER III

RESULT AND DISCUSSION

3.1 Process Description

The hydrodealkylation HDA of toluene process (alternative 1) by Douglas (1988) on conceptual design as in Fig. 3.1 contain 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

$$\text{Toluene} + H_2 \rightarrow \text{benzene} + CH_4$$

$$\text{2BenZene} \rightarrow \text{diphenyl} + H_2$$

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

$$r_1 = 3.6858 \times 10^6 \exp(-25616/T)\, p_T\, p_H^{1/2}$$

$$r_2 = 5.987 \times 10^4 \exp(-25616/T)\, p_B^2 - 2.553 \times 10^5\, p_D\, p_H$$

Where r_1 and r_2 have units of lb×mol/(min×ft^3) and T is the absolute temperature in Kelvin. The heats of reaction given by Douglas (1988) are -21500 Btu/lb×mol of toluene for r_1 and 0 Btu/lb×mol for r_2 .

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.

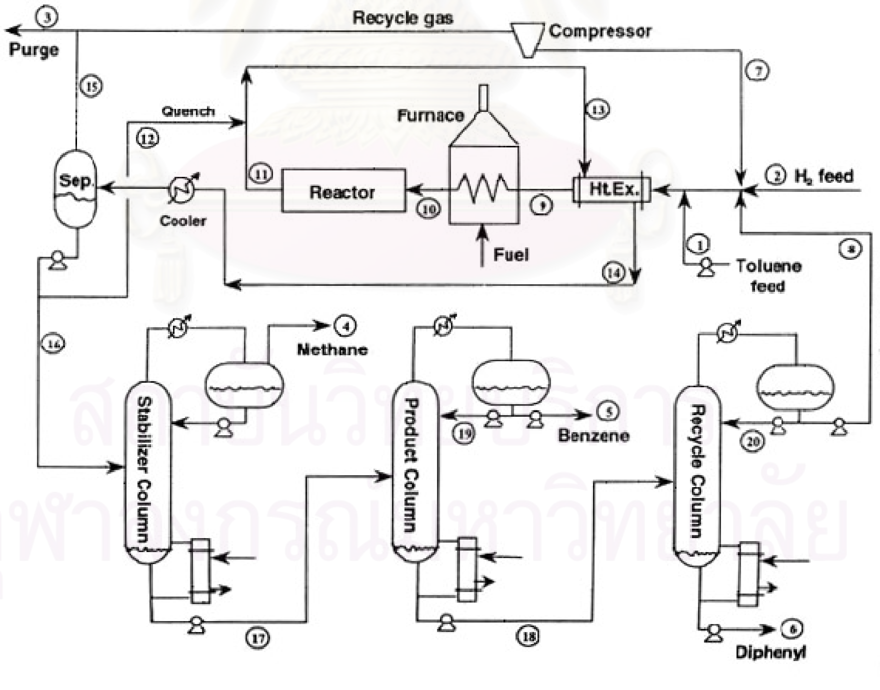

Figure 3.1: Hydrodealkylation HDA of toluene process (base case).

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

3.2 Hydrodealkylation Process Alternatives

Terrill and Douglas (1987b) design six different energy-saving alternatives to the base case. The simplest of these designs (alternative 1) recovers an additional 29% of the base case heat consumption by making the reactor preheated larger and the furnace smaller.

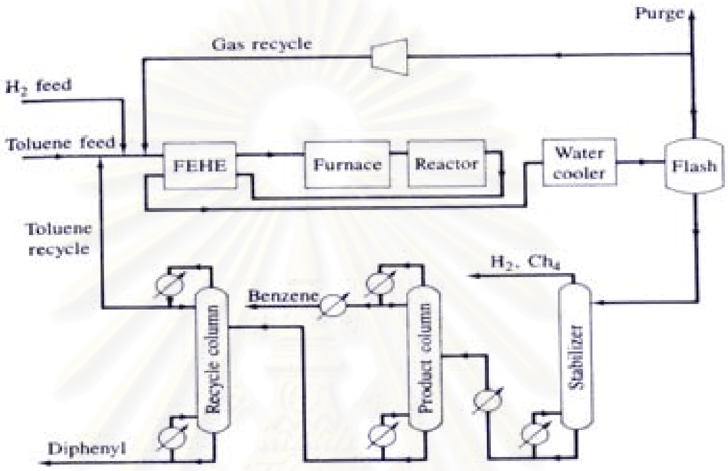

Figure 3.2: HDA process -alternative 1.

In alternative 2 (Figure 3.3) is not the same as alternative 1, heat was not recovered and used to drive stabilizer column, except that recycle column was pressure shifted to be above the pinch temperature, and the condenser for the recycle column is used to drive the product column reboiler.

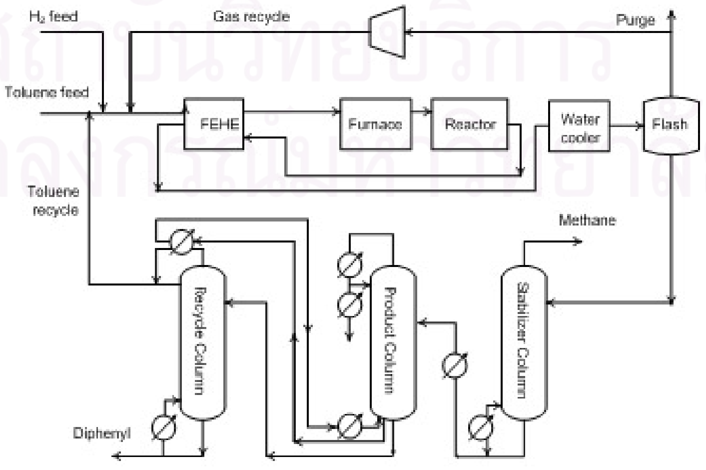

Figure 3.3: HDA process -alternative 2.

In alternative 3 part of the heat in the reactor effluent stream is used to drive the stabilizer reboiler, recycle column was pressure shifted to be above the pinch temperature, and the condenser for the recycle column is used to drive the product column reboiler as in Figure 3.3.

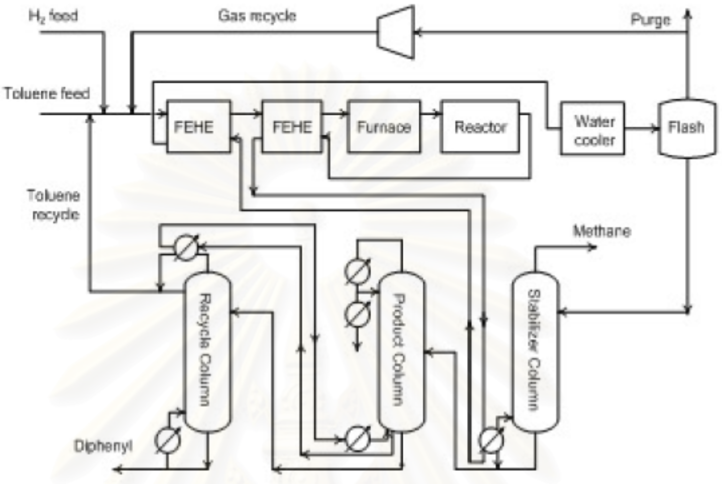

Figure 3.4: HDA process -alternative 3.

The benefit obtained from energy integration with the base-case flow rate for the three alternatives is given in table 3.1. The energy saving from the energy integration fall between 29 and 43 %, but the cost saving are in the range from -1 to 5 %. The cost saving are not as dramatic the raw-material costs dominate the process economics.

Table 3.1: Energy integration for HDA process

	Base Case	Alternatives		
		1	2	3
1. TAC ($\$10^6$/yr) base-case flows	6.38	6.40	6.45	6.38
2. Utility Usage (MW) base-case flows	12.70	9.06	7.68	7.34
3. Energy saving %		29	40	42
4. Cost saving %		-0.3	-1	0

3.3 Steady-State Modeling

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Douglas (1988); Luyben et al. (1998). Table A.2 presents the data and specifications for the equipment employed other than the three columns. For this work, 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 given in Douglas (1988). The detailed design data and specifications for the columns are summarized in Table A.3.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.

3.3.1 Steady State Simulation of HDA Process Alternative 1

Figure 3.5 shows the HYSYS flowsheet of HDA process alternative 1. The steady state simulation results are summarized in table A1.1 to A1.3. For the comparison, the steady state simulation results given by Luyben et al. (1999) are also listed in those tables. The data and specification for the different equipments are given in Appendix B.

Since there are four materials recycle streams in HDA process alternative 1, four recycle modules are inserted in the streams: hot stream to FEHE, gas recycle, quench, and toluene recycle stream. 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.

All of the three columns are simulated using the “distillation column” module. When columns are modeled in steady state, besides the specification of inlet streams, pressure profiles, number of trays and feed tray, two additional variables should be additionally specified for columns with condenser or reboiler. These could be the duties, reflux rate, draw stream rates, composition fraction, etc. We chose to specify a priori overhead and bottom component mole fraction for all columns. These mole fractions are specified to meet the required purity of product given in Douglas (1988). The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on sieve trays. The column specifications of HDA process alternative 1 are given in Appendix B . Although the tray diameter and spacing, weir length and height are not required for steady state modeling, they are required for dynamic simulation.

3.3.2 Steady State Simulation of HDA Process Alternative 2 and 3

The steady state simulation results of HDA process alternative 1 have been compared with the earlier study by Luyben et al. (1999), and the results are found consistent with those in the earlier study. Then, considering the consistency of the simulation results of the HDA process alternative 1 with respect to the previous work, the other alternatives considered in this work, i.e. alternative 2 and 3 are also developed in the HYSYS software environment. Figures 3.6 and 3.7

show the HYSYS flowsheets of the HDA process with energy integration schemes for alternative 2 and 3, respectively. The data for the selected streams for these alternatives are listed in Appendix A. The data and specifications for the equipments ate summarized in Appendix B.

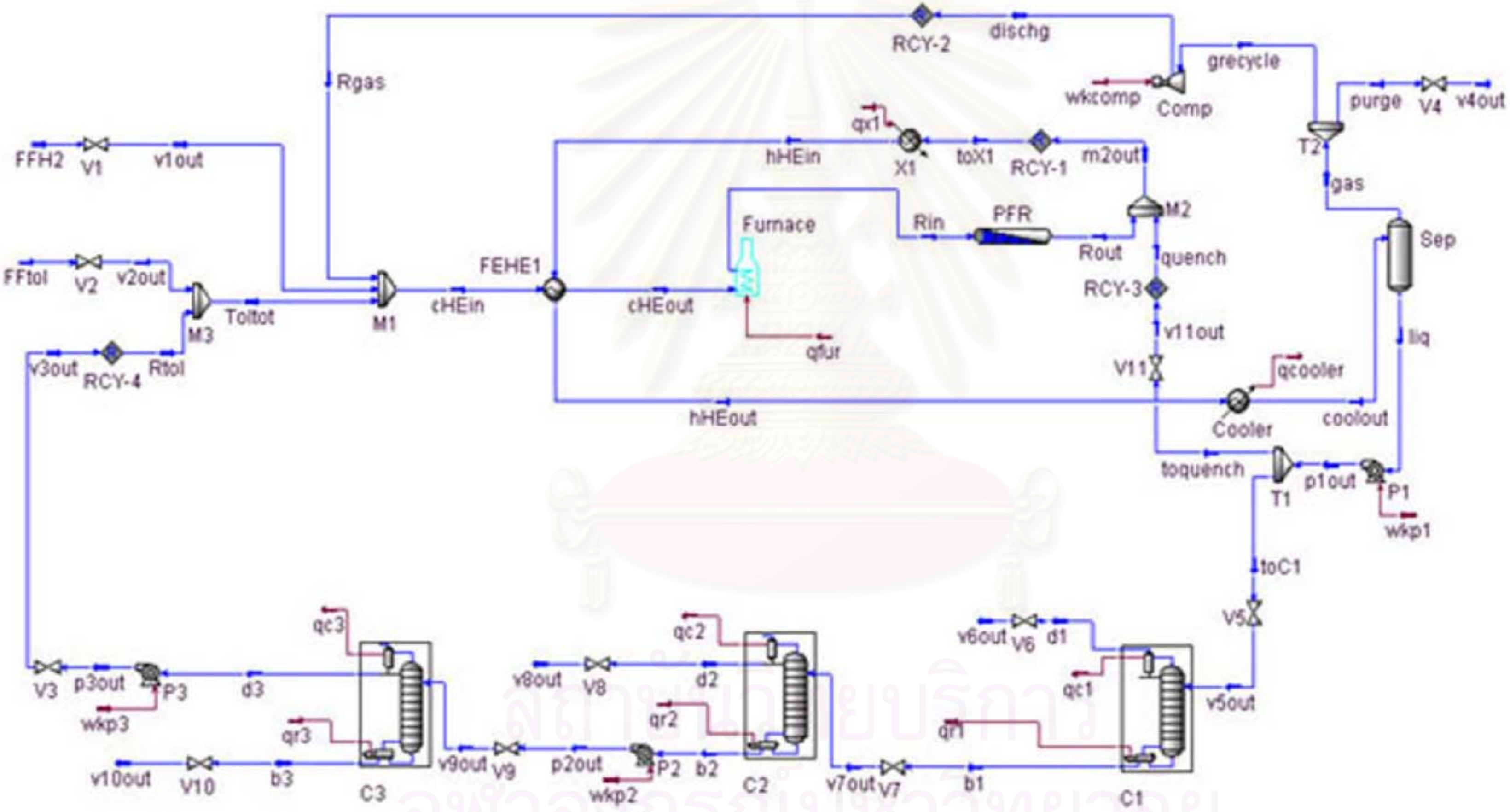

Figure 3.5: The simulated HDA process alternative 1 at steady-state by HYSYS

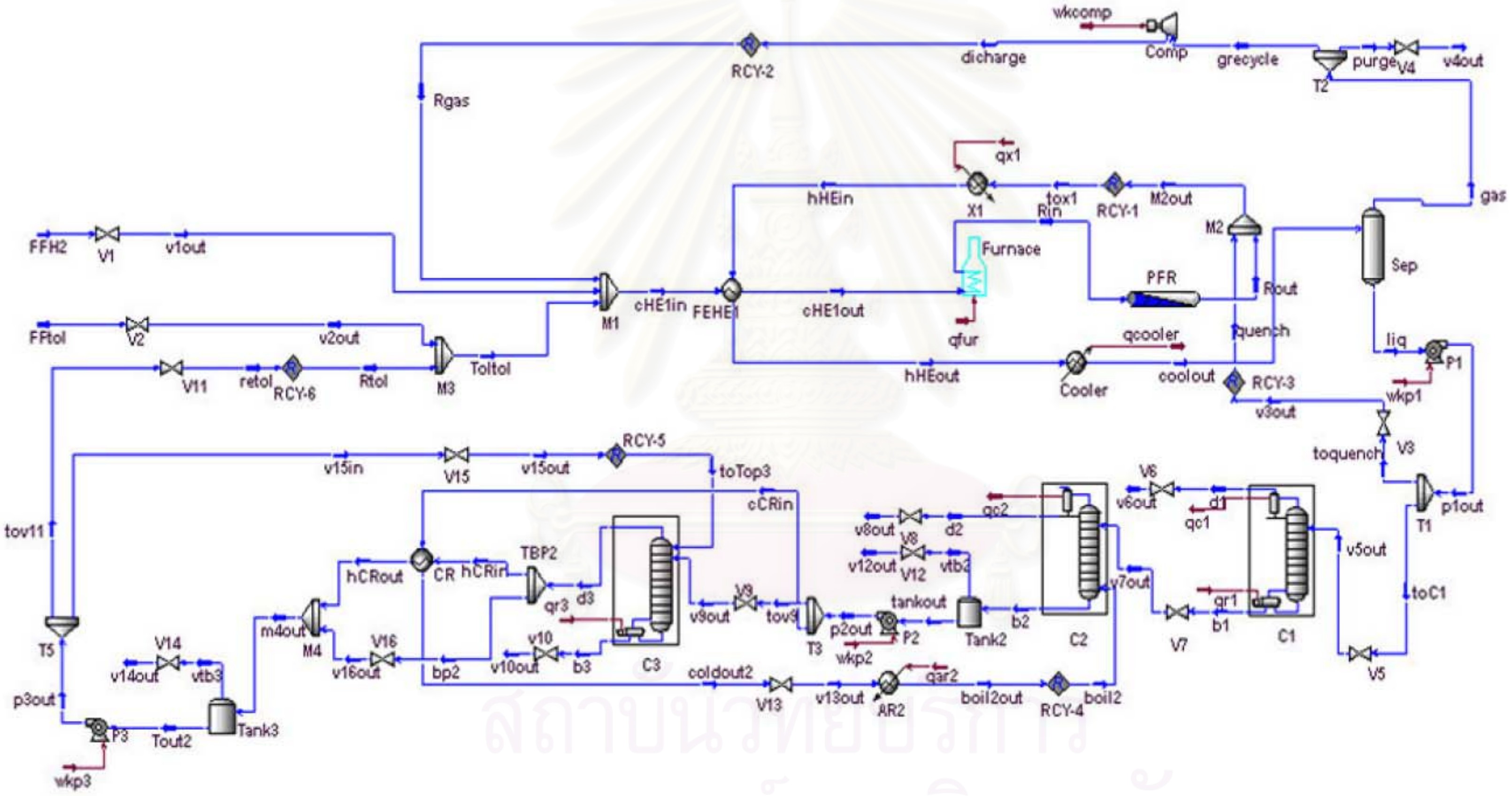

Figure 3.6: The simulated HDA process alternative 2 at steady-state by HYSYS

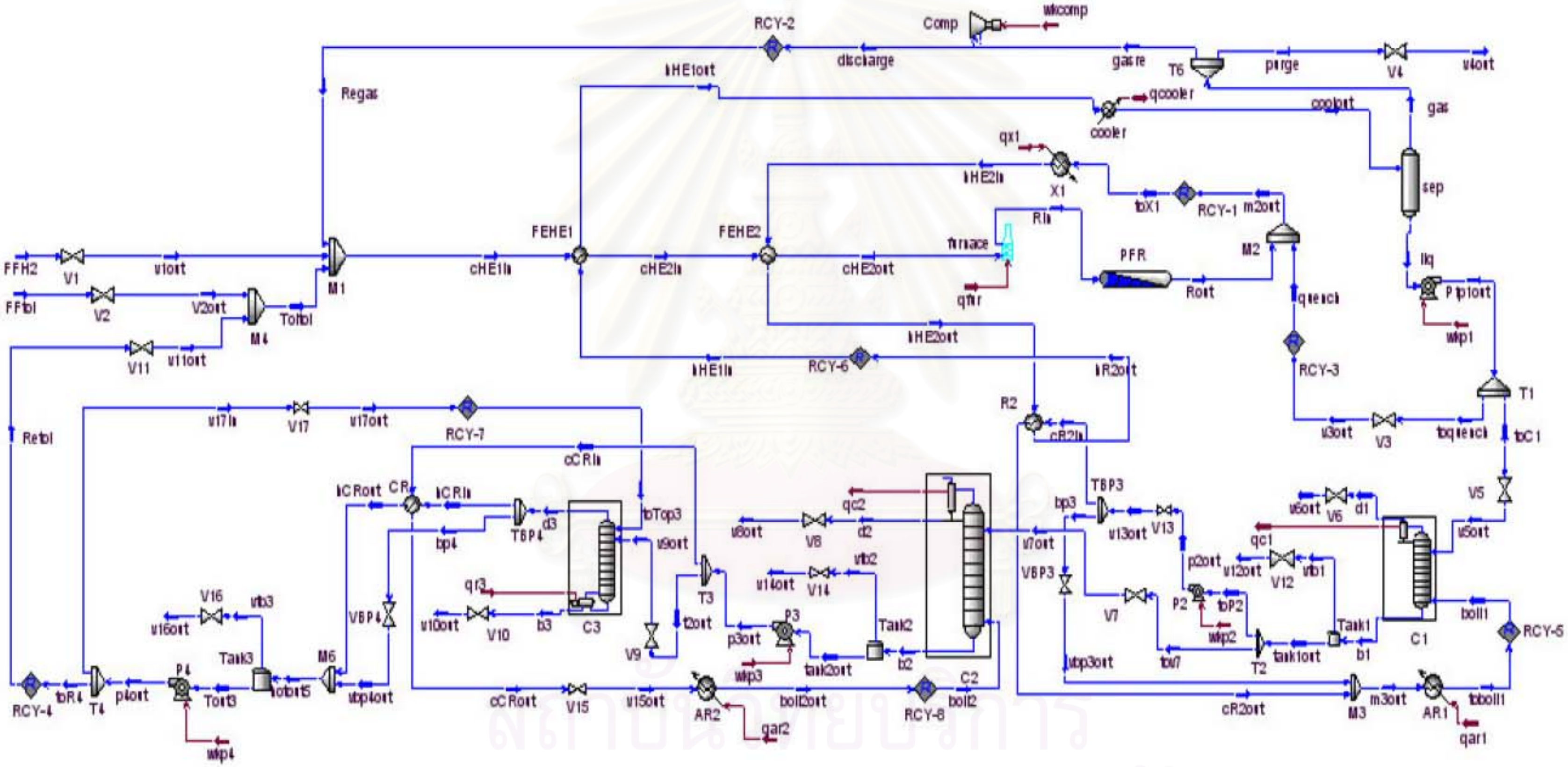

Figure 3.7: The simulated HDA process alternative 3 at steady-state by HYSYS

3.4 Plantwide control design procedure

Step 1. Establish Control Objectives.

For this process, the essential is to produce pure benzene while minimizing yield losses of hydrogen and diphenyl. The reactor effluent gas must be quenched to 621.11°C. The design a control structures for process associate with energy integration can be operated well.

Step 2. Determine Control Degree of Freedom.

There are 23 control degrees of freedom. They include; two fresh feed valves for hydrogen and toluene, purge valve, separator base and overhead valves, cooler cooling water valve, liquid quench valve, furnace fuel valve, stabilizer column steam, bottoms, reflux, cooling water, and vapor product valves; product column steam, bottoms, reflux, distillate, and cooling water valves; and recycle column steam, bottoms, reflux, distillate, and cooling water valves.

Step 3. Establish Energy management system.

The reactor operates adiabatically, so for a given reactor design the exit temperature depends upon the heat capacities of the reactor gases, reactor inlet temperature, and reactor conversion. Heat from the adiabatic reactor is carried in the effluent stream and is not removed from the process until it is dissipated to utility in the separator cooler.

Energy management of reaction section is handled by controlling the inlet and exit streams temperature of the reactor. Reactor inlet temperature must be controlled by adjusting fuel to the furnace and reactor exit temperature must be controlled by quench to prevent the benzene yield decreases from the side reaction. In the reference control structure, 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. But in alternative 3 part of the heat in the reactor effluent stream is used to drive the stabilizer reboiler before go to cooling water. And recycle column is pressure shifted to be above the pinch temperature, and the condenser for the recycle column is used to drive the product column reboiler for saving cost from the utility. However, this method gives up degree of freedom for temperature control. The solutions to restore one degree of freedom fairly easily have two ways. It is possible to oversize the P/P exchanger and provides a controlled bypass around it. And it is possible to combine the P/P exchanger with a utility exchanger.

Step 3. Set Production Rate.

Many control structures, there are not constrained to set production either by supply or demand. Considering of the kinetics equation is found that the three variables alter the reaction rate; pressure, temperature and toluene concentration (limiting agent).

- Pressure is not a variable choice for production rate control because of the compressor has to operate at maximum capacity for yield purposes.
- Reactor inlet temperature is controlled by specify the reactant fresh feed rate and reactant composition into the reactor constant. The reactor temperature is constrained below 703.44 C for preventing the cracking reaction that produces undesired byproduct.
- Toluene inventory can be controlled in two ways. Liquid level at the top of recycle column is measured to change recycle toluene flow and total toluene feed flow in the system is measured for control amount of fresh toluene feed flow.

For on demand control structure the production rate is set; distillate of product column is flow control instead of level control so condenser level is controlled by manipulating the total flow rate of the toluene. This on-demand structure might be used when the downstream customer desires immediate responses in the availability of the product stream from this unit.

Step 5. Control Product Quality and Handle Safety, Operational, and Environmental Constraints.

Benzene quality can be affected primarily by two components, methane and toluene. Any methane that leaves in the bottoms of the stabilizer column contaminates the benzene product. The separation in the stabilizer column is used to prevent this problem by using a temperature to set column stream rate (boilup). Toluene in the overhead of the product column also affects benzene quality. Benzene purity can be controlled by manipulating the column steam rate (boilup) to maintain temperature in the column.

Step 6. Control Inventories and Fix a Flow in Every Recycle Loop.

In most processes a flow control should be present in all recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows, while the process is perturbed by small disturbance. We call this high sensitivity of the recycle flowrates to small disturbances the ”snowball effect”.

Four pressures and seven liquid levels must be controlled in this process. For the pressures, there are in the gas loop and in the three distillation columns. In the gas loop, the separator overhead valve is opened and run the compressor at maximum gas recycle rate to improve yield so the gas loop control is related to the purge stream and fresh hydrogen feed flow. In the stabilizer column, vapor product flow is used to control pressure. In the product column, pressure control can be achieved by manipulating cooling water flow, and in the product column pressure control can be set by bypass valve of P/P heat exchanger to regulate overhead condensation rate.

For liquid control loops, there are a separator and two receivers in each column (base and overhead). The most direct way to control separator level is with the liquid flow to the stabilizer column. The stabilizer column overhead level is controlled with cooling water flow and base level is controlled with bottom flow. In several cases of this research; the product column, distillate flow controls overhead receiver level but on demand control structure condenser level is controlled by cascade the total flow rate of the toluene and bottom flow controls base level. In the recycle column manipulate the total toluene flow to control level. The base level of recycle column in the reference is controlled by manipulating the column steam flow because it has much larger effect than bottoms flow. But the column steam flow does not obtain a good controllability, so base level is controlled with bottom flow.

Step 7. Check Component Balances.

Component balances control loops consists of:

- Methane is purged from the gas recycle loop to prevent it from accumulating and its composition can be controlled with the purge flow.
- Diphenyl is removed in the bottom stream from the recycle column, where bottom stream controls base level. And control temperature (or concentration) with the reboiler steam.
- The inventory of benzene is accounted for via temperature and overhead receiver level control in the product column. But on demand structure the inventory of benzene is accounted for via temperature and distillate flow control in the product column.
- Toluene inventory is accounted for via level control in the recycle column overhead receiver.
- Gas loop pressure control accounts for hydrogen inventory.

Step 8. Control Individual Unit Operations.

The rest degrees of freedom are assigned for control loops within individual units. These include:

- Cooling water flow to the cooler controls process temperature to the separator.
- Refluxes to the stabilizer, product, and recycle columns are flow controlled.

Table 3.2: Component Material Balance

Component	Input	Generation	Output	Consumption	Accumulation Inventory Controlled by
H_2	Fresh Feed	$0.5V_Rr_2$	Purge Stream	V_Rr_1	Pressure control of recycle gas loop
CH_4	0	V_Rr_1	Purge Stream	0	Composition control of recycle gas loop
C_6H_6	0	V_Rr_1	Product Stream	$2V_Rr_2$	Temperature control in product column
C_7H_8	Fresh Feed	0	0	V_Rr_1	Level control in recycle column reflux drum
$C_{12}H_{10}$	0	$0.5V_Rr_2$	Purge Stream	0	Temperature control in recycle column

Where V_R= reactor volume
r_1 = first reaction rate
r_2 = second reaction rate

Step 9. Optimize Economics or Improve Dynamic Controllability.

The basic regulatory strategy has now been established. Some freedom is used to select several controller setpoints to optimize economics and plant performance. Such as, the setpoint for the methane composition controller in the gas recycle loop must balance the trade-off between yield loss and reactor performance. Reflux flows to the stabilizer, product, and recycle columns must be determined based upon column energy requirement and potential yield losses of benzene (in the overhead of the stabilizer and recycle columns) and toluene (in the base of the recycle column).

3.5 Design of plantwide control structure

In this current work three control structures were designed and compared, the first control structure Luyben et al. (2002) control system was modified, namely control structure 1 (CS1) to the HDA process as show in Figure 3.8 - 3.10. The second control structure we apply with control structure 1 with Kietawarin (2002) control system, namely control structure 2 (CS2) to the HDA process as show in Figure 3.11 - 3.13. The third control structures CS3 as show in Figure 3.14 - 3.16, this control structure a ratio control was induced to the second control scheme.

3.5.1 Design of control structure 1 (CS1).

The plant wide control structures in the HDA plant alternatives 1 to 3 are designed based on the heuristic design procedure given by Luyben et al. (2002). The major loops are the same as those used in Luyben et al. (1999), but we have used valve position control concept Luyben (1990) which can reduce energy-cost of utility. In this control structure both valve bypass of column heat exchanger and column auxiliary heater is used to control tray temperature of column. When valve bypass decreases to 5% open, temperature cannot achieve its setpoint. The auxiliary will operate to control temperature as show in figure 3.8 - 3.10. The size of disturbance in this study is about 5 to 10% according to Luyben's recommendations.

3.5.2 Design of control structure 2 (CS2).

For the second control structure, we apply control structure 1 with Kietawarin (2002) control system by adding a cooling unit to control the outlet temperature from reactor, instead of using internal process flow (from bottom of vapor-liquid separator) to reduce material and separation ratio fluctuations within the process flow.

3.5.3 Design of new plantwide control structure 3 (CS3)

In this control structure, a ratio control of fresh feed toluene and fresh feed toluene hydrogen was induced to the second control scheme for controlling the ratio of hydrogen and toluene within the process.

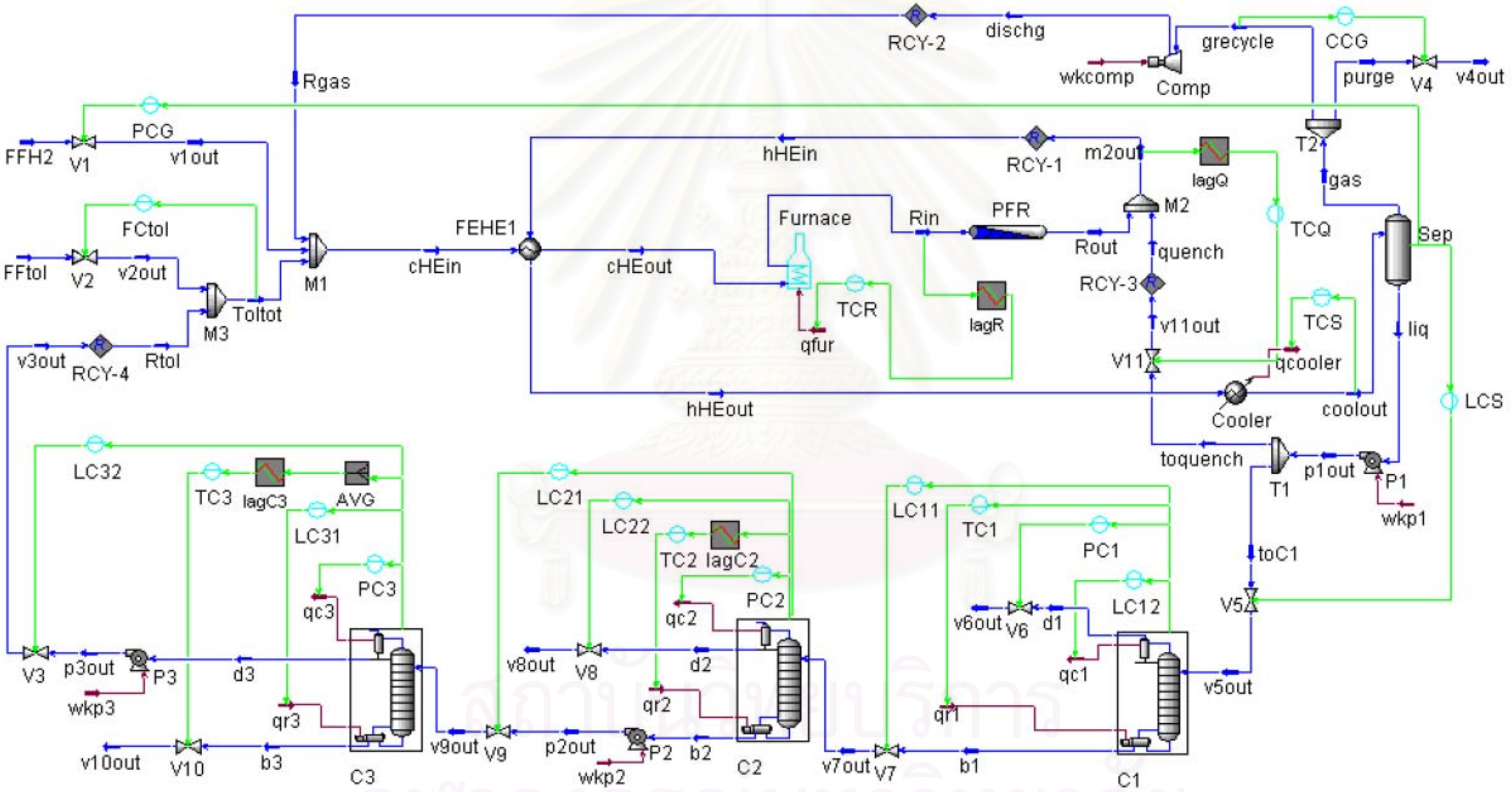

Figure 3.8: Application of control structure 1 to HDA plant alternative 1

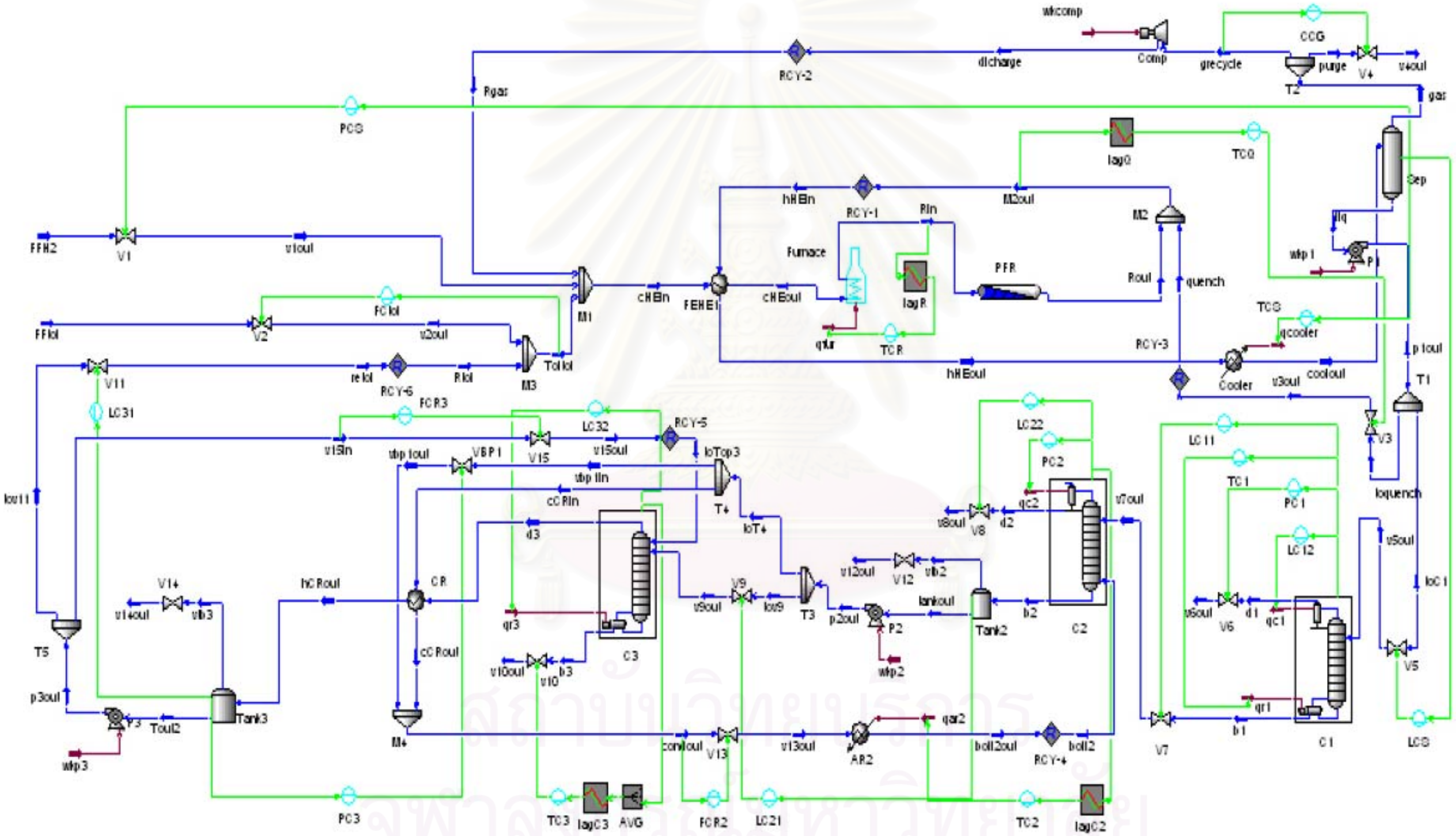

Figure 3.9: Application of control structure 1 to HDA plant alternative 2

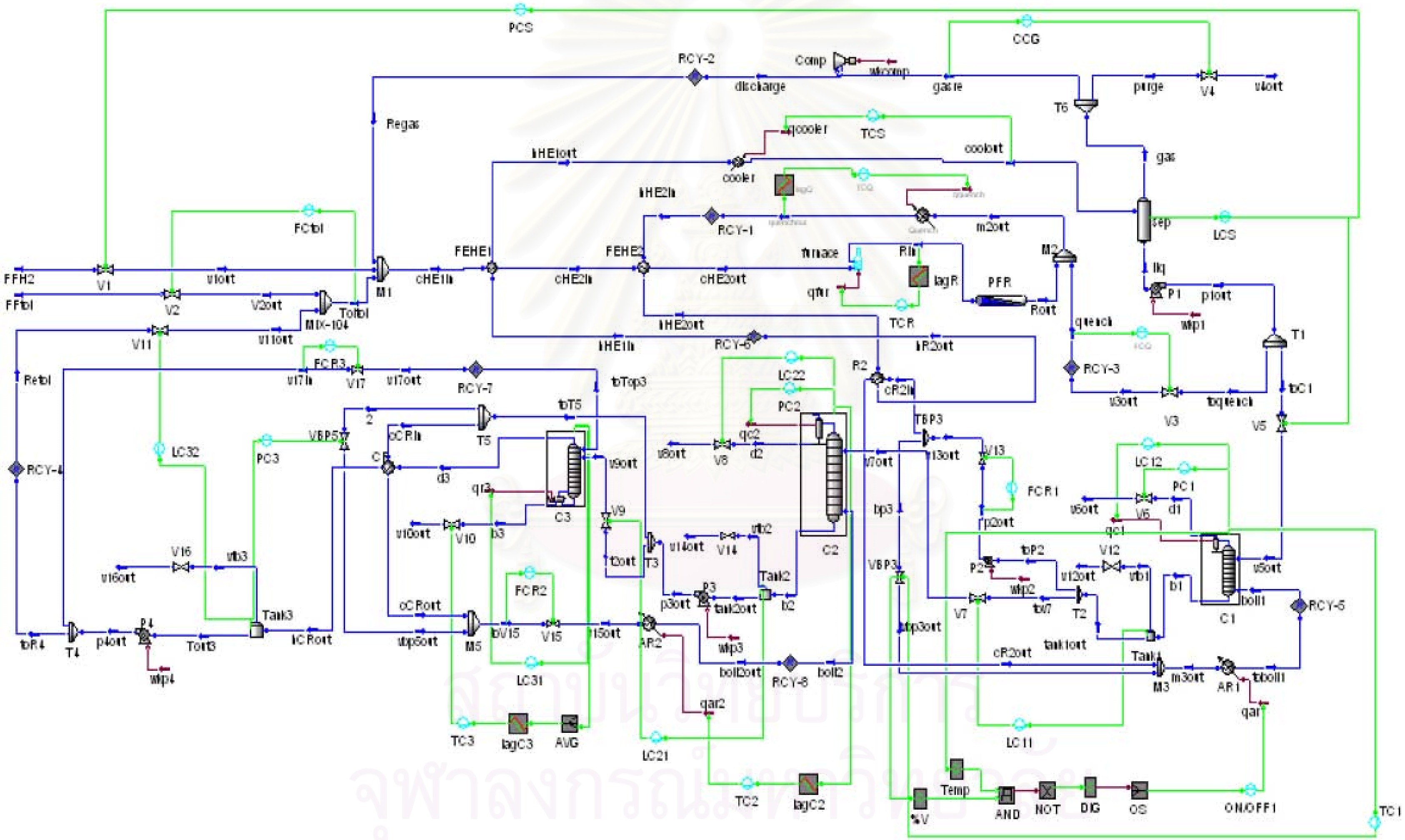

Figure 3.10: Application of control structure 1 to HDA plant alternative 3

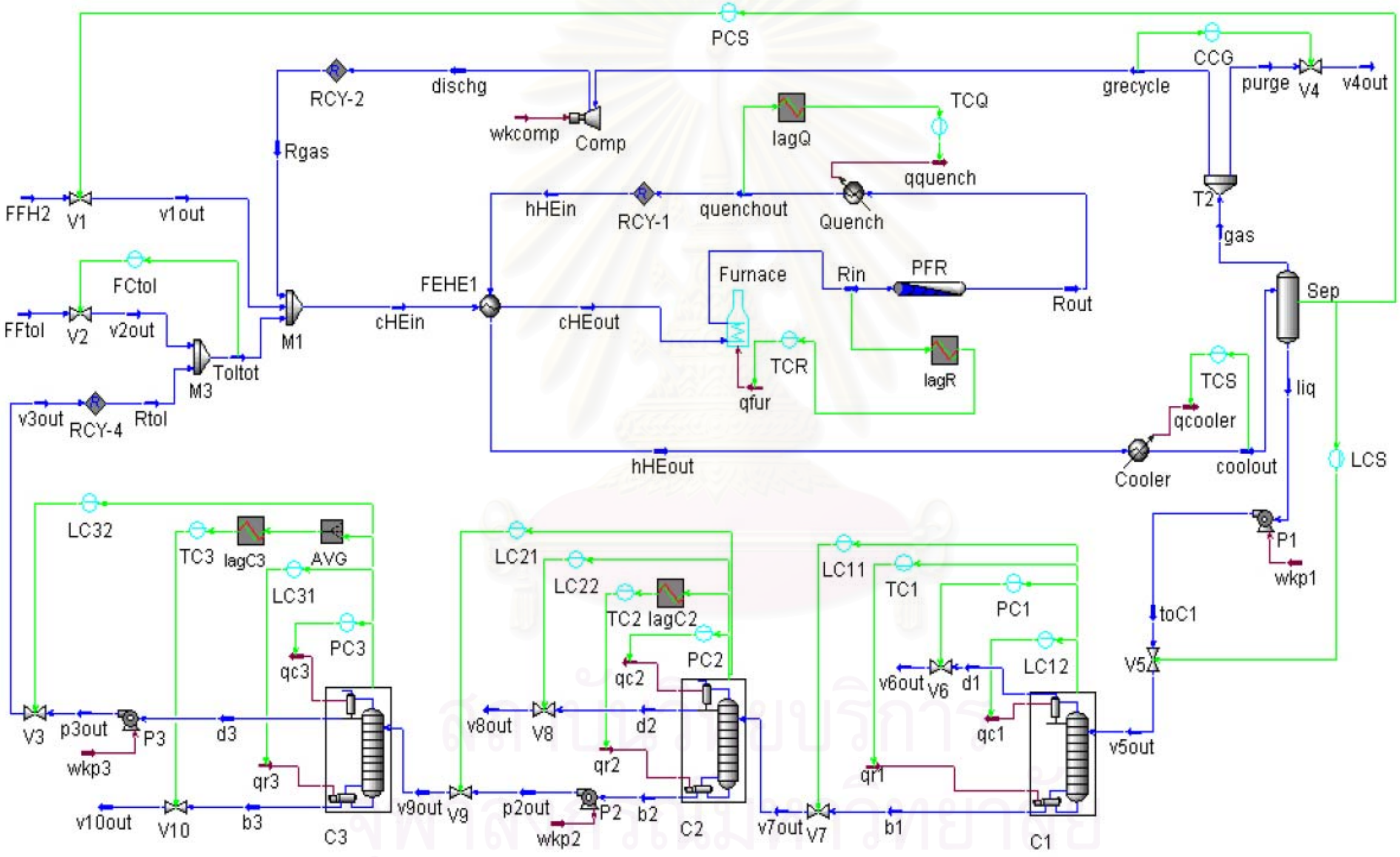

Figure 3.11: Application of control structure 2 to HDA plant alternative 1

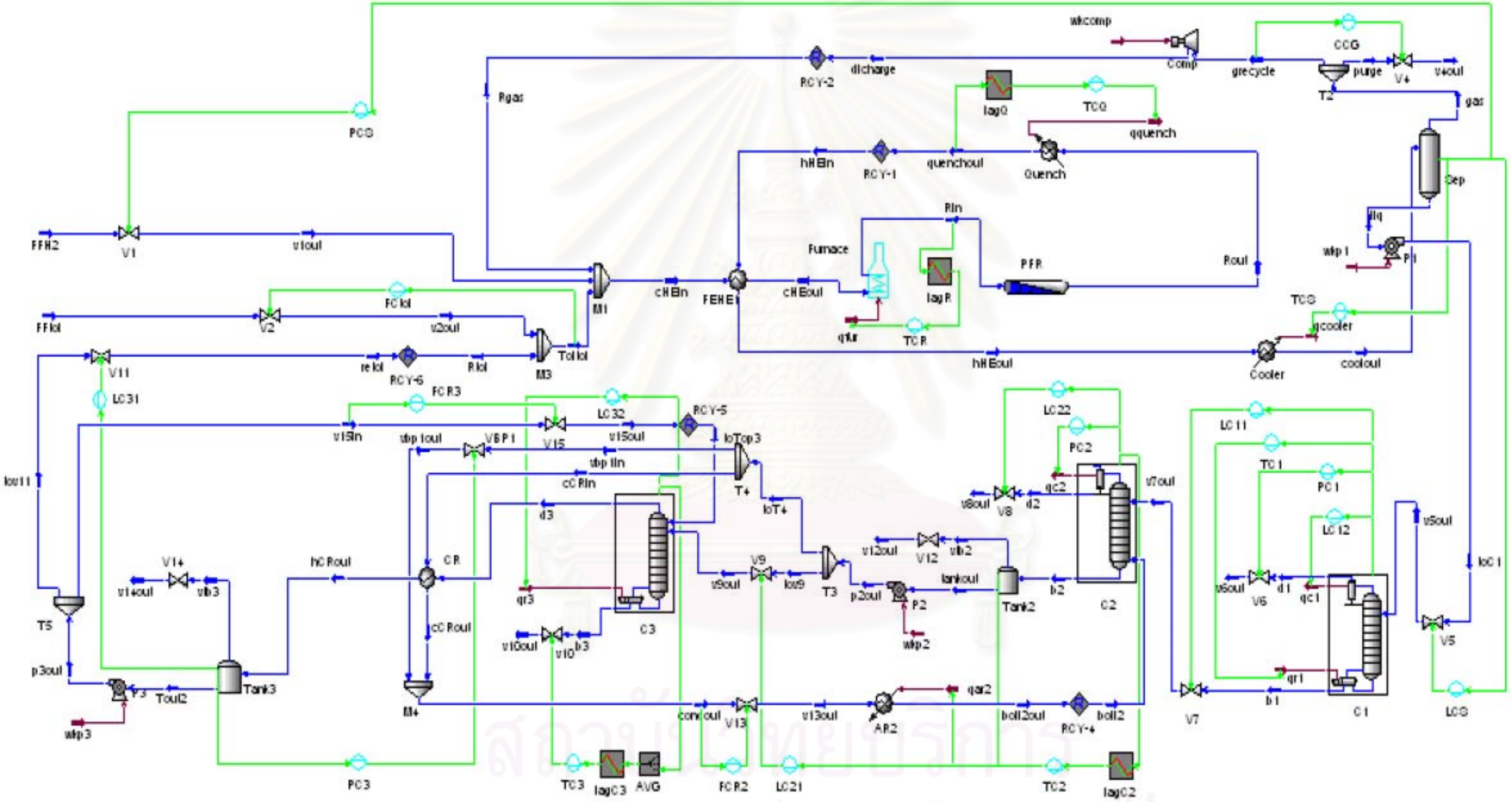

Figure 3.12: Application of control structure 2 to HDA plant alternative 2

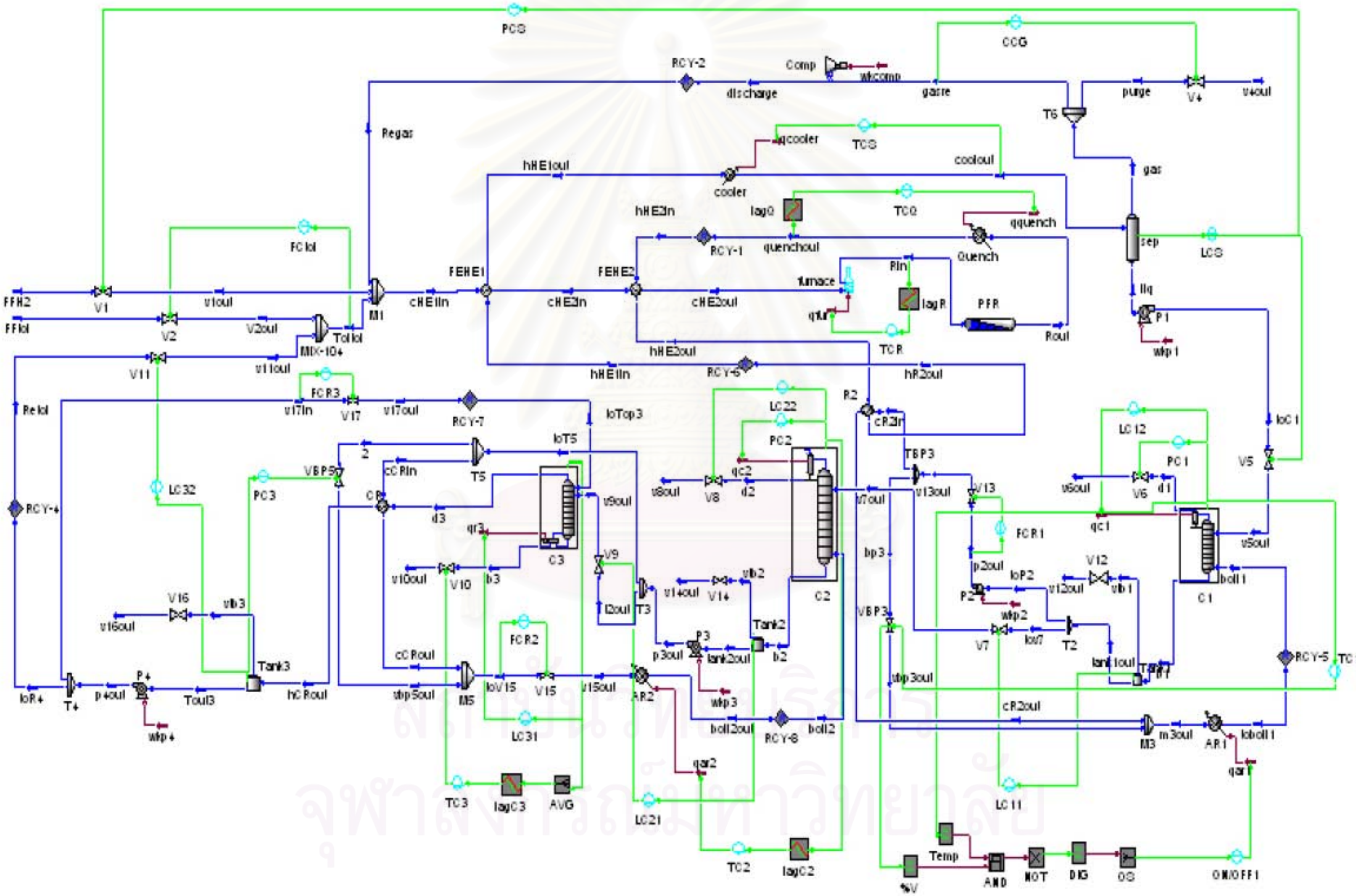

Figure 3.13: Application of control structure 2 to HDA plant alternative 3

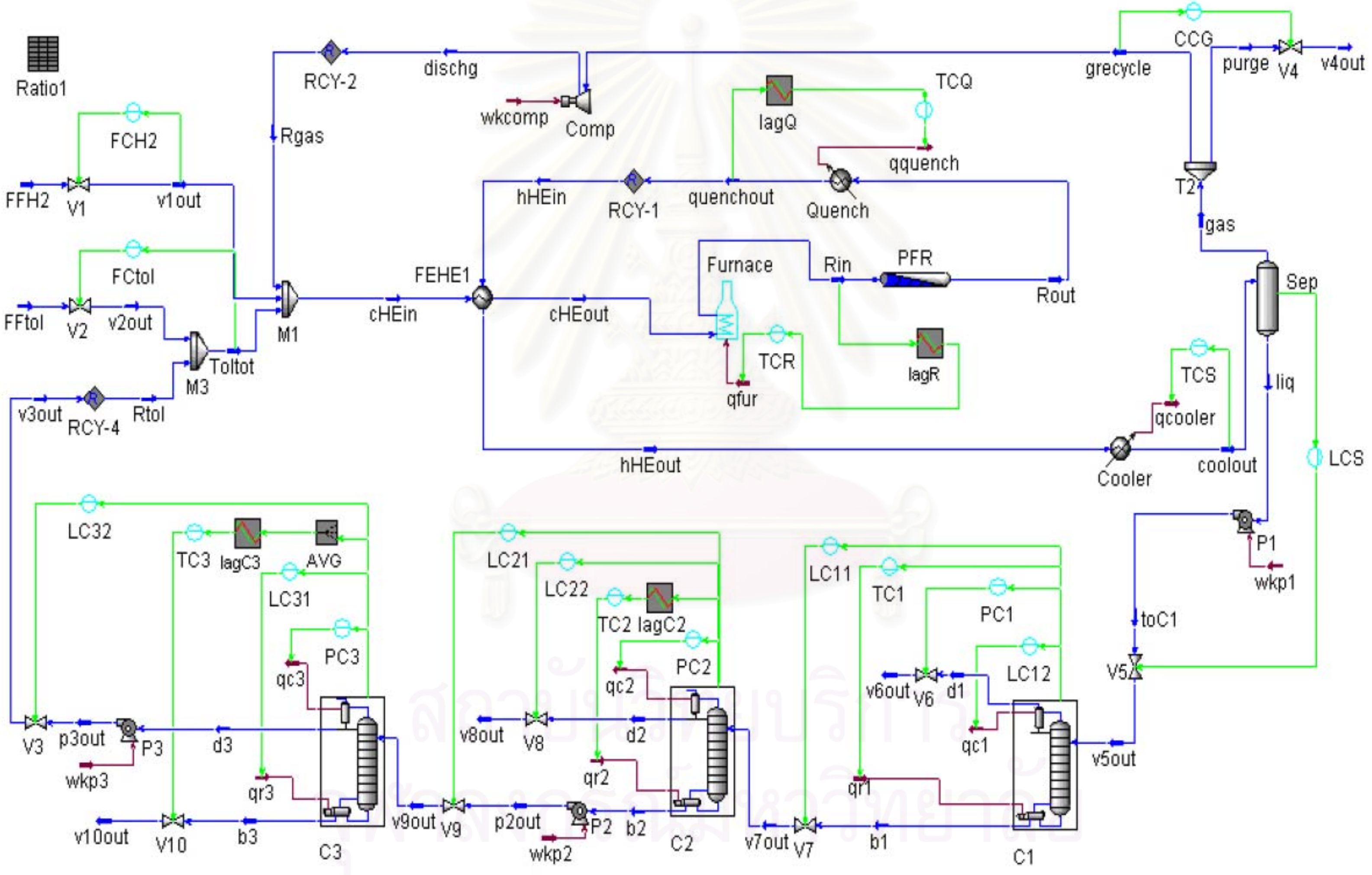

Figure 3.14: Application of control structure 3 to HDA plant alternative 1

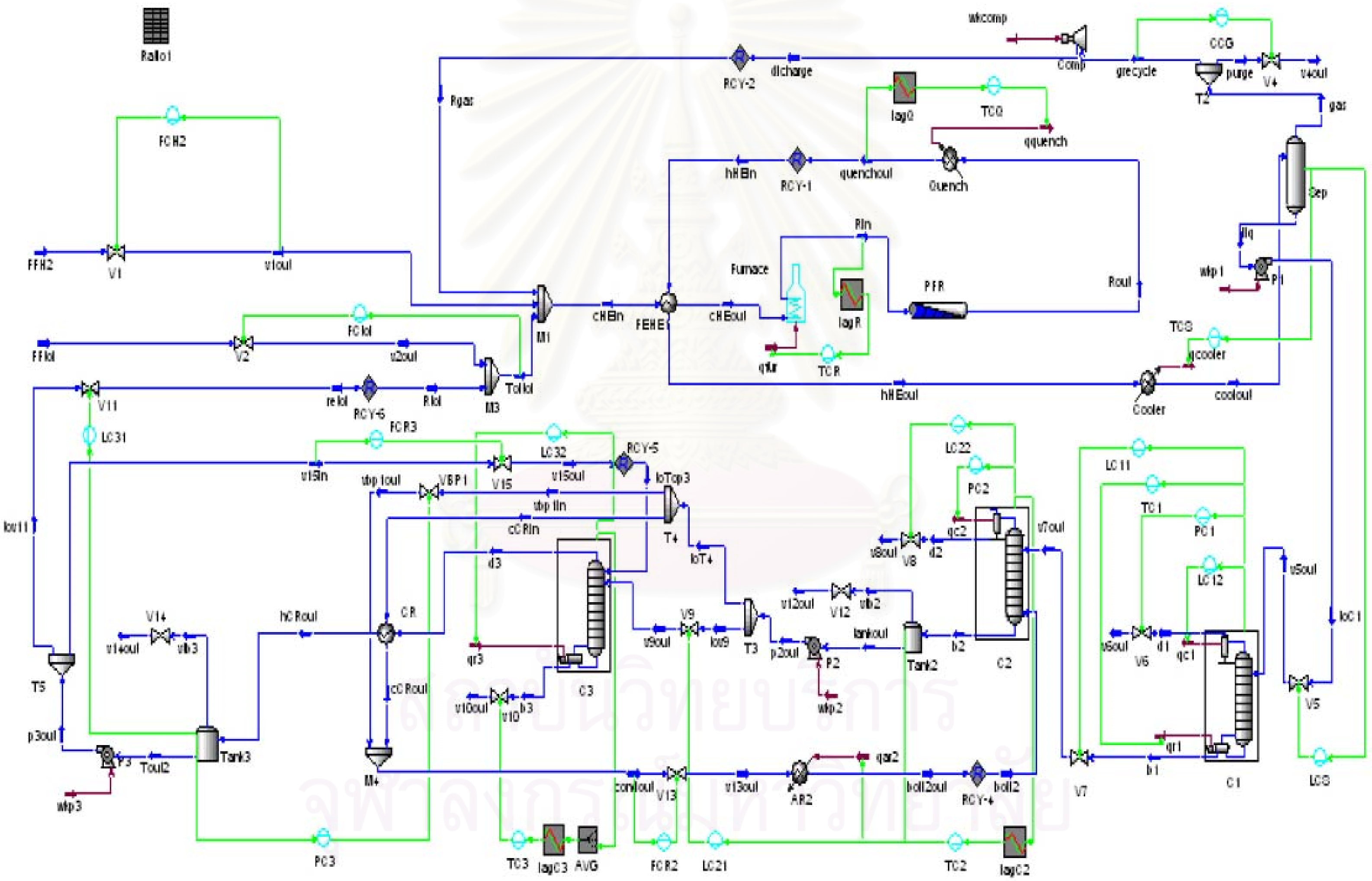

Figure 3.15: Application of control structure 3 to HDA plant alternative 2

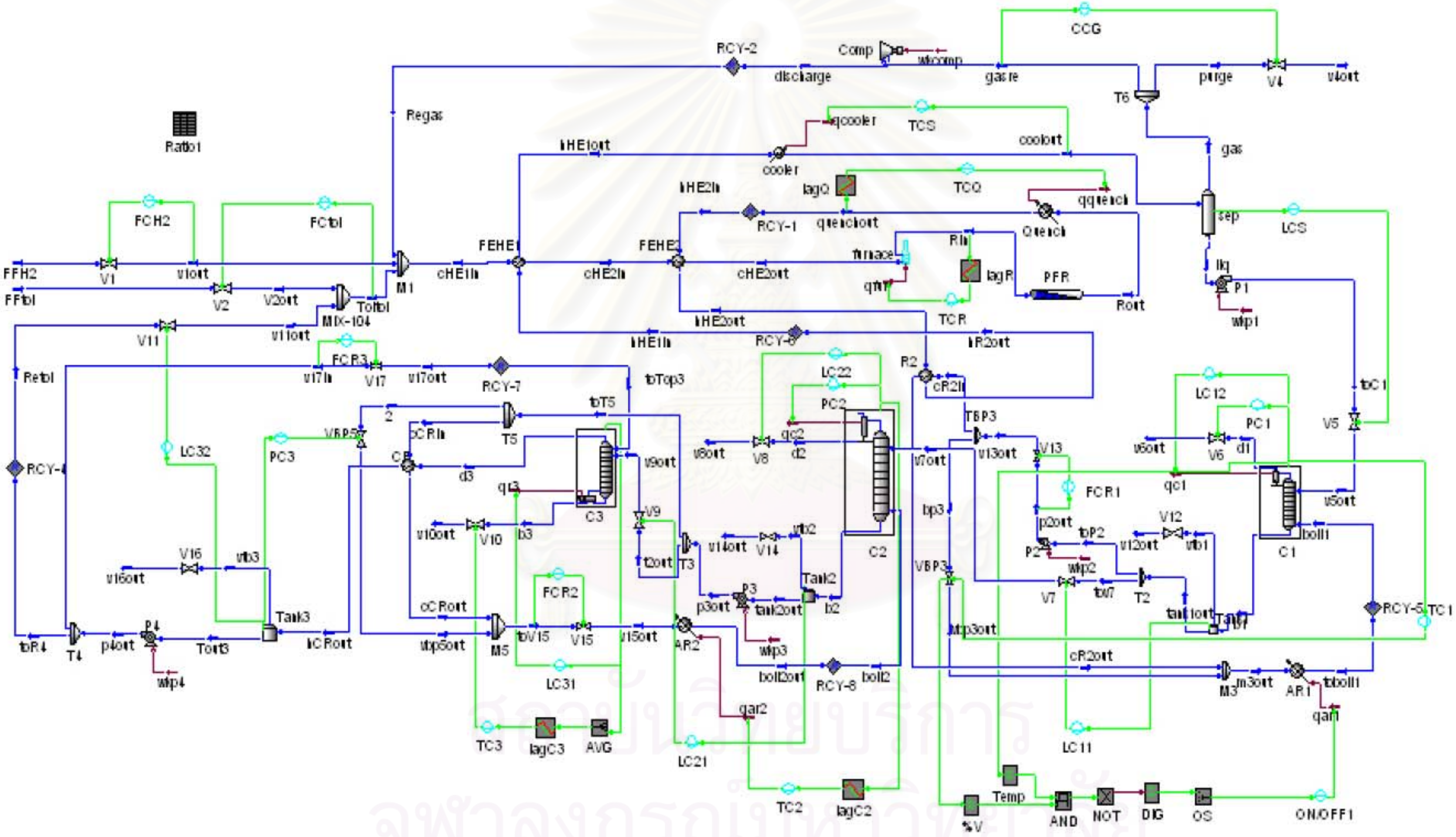

Figure 3.16: Application of control structure 3 to HDA plant alternative 3

3.6 Dynamic simulation results

In order to illustrate the dynamic behaviors of the new control structures in HDA plant alternatives 1, 2 and 3 several disturbance loads were made. The dynamic responses of our control structure are shown in Figures 3.17 to 3.22. In general, CS1 has better responses of utility consumptions are achieved here compared to CS2 and CS3. Results for individual disturbance load changes are as follows:

3.6.1 Change in the heat load disturbance of cold stream for HDA plant alternative 1

Figure 3.17 shows the dynamic responses of the HDA plant alternative 1 to a change in the heat load disturbance of the cold stream (reactor feed stream).This disturbance is made as follows: first the fresh toluene feed temperature is decreased from 30 to 20 ^{o}C at time equal to 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equal to 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equal to 200 minutes .The dynamic response of control structure 1 same as CS2 and CS3 but CS3 control system can handle more disturbance and faster than other.

As can be seen, in this study the reactor inlet temperature (Figure 3.17.a), the reactor outlet temperature (Figure 3.17.b), and the separator temperature (Figure 3.17.c) are slightly well controlled. But, for CS1 control system has more oscillations occur in the tray temperature of stabilizer column (Figure 3.17.e) and tray temperature of recycle column (Figure 3.17.g)

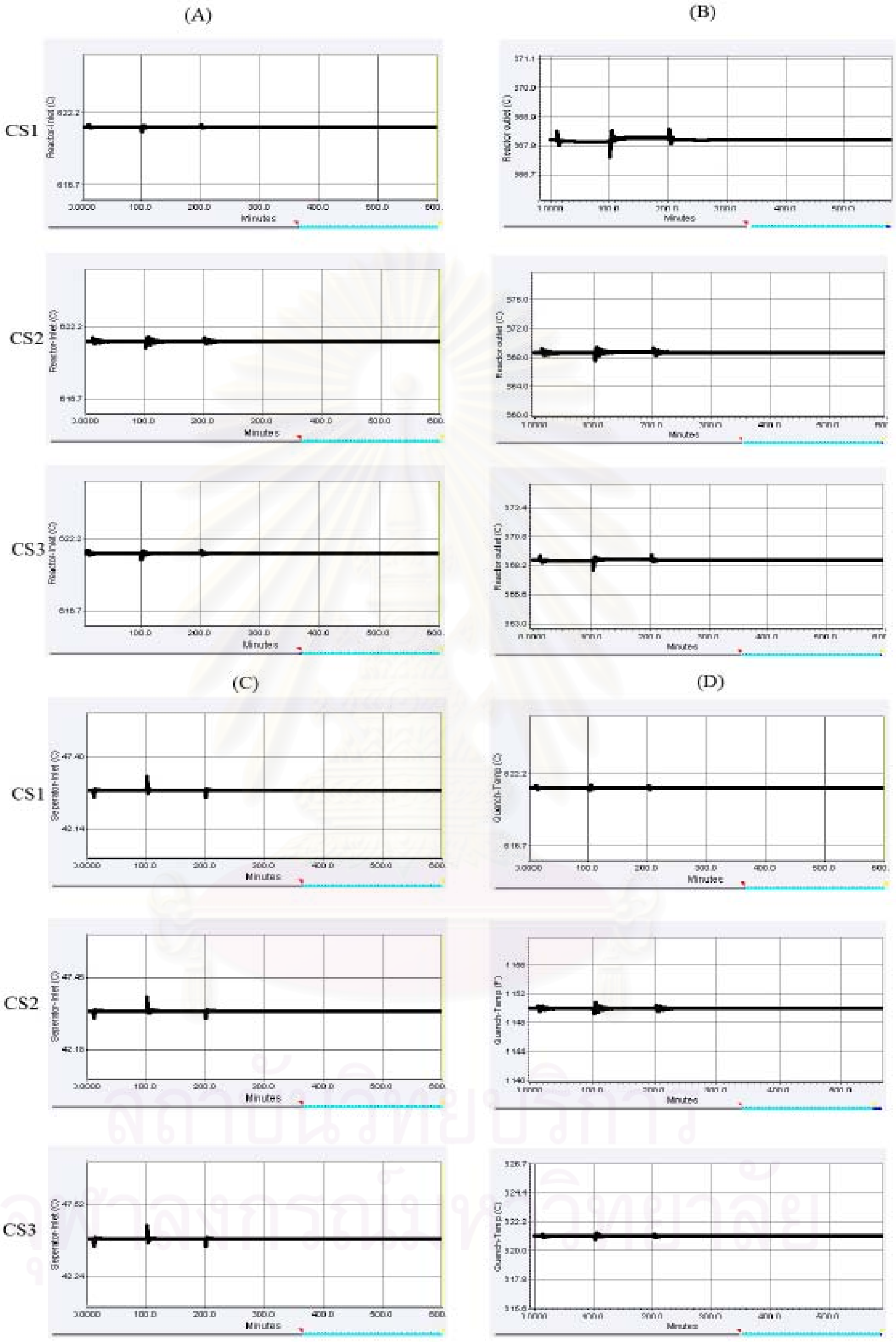

Figure 3.17: Dynamic responses of the HDA plant alternative 1 to a change in the heat load disturbance of cold stream (reactor feed stream), where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature, (e) tray temperature of stabilizer column, (f)tray temperature of product column, (g) tray temperature of recycle column; comparison between CS1, CS2 and CS3.

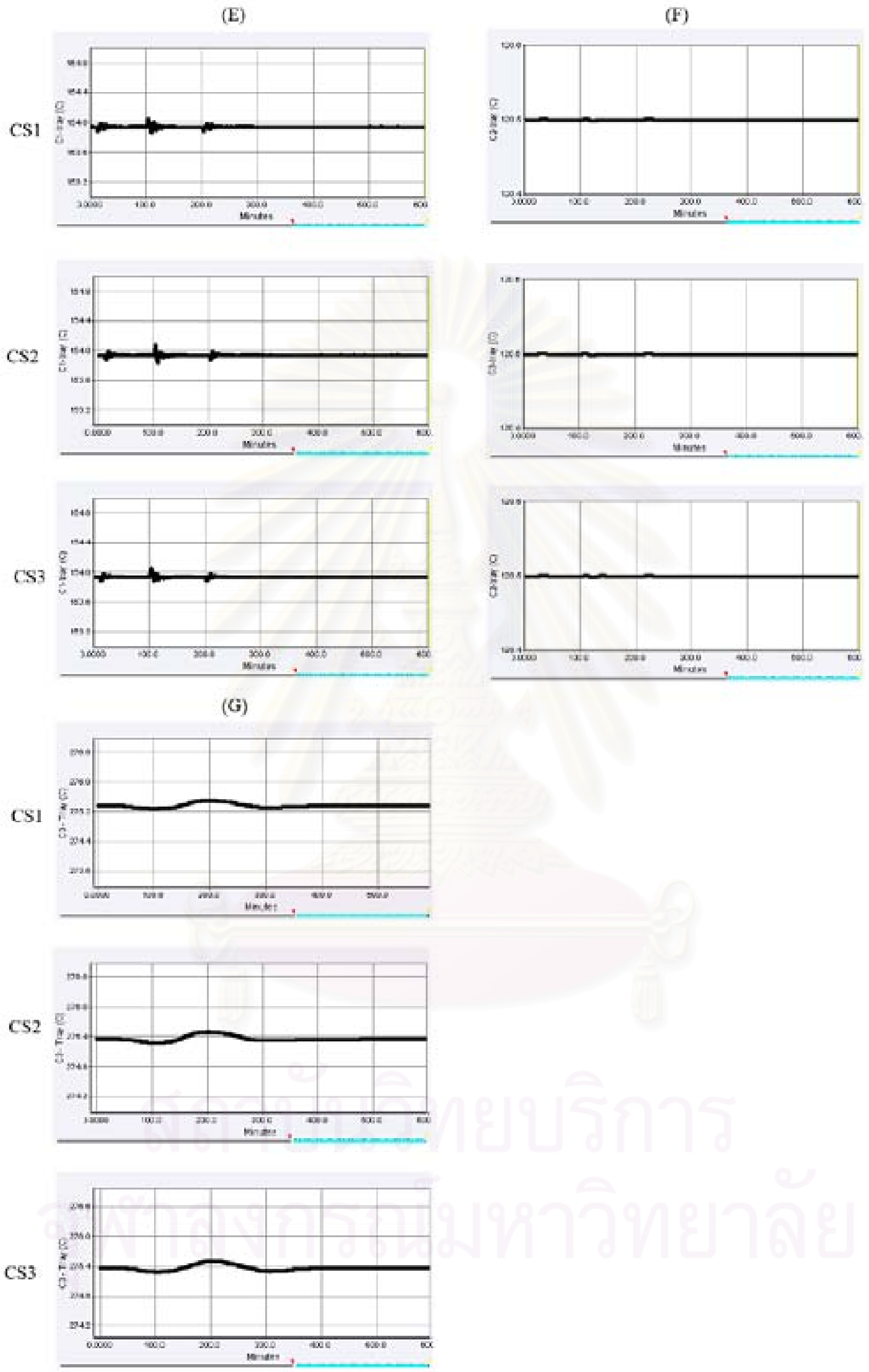

Figure 3.17: Continued.

3.6.2 Change in the heat load disturbance of cold stream for HDA plant alternative 2 and 3

Figure 3.18-3.19 show the dynamic responses of the HDA plant alternative 2 and 3 to a change in the heat load disturbance of the cold stream (reactor feed stream).This disturbance is made as follows: first the fresh toluene feed temperature is decreased from 30 to 20 ^{o}C at time equals 10 minutes, and the temperature is increased from 20 to 40 ^{o}C at time equals 100 minutes, then its temperature is returned to its nominal value of 30 ^{o}C at time equals 200 minutes.

As shown in figure 3.18, the dynamic response of HDA process alternative 2 are slower than those in HDA process alternative 1. The reactor inlet temperature (Figure3.18.a) , the reactor outlet temperature(Figure3.18.b), and the separator temperature (FIgure3.18.c) are slightly well controlled. But, for tray temperature of recycle column (Figure3.19.g) has more oscillations occur.

Again, the dynamic response of HDA process alternative 3 are slower than those in HDA process alternative 2 .Most of control loop more oscillations occur compared with previous case. The reactor inlet temperature, the reactor outlet temperature, the separator temperature, and tray temperature of product column are slightly well controlled. But, for CS1 control system has more oscillations occur in the tray temperature of stabilizer column (Figure3.19.e) and tray temperature of recycle column (Figure3.19.g).

For complex heat integration plant more oscillations occur in the tray temperature of stabilizer column, tray temperature of product column and tray temperature of recycle column. Those results indicate that the implementation of complex energy integration to the process deteriorates the dynamic performance of the process. CS3 control system can handle more disturbance and faster than other, but for first control system has better responses of utility consumptions are achieved here compared to CS2 and CS3 because in CS2 and CS3 control system as modified from the first control system by adding a cooling unit to control the outlet temperature from reactor, instead of using internal process flow. So, first control system requires less furnace utility consumptions are achieved compare to other control system.

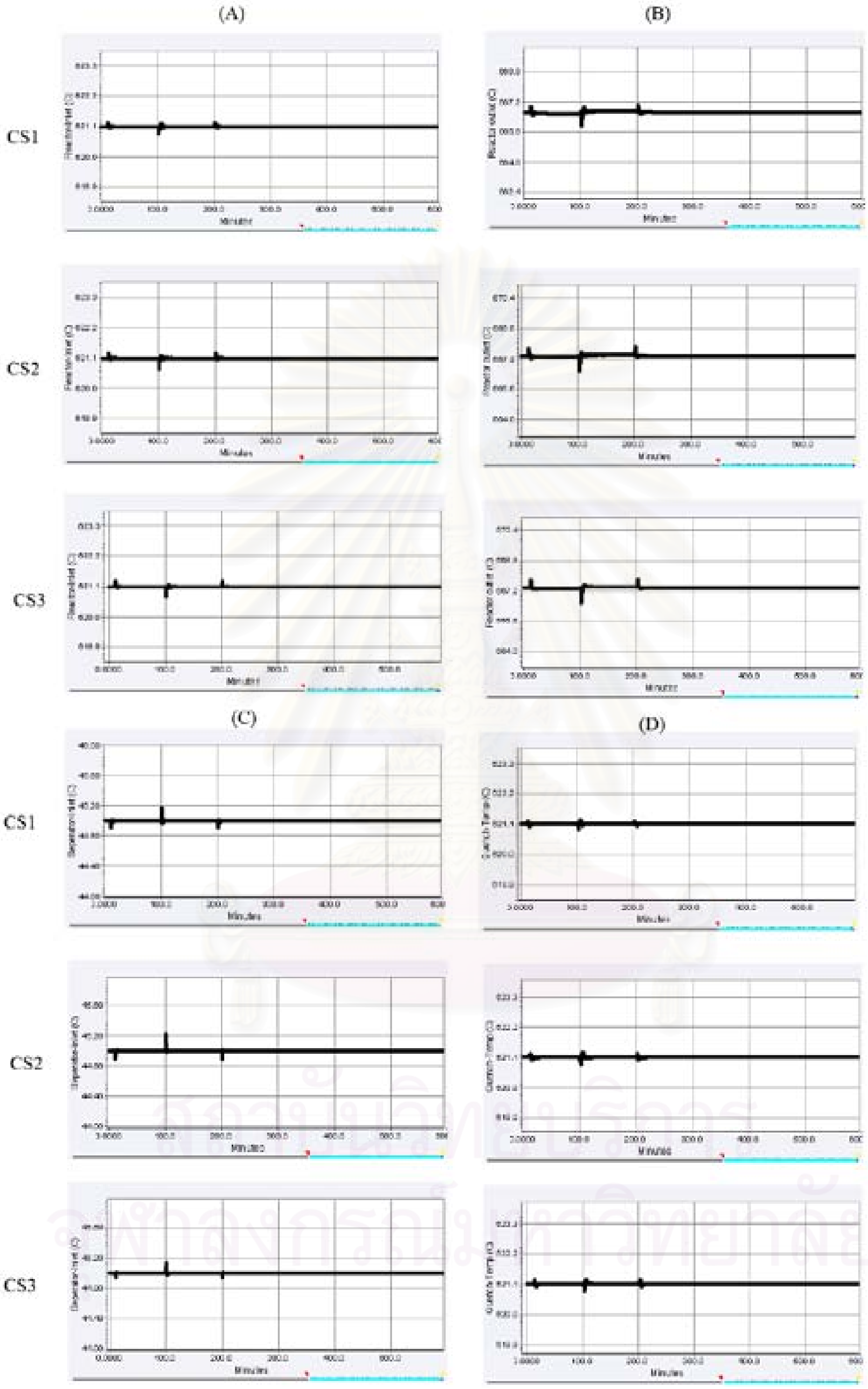

Figure 3.18: Dynamic responses of the HDA plant alternative 2 to a change in the heat load disturbance of cold stream (reactor feed stream), where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature, (e) tray temperature of stabilizer column, (f)tray temperature of product column, (g) tray temperature of recycle column; comparison between CS1, CS2 and CS3.

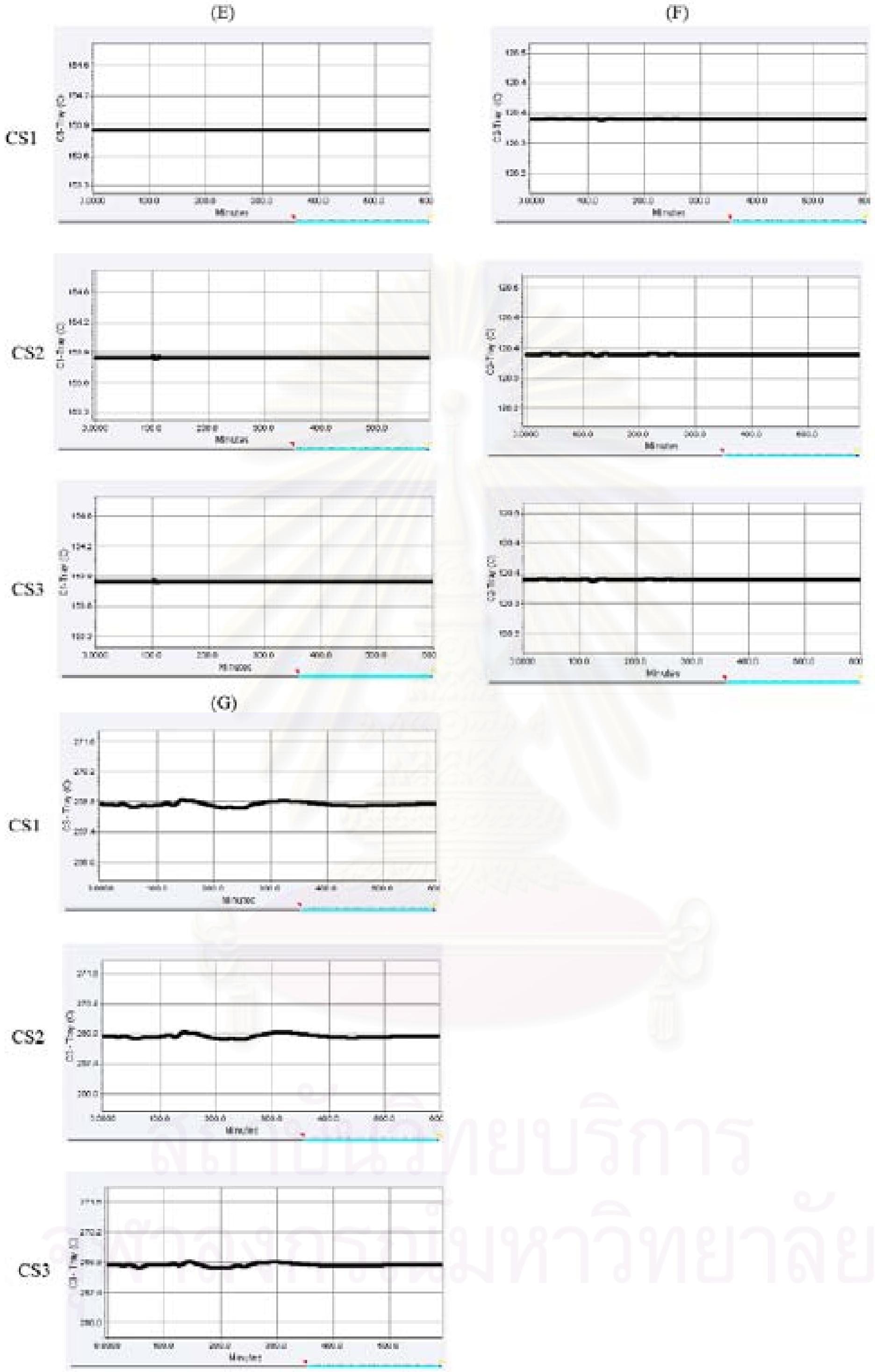

Figure 3.18: Continued.

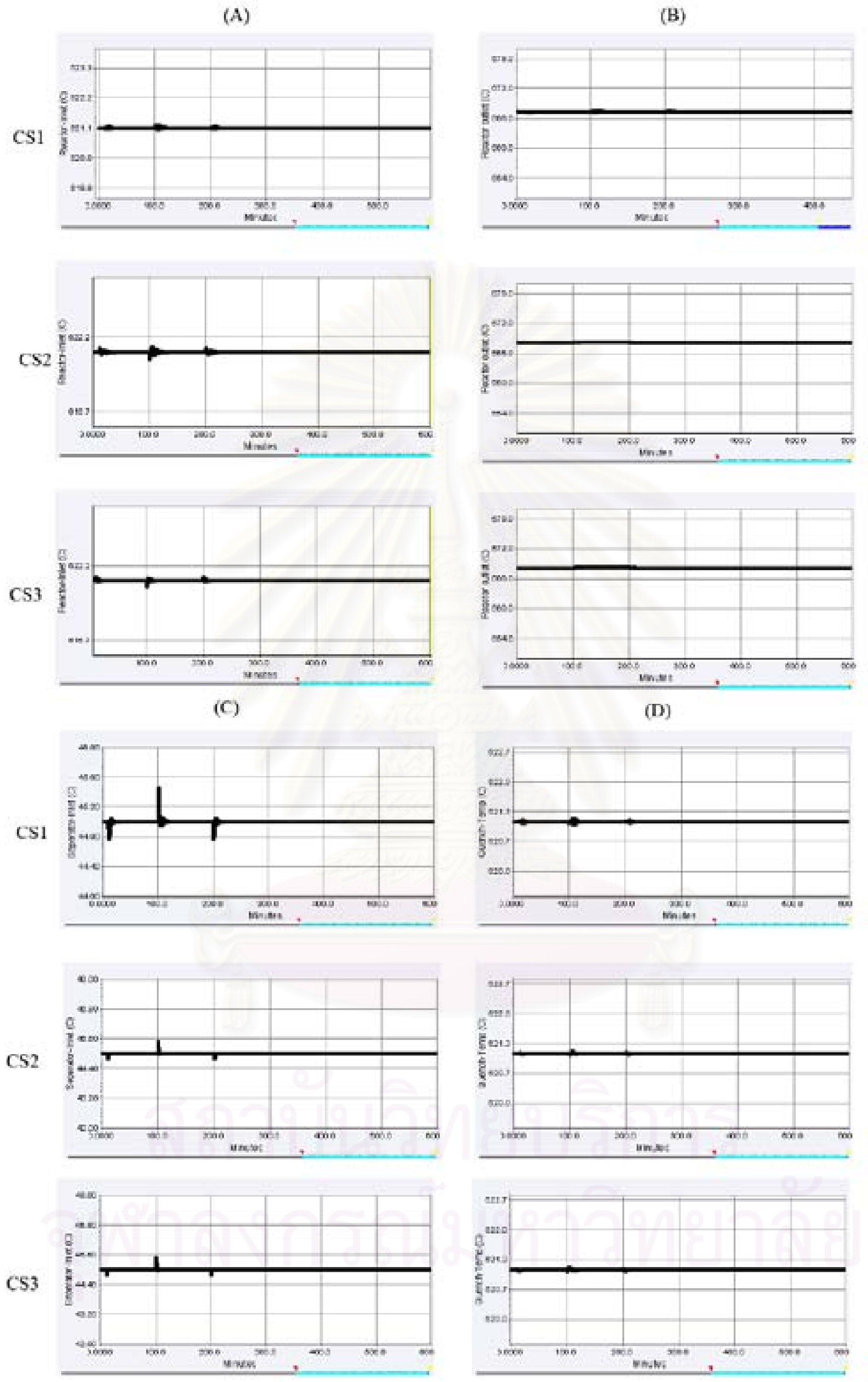

Figure 3.19: Dynamic responses of the HDA plant alternative 3 to a change in the heat load disturbance of cold stream (reactor feed stream), where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature , (e) tray temperature of stabilizer column , (f) tray temperature of product column , (g) tray temperature of recycle column; comparison between CS1 , CS2 and CS3.

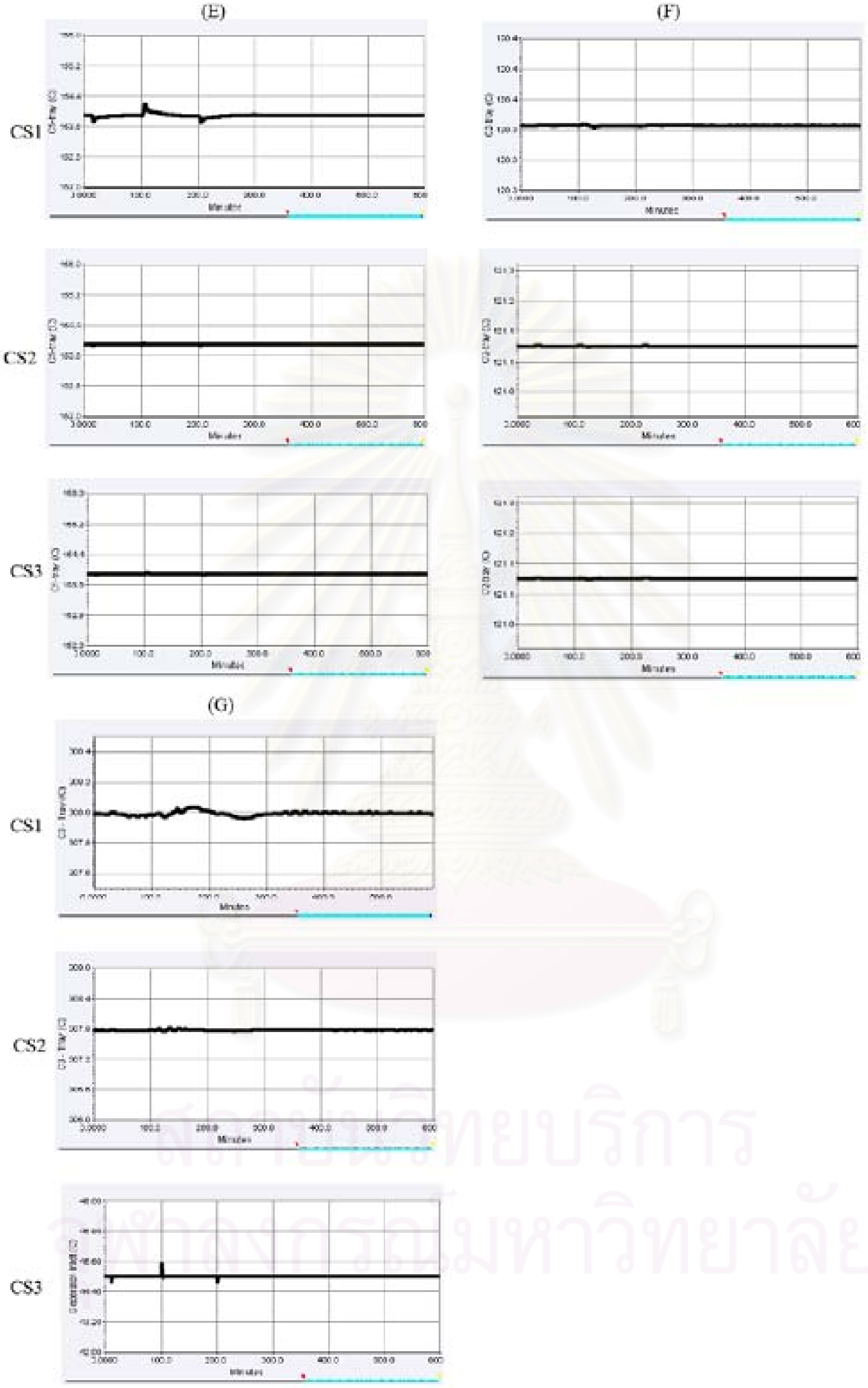

Figure 3.19: Continued.

3.6.3 Change in the recycle toluene flowrates for HDA plant alternative 1

On the other case, a disturbance in the production rate is also made for this study. Figure 3.20 shows the dynamic responses of the HDA plant alternative 1 to a disturbance in the recycle toluene flowrates from 168.6 to 158.6 kgmole/h at time equal to 10 minutes, and the flowrates is increased from 158.6 to 178.6 kgmole/h at time equal to 100 minutes, then its flowrates is returned to its nominal value of 168.6 kgmole/h at time equal to 200 minutes.

The dynamic response of control structure 1 when change in the recycle toluene flowrates for HDA plant alternative 1 are similar with those to change in the heat load disturbance of cold stream case. As can be seen, in this case has more oscillations occur in the most of temperature control loop are compare with previous case. The tray temperature of recycle column (Figure 3.20.g) has a large deviation.

The dynamic response of control structure 1 same as CS2 and CS3 but CS3 control system can handle more disturbance and faster than others. As can be seen, in our study the reactor inlet temperature (Figure 3.20.a), the reactor outlet temperature Figure 3.20.b), and the separator temperature (Figure 3.20.c) are slightly well controlled.

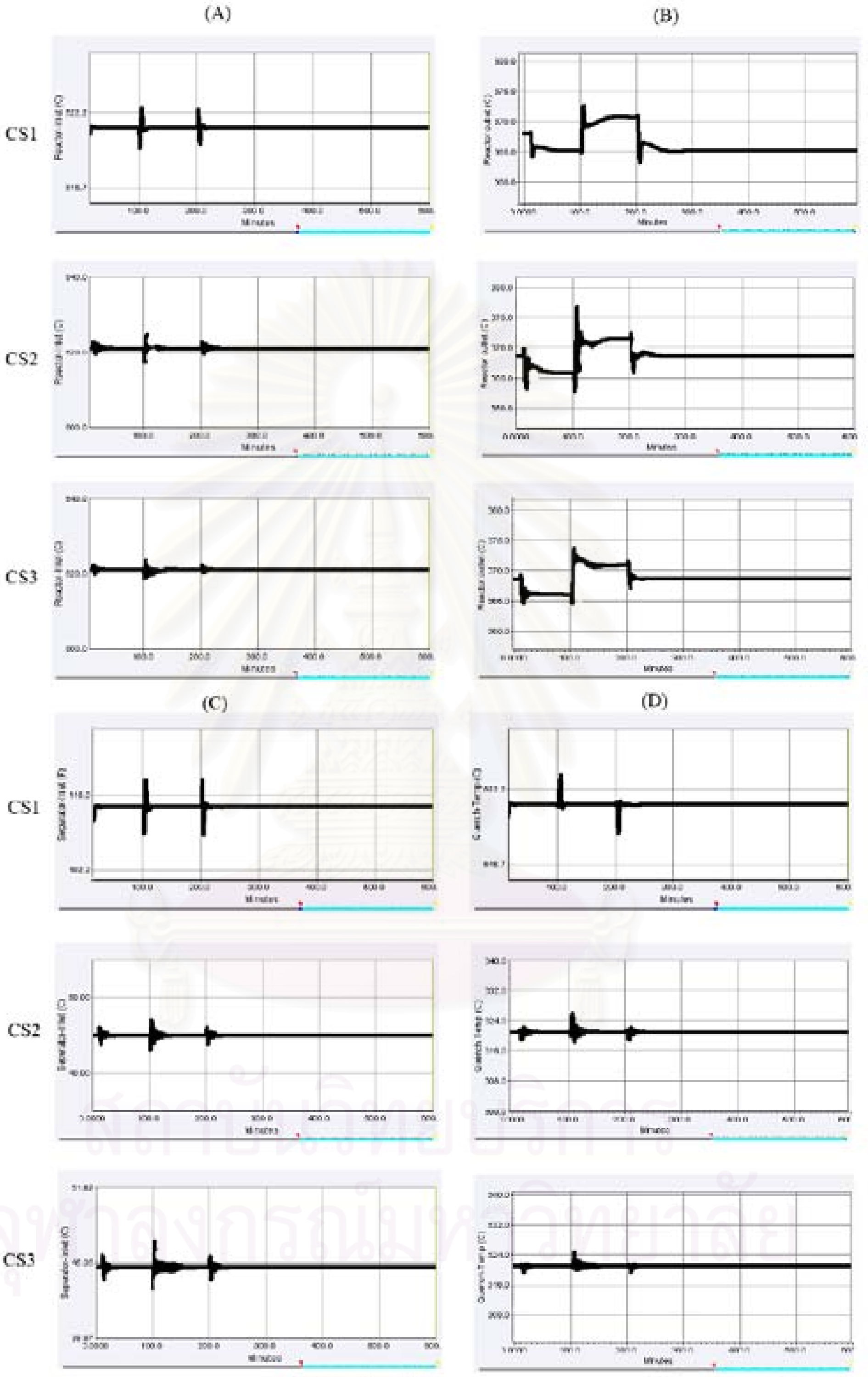

Figure 3.20: Dynamic responses of the HDA plant alternative 1 to a change in the recycle toluene flowrates, where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature, (e) tray temperature of stabilizer column, (f) tray temperature of product column, (g) tray temperature of recycle column; comparison between CS1, CS2 and CS3.

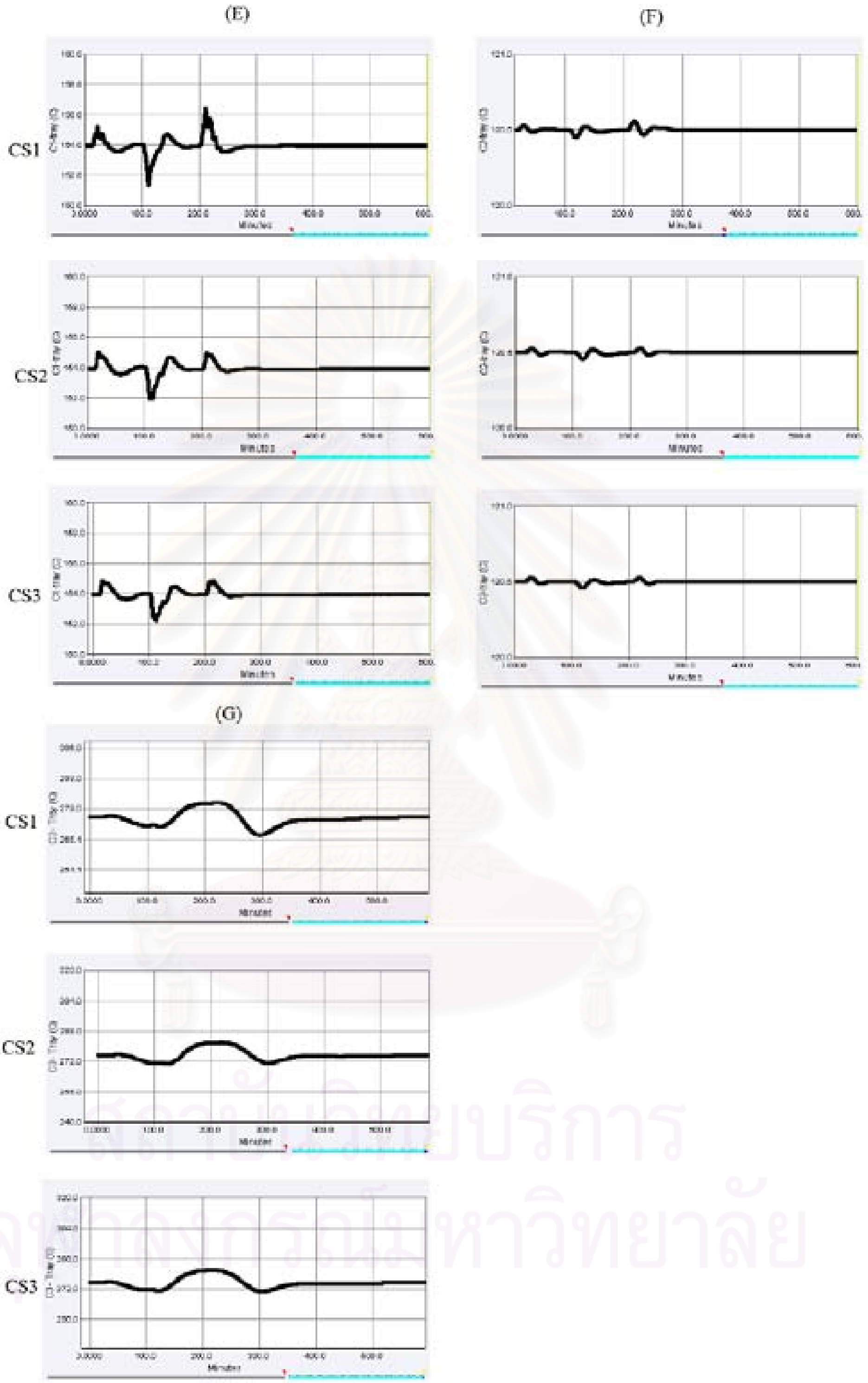

Figure 3.20: Continued.

3.6.4 Change in the recycle toluene flowrates for HDA plant alternative 2 and 3

On the other case, a disturbance in the production rate is also made for this study. Figure 3.21-3.22 show the dynamic responses of the HDA plant alternative 2 and 3 to a disturbance in the recycle toluene flowrates from 168.6 to 158.6 kgmole/h at time equal to 10 minutes, and the flowrates is increased from 158.6 to 178.6 kgmole/h at time equal to 100 minutes, then its flowrates is returned to its nominal value of 168.6 kgmole/h at time equal to 200 minutes.

As can be seen, the dynamic responses of HDA process alternative 2 are slower than those in HDA process alternative 1. In our study the reactor inlet temperature (Figure 3.21.a), the reactor outlet temperature (Figure 3.21.b), and the separator temperature(Figure 3.21.c) are slightly well controlled. But, the tray temperature of recycle column (Figure 3.21.g) has more oscillations. The tray temperature of column it takes long time to return to it nominal value.

Again, the dynamic responses of HDA process alternative 3 are slower than those in HDA process alternative 2. The reactor inlet temperature, the separator temperature, tray temperature of stabilizer column, and tray temperature of product column are slightly well controlled. But, CS1 control system shows more oscillating in the tray temperature of stabilizer column and tray temperature of recycle column.

In this case has more oscillations occur in the most of temperature control loop are compare with change in the heat load disturbance of cold stream case. For complex heat integration plant more oscillations occur in the tray temperature of stabilizer column, tray temperature of product column, and tray temperature of recycle column.

In tray temperature of recycle column has a large deviation and it takes long time to return to its nominal value. Those results indicate that the implementation of complex energy integration to the process deteriorates the dynamic performance of the process. CS3 control system can handle more disturbance and faster than other, but for first control system has better responses of utility consumptions are achieved here compared to CS2 and CS3 because in CS2 and CS3 control system as modified from the first control system by adding a cooling unit to control the outlet temperature from reactor, instead of using internal process flow. So, first control system requires less furnace utility consumptions are achieved compare to other control system.

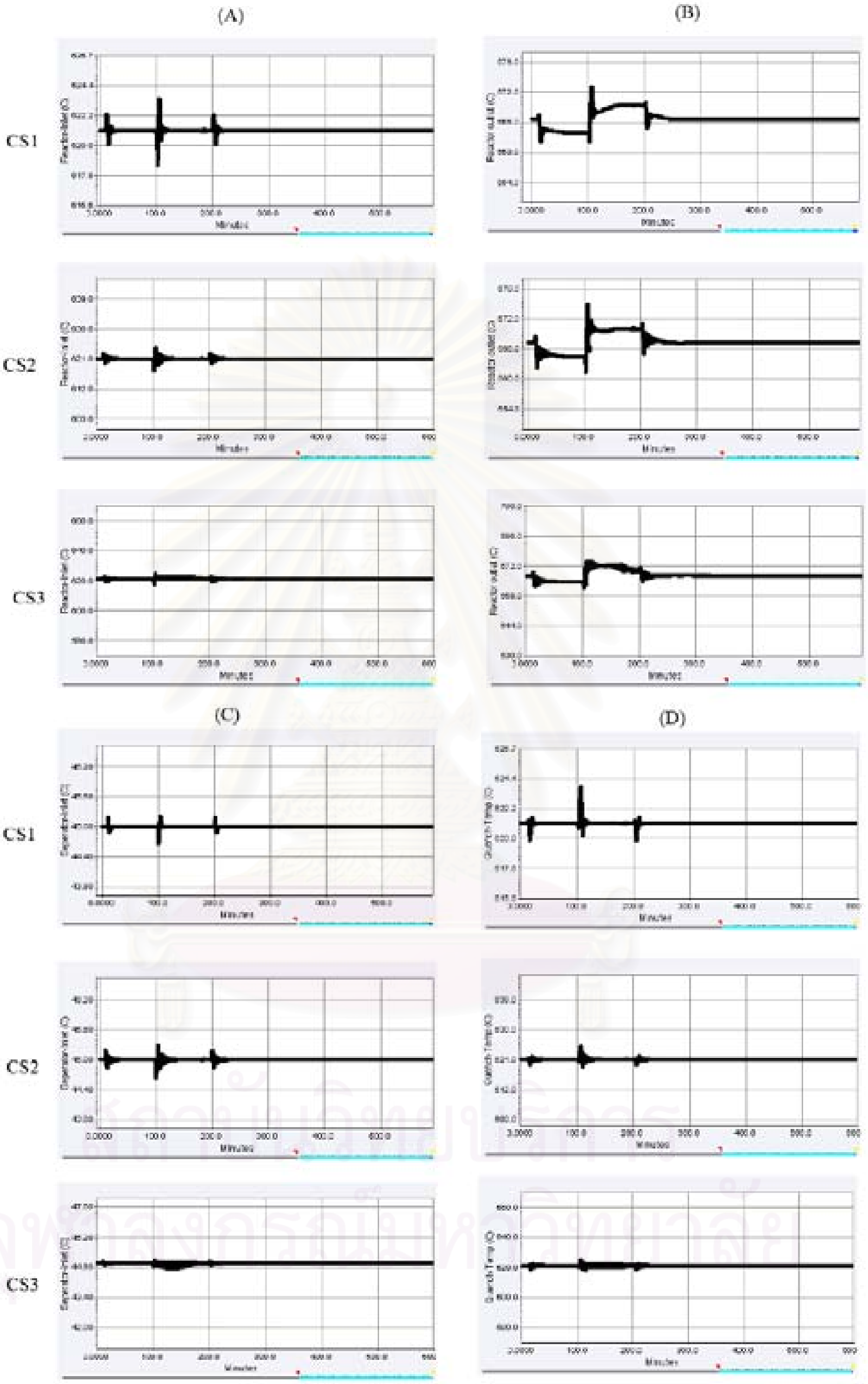

Figure 3.21: Dynamic responses of the HDA plant alternative 2 to a change in the recycle toluene flowrates, where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature, (e)tray temperature of stabilizer column, (f)tray temperature of product column, (g) tray temperature of recycle column; comparison between CS1, CS2 and CS3.

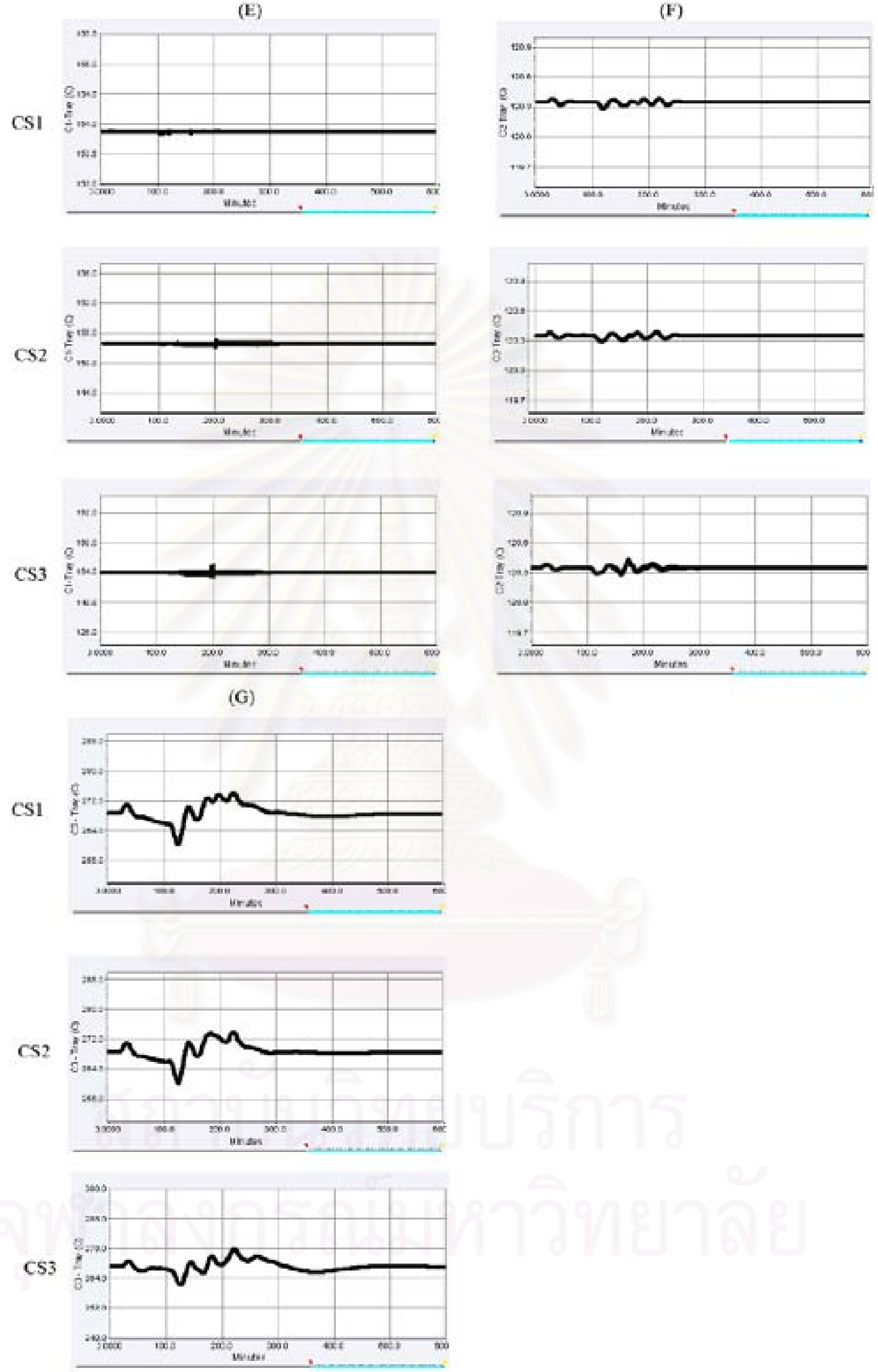

Figure 3.21: Continued.

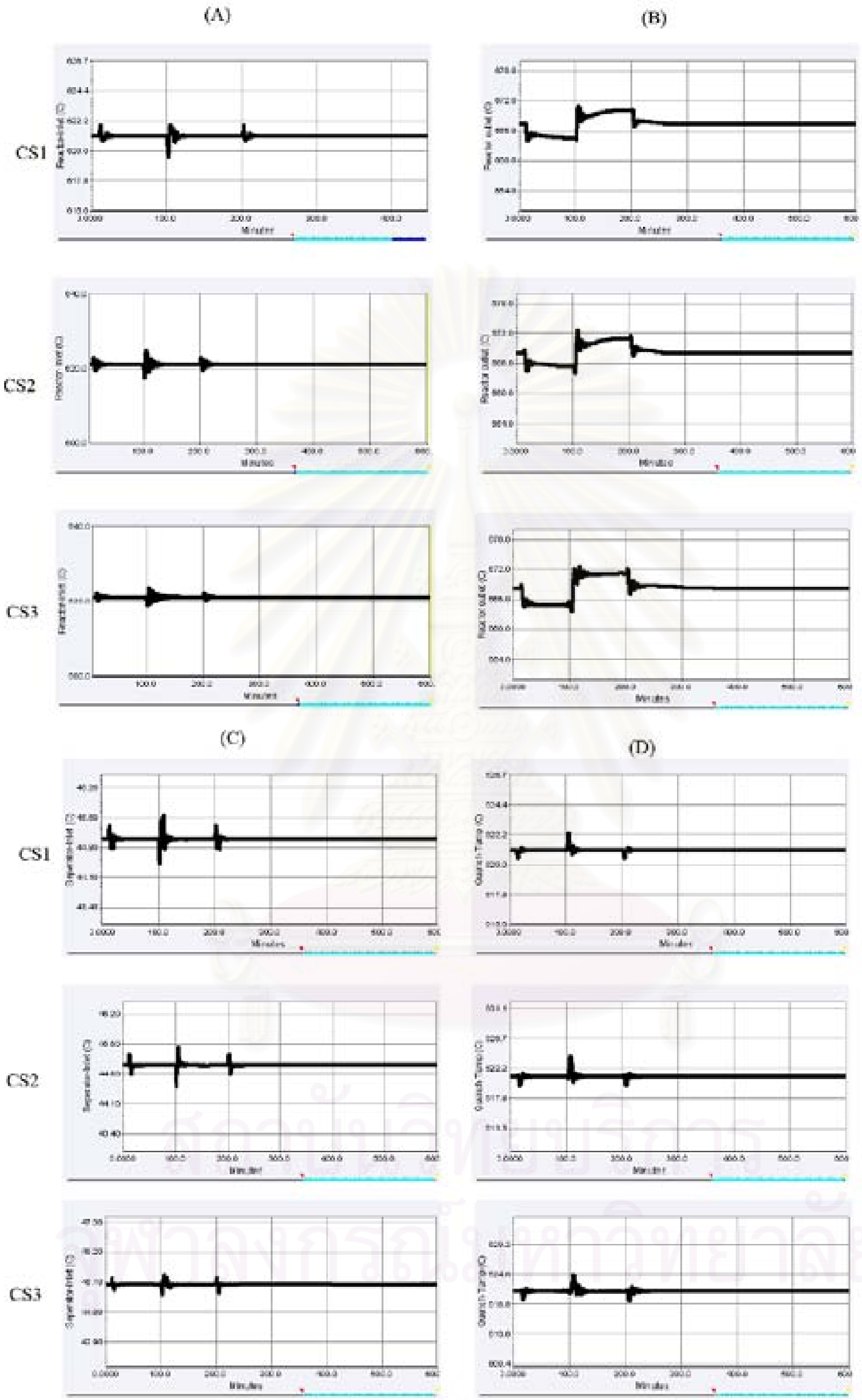

Figure 3.22: Dynamic responses of the HDA plant alternative 3 to a change in the recycle toluene flowrates, where (a) reactor inlet temperature, (b) the reactor outlet temperature (C) separator temperature, (d) quench temperature, (e)tray temperature of stabilizer column, (f)tray temperature of product column, (g) tray temperature of recycle column; comparison between CS1, CS2 and CS3.

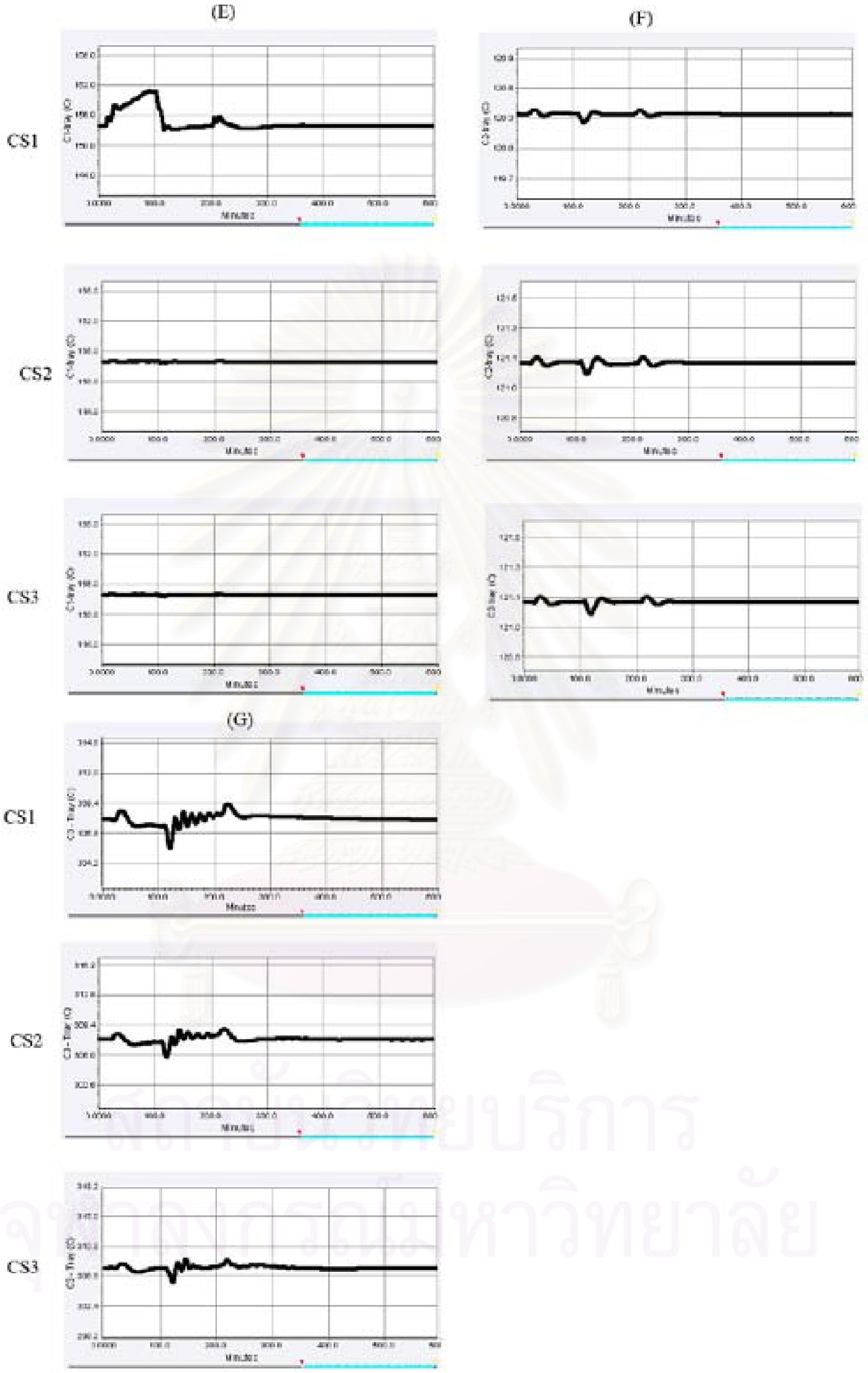

Figure 3.22: Continued.

3.7 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:

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

In this study, IAE method is used to evaluate the dynamic performance of the designed control system. Table 3.3a to 3.5a show the IAE results for the change in the disturbance loads of cold steam in HDA process with different energy integration schemes (alternative 1, 2 and 3) for CS1 control structure to CS3 control structure respectively. Table 3.3b to 3.5b shows the IAE results for the change in the total toluene feed flowrates in HDA process with different energy integration schemes (alternative 1, 2 and 3) for CS1 control structure to CS3 control structure respectively.

3.7.1 Evaluation of the dynamic performance for CS1 control structure case

Table 3.3a and 3.3b show the IAE results for the change in the disturbance loads of cold steam in HDA process and the IAE results for the change in the disturbance loads of cold steam in HDA process the IAE results for the change in the total toluene feed flowrates in HDA process respectively.

For the change in the disturbance loads of cold steam on HDA process case the control system of HDA process alternative 1 for CS1 control structure case is the most effective on compared with those in HDA process alternatives 2 and 3, i.e. the value of IAE in HDA process alternative 1 is smaller than those in alternatives 2 and 3.

As can be seen, the similarity result between the change in the total toluene feed flowrates on HDA process case and change in the disturbance loads of cold steam on HDA process case, the value of IAE in HDA process alternative 1 is smaller than the other alternatives.

Table 3.3a The IAE results of the CS1 control structure to a change in the disturbance load of cold stream (reactor feed stream)

	Alternative 1	Alternative 2	Alternative 3
FCtol	3.9322	2.7887	2.2578
TC1	1.6467	0.3617	3.5314
TC2	0.1349	0.1678	0.0205
TC3	12.099	23.814	26.8507
TCS	2.1409	0.2191	1.0365
TCQ	0.9391	1.4588	0.5108
TCR	0.9348	1.0316	0.8482
sum	21.6276	29.7417	35.0559

Table 3.3b The IAE results of the CS1 control structure to a change the total toluene feed flowrates

	Alternative 1	Alternative 2	Alternative 3
FCtol	40.944	35.989	28.06
TC1	69.1	43.4627	70.88
TC2	2.1064	2.3572	1.9392
TC3	533.316	568.12	723.32
TCS	17.464	11.2492	13.3816
TCQ	11.463	13.079	11.283
TCR	9.8217	15.124	12.4447

3.7.2 Evaluation of the dynamic performance for CS2 control structure case

Table 3.4a and 3.4b shows the IAE results for the change in the disturbance loads of cold steam in HDA process and the IAE results for the change in the disturbance loads of cold steam in HDA process the IAE results for the change in the total toluene feed flowrates in HDA process respectively.

For the change in the disturbance loads of cold steam on HDA process case the control system of HDA process alternative 1 for CS2 control structure case is the most effective on compared with the others. the value of IAE in HDA process alternative 1 is smaller than those in alternatives 2, 3, 4, 5, and 6. As can be seen the similarity result between the change in the total toluene feed flowrates on HDA process case and change in the disturbance loads of cold steam on HDA process case, the value of IAE in HDA process alternative 1 is smaller than another alternatives.

As can be seen that the IAE results for CS3 control structure look just the same as CS2 control structure results, but IAE results for CS1 control structure are smaller than CS2 control structure.

Table 3.4a The IAE results of the CS2 control structure to a change in the disturbance load of cold stream (reactor feed stream)

	Alternative 1	Alternative 2	Alternative 3
FCtol	3.0015	2.8313	1.9967
TC1	1.5725	0.124	3.4921
TC2	0.13815	0.0585	0.05275
TC3	12.099	22.981	23.844
TCS	2.1523	0.27362	0.72413
TCQ	0.8261	1.2175	0.29925
TCR	0.945	1.0869	0.67145
sum	22.73455	28.57282	31.08038

Table 3.4b The IAE results of the CS2 control structure to a change the total toluene feed flowrates

	Alternative 1	Alternative 2	Alternative 3
FCtol	48.126	50.539	30.057
TC1	56.213	46.82	68.4584
TC2	1.6549	2.358	1.899
TC3	417.45	448.41	545.3928
TCS	15.323	28.521	12.9497
TCQ	27.67	23.025	19.947
TCR	26.217	28.521	17.784
sum	593.6539	628.194	696.4879

3.7.3 Evaluation of the dynamic performance for CS3 control structure case

Table 3.5a and 3.5b shows the IAE results for the change in the disturbance loads of cold steam in HDA process and the IAE results for the change in the disturbance loads of cold steam in HDA process the IAE results for the change in the total toluene feed flowrates in HDA process respectively.

For the change in the disturbance loads of cold steam on HDA process case the control system of HDA process alternative 1 for CS3 control structure case is the most effective on compared with those in HDA process alternatives 2 and 3, the value of IAE in HDA process alternative 1 is smaller than those in alternatives 2 and 3. As can be seen the similarity result between the change in the total toluene feed flowrates on HDA process case and change in the disturbance loads of cold steam on HDA process case, the value of IAE in HDA process alternative 1 is smaller than the another alternatives.

As can be seen that the IAE results for CS3 control structure look just the same as CS2 control structure results, but IAE results for CS2 control structure are larger than CS1 control structure. The performance of these control structures can be arranged from the best to the worst performance (error of controllability point of view) as the following sequences: CS3, CS2, and CS1.

Table 3.5a The IAE results of the CS3 control structure to a change in the disturbance load of cold stream (reactor feed stream)

	Alternative 1	Alternative 2	Alternative 3
FCtol	3.0092	2.8765	3.1596
TC1	1.3124	0.11795	3.0605
TC2	0.13285	0.07645	0.09
TC3	12.094	21.874	21.393
TCS	2.1534	0.12116	0.79715
TCQ	0.8838	1.2901	0.51205
TCR	1.0957	0.8968	1.1685
sum	22.68135	27.25296	30.1809

Table 3.5b The IAE results of the CS3 control structure to a change the total toluene feed flowrates

	Alternative 1	Alternative 2	Alternative 3
FCtol	63.719	73.44	49.374
TC1	50.608	47.82	61.3601
TC2	1.3617	2.678	1.5831
TC3	406.532	423.87	543.896
TCS	19.411	13.0951	13.0951
TCQ	22.812	23.7	23.839
TCR	23.764	22.77	27.071
Sum	591.2077	609.3731	723.2183

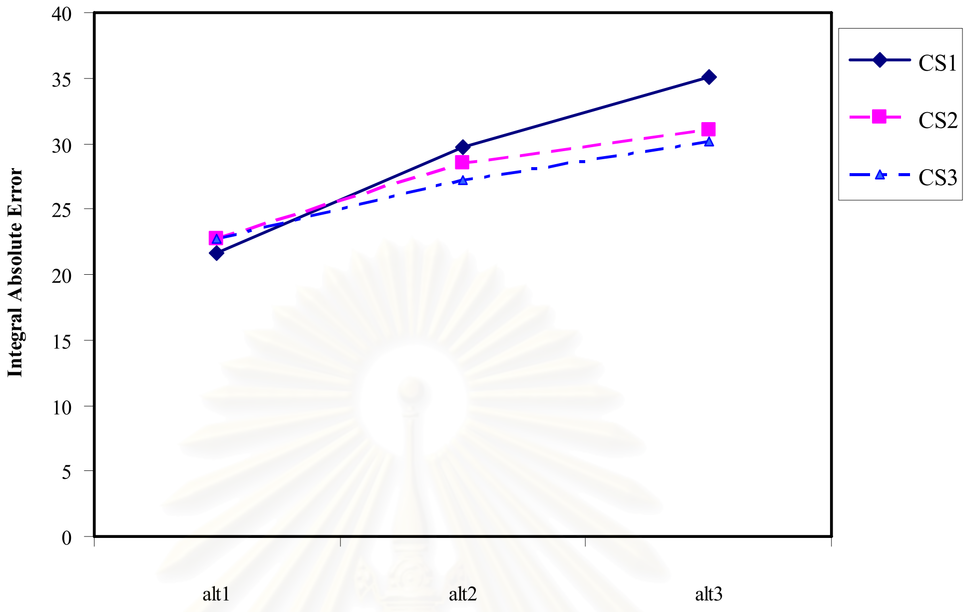

Figure 3.23: The IAE results of a change in the disturbance load of cold stream (reactor feed stream).

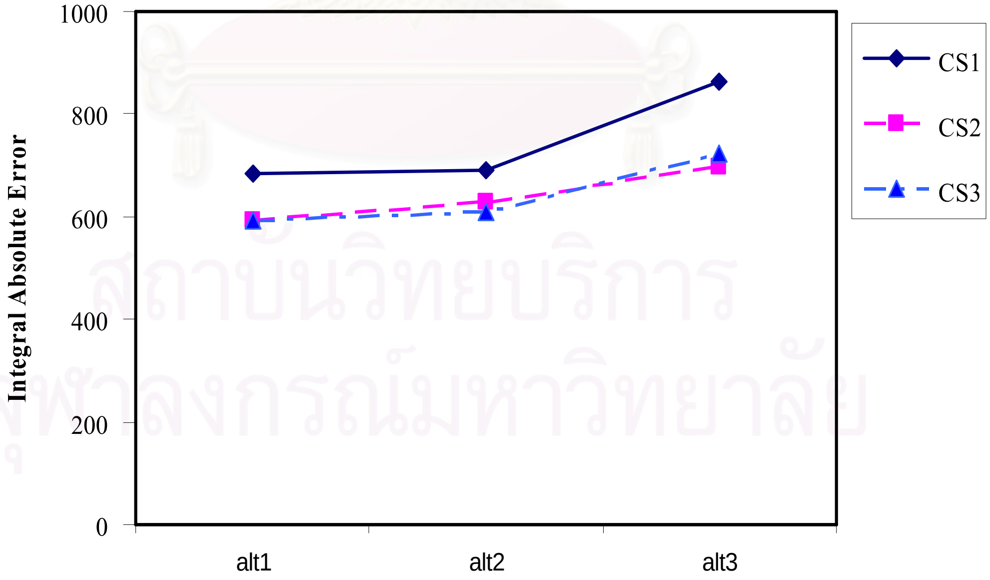

Figure 3.24: The IAE results of a change the total toluene feed flowrates.

3.8 Economic analysis for HDA process

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

From steady state point of view, 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. The benefit obtained from energy integration with the alternatives 1 to the others is given in Table 3.6. The energy cost savings from the energy integration of CS2 and CS3 are 3.68 and 12.95 %, respectively, but the capital cost rising of those are 2.20 and 3.71%, respectively.

Table 3.6 Results of cost estimation for HDA process with different energy integration schemes

Process alternative	Grass Roots Cost (US dollar)	Capital Cost Increasing from alternative 1 (%)	Annual Utility cost (US dollar)	Utility Saving from alternative 1 (%)
1	9,550,000	0.00	2,780,000	0.00
2	9,760,000	2.20	2,650,000	3.68
3	10,000,000	3.71	2,420,000	12.95

For evaluation of operating cost of control system are show in figure 3.25 - 3.28 control system has better responses of utility consumptions are achieved here compared to CS2 and CS3. Because both CS2 and CS3 control system require more furnace and quench utility compared to CS1 .Economic analysis shows that the improved energy integration has allowed us to increase the recycle flows. The increased recycle flows actually decrease the utilities consumption.

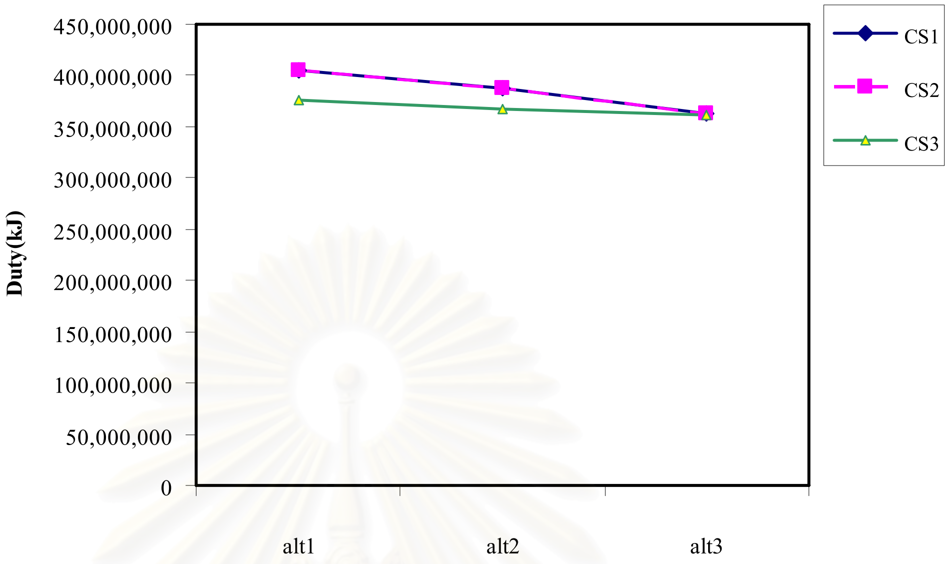

Figure 3.25: The utility consumptions (exclude cooler and quench duty) of HDA process when change in the disturbance load of cold stream (reactor feed stream).

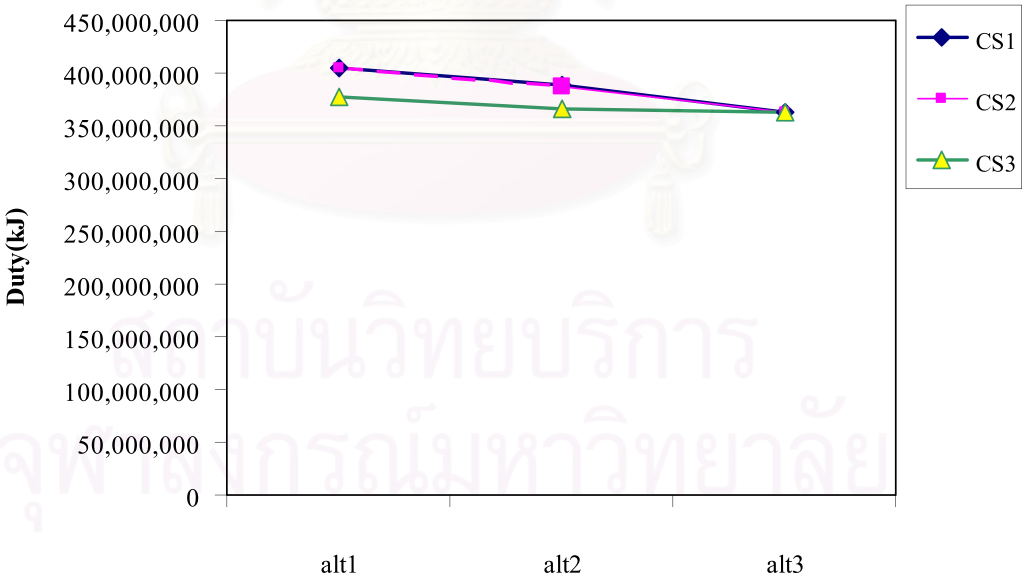

Figure 3.26: The utility consumptions (exclude cooler and quench duty) of HDA process when change the total toluene feed flowrates.

CHAPTER IV

CONCLUSIONS AND SUGGESTION FOR FURTHER WORK

4.1 Conclusion

In this research, HDA process with different energy integration schemes (alternative 1, 2 and 3) were studied, since three HEN alternative can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduce a feedback of material and energy among unit upstream and downstream. This work presents three plantwide designed control structures with three different energy integration schemes. The commercial software HYSYS was utilized to carry out both the steady state and dynamic simulations.

4.1.1 Steady State Simulation Results of HDA process

The steady state simulation results of HDA process alternative 1 have been compared with the earlier study by Luyben et al. (1998 and 2002), and the results are found consistent with those in the earlier study. Then, considering the consistency of the simulation results of the HDA process alternative 1 with respect to the previous work, the other alternatives considered in this work, alternative 2 and 3 are also developed in the HYSYS software environment. However, there are also some differences: for example, in the current study the flowrates of the reflux streams in the product and the recycle columns are larger and the reactor effluent temperature is lower than Luyben’s work. The reasons for these differences may be in current study vapor-liquid equilibrium behavior is base on the Peng-Robinson equation of state and the stabilizer column is modeled rigorously, whereas in Luyben’s work vapor-liquid equilibrium behavior was assumed to be ideal and stabilizer column was modeled as a component splitter and tank.

4.1.2 Dynamic Simulation Results of HDA process

In order to illustrate the dynamic behaviors of the control structures in HDA plant alternatives 1, 2 and 3 change in the heat load disturbance of cold stream and change in the recycle toluene flowrates were made. The dynamic simulation results have been compared with three difference control structure.

As can be seen in change in the heat load disturbance of cold stream case, when the cold inlet temperature of FEHE1 decreases, CS1 has better responses of the furnace and cooler utility consumptions are achieved here compared to CS2 and CS1. CS3 control system can handle more disturbance and responds faster than others. In CS3 control system the tray temperature of column has large deviation and takes long time to return to its nominal value.

On the other case, a disturbance in the production rate is also made for this study. In this case has more oscillations occur in the most of temperature control loop are compared with change in the heat load disturbance of cold stream case. As can be seen that, the dynamic response of HDA process alternative 3 are the slowest compared with those in HDA process alternative 2 and 1 . Those results indicate that the implementation of complex energy integration to the process deteriorates the dynamic performance of the process.

4.1.3 Evaluation of the dynamic performance

In this study, IAE method is used to evaluate the dynamic performance of the control system. For the change in the disturbance loads of cold steam on HDA process case the control system of HDA process alternative 1 for case is the most effective on compared with those in HDA process alternatives 2 and 3, the value of IAE in HDA process alternative 1 is smaller than those in alternatives 2 and 3.

As can be seen the similarity result between the change in the total toluene feed flowrates on HDA process case and change in the disturbance loads of cold steam on HDA process case, the value of IAE in HDA process alternative 1 is smaller than the other alternatives. Therefore, those results indicate that the implementation of complex energy integration to the process deteriorates the dynamic performance of the process.

The IAE results for CS3 control structure look just the same as CS2 and CS1 control structure results. The performance of these control structures can be arranged from the best to the worst performance (error of controllability point of view) as the following sequences: CS3, CS2, and CS1.

4.1.4 Economic analysis for HDA process

In this study, we concentrate on the evaluation of the economics of a HDA process. From steady state point of view the benefit obtained from energy integration with the alternatives 1 to the others is given the energy cost savings from the energy integration of alternative 2 and alternative 3 are 3.68 and 12.95 %, respectively, but the capital cost rising of those are 2.20 and 3.71%, respectively.

In order to evaluation of operating cost the result show that the improved energy integration has allowed us to increase the recycle flows. The increased recycle flows actually decrease the utilities consumption. Economics of these control structures can be arranged from the best to lowest as the following sequences: CS1, CS3 and CS2.

It can be conclude that the HDA alternative 3 is the appropriate process for implementation because it gives the significant cost saving while the capital cost rising is small. The HDA alternative 3 should be controlled by control structure 1 (CS1) because the CS1 give the appropriate responses and economics compared with other control structures.

4.2 Suggestion for Further Work

1. Study on the other control structure of HDA process.
2. Improve the methodology to accelerate the dynamic performance of complex chemical process.
3. Study and improve the methodology of MPC plantwide control of HDA process.

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APPENDICES

APPENDIX A

Table A.1.1 Process data of HDA plant alternative 1

Name	FFtol		FFH2		Rtol		v1out		bp1	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000	0.90932	0.90878
Temperature [oC]	30.00000	30.00000	30.00000	30.00000	140.27199	142.46194	29.99705	29.99705	63.51789	61.10720
Pressure [Psia]	635.00000	635.00000	635.00000	635.00000	605.00000	605.00000	605.00000	605.00000	605.00000	605.00000
Molar Flow [kgmole/h]	130.00000	144.64374	222.71614	245.70197	38.61616	23.97238	222.71614	245.70197	104.35062	124.64123
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.97000	0.97000	0.00000	0.00000	0.97000	0.97000	0.42902	0.43533
Comp Mole Frac (Methane)	0.00000	0.00000	0.03000	0.03000	0.00000	0.00000	0.03000	0.03000	0.47709	0.47086
Comp Mole Frac (Benzene)	0.00000	0.00000	0.00000	0.00000	0.00064	0.00086	0.00000	0.00000	0.00815	0.00880
Comp Mole Frac (Toluene)	1.00000	1.00000	0.00000	0.00000	0.99934	0.99912	0.00000	0.00000	0.08574	0.08500
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.00002	0.00002	0.00000	0.00000	0.00000	0.00000
Name	cHEin		cHEout		vbp1out		m4out		Rin	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.90932	0.90878	1.00000	1.00000	0.91025	0.90966	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	63.51789	61.10720	609.99576	610.32853	62.88729	60.51198	584.02005	579.24967	621.11111	621.11111
Pressure [Psia]	605.00000	605.00000	543.00000	544.18300	543.00000	544.18300	543.00000	544.18300	503.00000	502.64000
Molar Flow [kgmole/h]	1883.28032	1872.81170	1883.28032	1872.81170	104.35062	124.64123	1987.63094	1997.45293	1987.63094	1997.45293
Comp Mole Frac (Hydrogen)	0.42902	0.43533	0.42902	0.43533	0.42902	0.43533	0.42902	0.43533	0.42902	0.43533
Comp Mole Frac (Methane)	0.47709	0.47086	0.47709	0.47086	0.47709	0.47086	0.47709	0.47086	0.47709	0.47086
Comp Mole Frac (Benzene)	0.00815	0.00880	0.00815	0.00880	0.00815	0.00880	0.00815	0.00880	0.00815	0.00880
Comp Mole Frac (Toluene)	0.08574	0.08500	0.08574	0.08500	0.08574	0.08500	0.08574	0.08500	0.08574	0.08500
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Table A.1.1 Process data of HDA plant alternative 1 (cont)

Name	Rout		quench		m4out		Rin		Rout	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	665.67038	669.18903	45.46224	45.45683	584.02005	579.24967	621.11111	621.11111	665.67038	669.18903
Pressure [Psia]	486.00000	485.48200	486.00000	485.48200	543.00000	544.18300	503.00000	502.64000	486.00000	485.48200
Molar Flow [kgmole/h]	1987.63098	1997.45296	49.00000	52.93976	1987.63094	1997.45293	1987.63094	1997.45293	1987.63098	1997.45296
Comp Mole Frac (Hydrogen)	0.36518	0.36525	0.00465	0.00453	0.42902	0.43533	0.42902	0.43533	0.36518	0.36525
Comp Mole Frac (Methane)	0.54233	0.54317	0.04505	0.04461	0.47709	0.47086	0.47709	0.47086	0.54233	0.54317
Comp Mole Frac (Benzene)	0.07058	0.07667	0.70969	0.78335	0.00815	0.00880	0.00815	0.00880	0.07058	0.07667
Comp Mole Frac (Toluene)	0.02050	0.01270	0.22442	0.14139	0.08574	0.08500	0.08574	0.08500	0.02050	0.01270
Comp Mole Frac (BiPhenyl)	0.00140	0.00222	0.01619	0.02612	0.00000	0.00000	0.00000	0.00000	0.00140	0.00222

Name	quench		m2out		toX1		hHEin		hHEout	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.97042	0.97836
Temperature [oC]	45.46224	45.45683	621.06708	621.11113	621.06708	621.11113	621.06708	621.11096	119.43767	123.55475
Pressure [Psia]	486.00000	485.48200	486.00000	485.48200	486.00000	485.48200	486.00000	485.33000	480.00000	479.16300
Molar Flow [kgmole/h]	49.00000	52.93976	2036.63098	2050.39272	2036.63098	2050.39272	2036.63098	2050.39271	2036.63098	2050.39268
Comp Mole Frac (Hydrogen)	0.00465	0.00453	0.35651	0.35593	0.35651	0.35593	0.35651	0.35593	0.35651	0.35593
Comp Mole Frac (Methane)	0.04505	0.04461	0.53036	0.53030	0.53036	0.53030	0.53036	0.53030	0.53036	0.53030
Comp Mole Frac (Benzene)	0.70969	0.78335	0.08596	0.09492	0.08596	0.09492	0.08596	0.09492	0.08596	0.09492
Comp Mole Frac (Toluene)	0.22442	0.14139	0.02541	0.01602	0.02541	0.01602	0.02541	0.01602	0.02541	0.01602
Comp Mole Frac (BiPhenyl)	0.01619	0.02612	0.00176	0.00284	0.00176	0.00284	0.00176	0.00284	0.00176	0.00284

Table A.1.1 Process data of HDA plant alternative 1 (cont)

Name	coolout		gas		liq		purge		grecycle	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.89149	0.89145	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	45.00000	45.00000	45.00000	45.00002	45.00000	45.00002	45.00000	45.00002	45.00000	45.00002
Pressure [Psia]	476.80000	475.85900	476.80000	475.85900	476.80000	475.85900	476.80000	475.85900	476.80000	475.85900
Molar Flow [kgmole/h]	2036.63098	2050.39266	1815.63910	1827.83135	220.99188	222.56130	219.34045	244.69651	1596.29865	1583.13483
Comp Mole Frac (Hydrogen)	0.35651	0.35593	0.39934	0.39872	0.00465	0.00453	0.39934	0.39872	0.39934	0.39872
Comp Mole Frac (Methane)	0.53036	0.53030	0.58944	0.58944	0.04505	0.04461	0.58944	0.58944	0.58944	0.58944
Comp Mole Frac (Benzene)	0.08596	0.09492	0.01004	0.01109	0.70969	0.78335	0.01004	0.01109	0.01004	0.01109
Comp Mole Frac (Toluene)	0.02541	0.01602	0.00119	0.00075	0.22442	0.14139	0.00119	0.00075	0.00119	0.00075
Comp Mole Frac (BiPhenyl)	0.00176	0.00284	0.00000	0.00000	0.01619	0.02612	0.00000	0.00000	0.00000	0.00000

Name	v4out		dischg		p1out		toquench		toC1	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	44.97574	44.60401	70.31439	70.50648	45.25334	45.25212	45.25334	45.25212	45.25334	45.25212
Pressure [Psia]	475.00000	446.80000	605.00000	605.00000	551.60000	550.75400	551.60000	550.75400	551.60000	550.75400
Molar Flow [kgmole/h]	219.34045	244.69651	1596.29865	1583.13483	220.99188	222.56130	49.00000	52.93976	171.99188	169.62154
Comp Mole Frac (Hydrogen)	0.39934	0.39872	0.39934	0.39872	0.00465	0.00453	0.00465	0.00453	0.00465	0.00453
Comp Mole Frac (Methane)	0.58944	0.58944	0.58944	0.58944	0.04505	0.04461	0.04505	0.04461	0.04505	0.04461
Comp Mole Frac (Benzene)	0.01004	0.01109	0.01004	0.01109	0.70969	0.78335	0.70969	0.78335	0.70969	0.78335
Comp Mole Frac (Toluene)	0.00119	0.00075	0.00119	0.00075	0.22442	0.14139	0.22442	0.14139	0.22442	0.14139
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.01619	0.02612	0.01619	0.02612	0.01619	0.02612

Table A.1.1 Process data of HDA plant alternative 1 (cont)

Name	v11out		v5out		d1		b1		v6out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.02954	0.02943	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000
Temperature [oC]	45.46224	45.45683	45.97125	45.93972	51.04971	50.32124	190.51377	187.46922	50.14766	49.41655
Pressure [Psia]	486.00000	485.48200	152.00000	150.22700	150.00000	150.00000	153.00000	150.56700	120.00000	120.00000
Molar Flow [kgmole/h]	49.00000	52.93976	171.99188	169.62154	8.92567	8.69490	163.06621	160.92649	8.92567	8.69490
Comp Mole Frac (Hydrogen)	0.00465	0.00453	0.00465	0.00453	0.08965	0.08834	0.00000	0.00000	0.08965	0.08834
Comp Mole Frac (Methane)	0.04505	0.04461	0.04505	0.04461	0.86801	0.87017	0.00000	0.00000	0.86801	0.87017
Comp Mole Frac (Benzene)	0.70969	0.78335	0.70969	0.78335	0.04200	0.04130	0.74623	0.82344	0.04200	0.04130
Comp Mole Frac (Toluene)	0.22442	0.14139	0.22442	0.14139	0.00034	0.00019	0.23669	0.14902	0.00034	0.00019
Comp Mole Frac (BiPhenyl)	0.01619	0.02612	0.01619	0.02612	0.00000	0.00000	0.01708	0.02754	0.00000	0.00000

Name	v7out		d2		b2		v8out		p2out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.45070	0.43494	0.00000	0.00000	0.00000	0.00000	0.11624	0.11625	0.00000	0.00000
Temperature [oC]	116.79289	116.68007	105.54995	105.54983	144.66713	153.90518	80.85270	80.85093	144.74760	154.00755
Pressure [Psia]	32.00000	33.58400	30.00000	30.00000	33.00000	36.89400	15.00000	15.00000	53.00000	64.86300
Molar Flow [kgmole/h]	163.06621	160.92649	121.69729	132.52128	41.36892	28.40474	121.69729	132.52128	41.36892	28.40474
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.74623	0.82344	0.99970	0.99978	0.00060	0.00073	0.99970	0.99978	0.00060	0.00073
Comp Mole Frac (Toluene)	0.23669	0.14902	0.00030	0.00021	0.93208	0.84327	0.00030	0.00021	0.93208	0.84327
Comp Mole Frac (BiPhenyl)	0.01708	0.02754	0.00000	0.00000	0.06732	0.15600	0.00000	0.00000	0.06732	0.15600

Table A.1.1 Process data of HDA plant alternative 1 (cont)

Name	v9out		d3		b3		v10out		p3out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00932	0.06255	0.00000	0.00000	0.00000	0.00000	0.35924	0.35353	0.00000	0.00000
Temperature [oC]	143.37335	145.57140	137.63744	137.62778	292.68143	292.15065	259.38998	259.37957	140.21783	141.72702
Pressure [Psia]	32.00000	30.23400	30.00000	30.00000	31.00000	30.72800	16.00000	16.00000	635.00000	1003.80800
Molar Flow [kgmole/h]	41.36892	28.40474	38.58418	23.97238	2.78474	4.43221	2.78474	4.43221	38.58418	23.97238
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00060	0.00073	0.00064	0.00086	0.00000	0.00000	0.00000	0.00000	0.00064	0.00086
Comp Mole Frac (Toluene)	0.93208	0.84327	0.99934	0.99912	0.00026	0.00035	0.00026	0.00035	0.99934	0.99912
Comp Mole Frac (BiPhenyl)	0.06732	0.15600	0.00002	0.00002	0.99974	0.99965	0.99974	0.99965	0.00002	0.00002

Name	v3out	
	steady state	dynamic
Vapour Fraction	0.00000	0.00000
Temperature [oC]	140.27200	142.46194
Pressure [Psia]	605.00000	605.00000
Molar Flow [kgmole/h]	38.58418	23.97238
Comp Mole Frac (Hydrogen)	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00064	0.00086
Comp Mole Frac (Toluene)	0.99934	0.99912
Comp Mole Frac (BiPhenyl)	0.00002	0.00002

Table A.1.2 Energy stream data of HDA plant alternative 1

Name	qfur		qcooler		qc1		qc2		qc3		qr1		qr2		qr3		wkcomp		wkp1		wkp2		wkp3	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	1388.74257	1566.50954	3189.62955	3434.00391	189.60023	179.57246	4007.46522	4074.92418	427.00988	297.126798	1272.24116	1222.66819	3413.66888	3511.35683	467.81367	359.89953	377.81969	377.819699	3.97953	3.979538	0.2669872	0.26661706	7.30638249	7.30638218

Table A.2.1 Process data of HDA plant alternative 2

Name	FFH2		v1out		FFtol		v2out		Rtol	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	30.00000	30.00000	29.99705	29.99686	30.00000	30.00000	30.11499	30.12150	182.60467	181.97799
Pressure [Psia]	635.00000	635.00000	605.00000	603.30262	635.00000	635.00000	605.00000	603.30262	605.00000	603.30262
Molar Flow [kgmole/h]	222.71614	221.29956	222.71614	221.29956	131.08954	129.41345	131.08954	129.41345	33.49568	40.03108
Comp Mole Frac (Hydrogen)	0.97000	0.97000	0.97000	0.97000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.03000	0.03000	0.03000	0.03000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00087	0.00123
Comp Mole Frac (Toluene)	0.00000	0.00000	0.00000	0.00000	1.00000	1.00000	1.00000	1.00000	0.99870	0.99833
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00043	0.00044

Name	toX1		cHEout		hHEout		Rin		Rout	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	-	1.00000	1.00000	1.00000	0.98744	0.98603	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	-	621.11112	596.66667	604.56530	129.46983	128.75233	621.11111	621.11112	665.47890	665.07352
Pressure [Psia]	-	487.05487	543.00000	545.90695	480.00000	480.57736	503.00000	504.23495	486.00000	487.05487
Molar Flow [kgmole/h]	-	2064.19859	1879.46101	1886.07211	2032.81533	2064.19870	1983.60001	2015.37945	1983.60005	2015.37940
Comp Mole Frac (Hydrogen)	-	0.35869	0.43904	0.43001	0.36721	0.35869	0.43904	0.43001	0.37620	0.36727
Comp Mole Frac (Methane)	-	0.52924	0.46895	0.47692	0.52130	0.52924	0.46895	0.47692	0.53314	0.54097
Comp Mole Frac (Benzene)	-	0.08446	0.00813	0.00804	0.08528	0.08446	0.00813	0.00804	0.06962	0.06946
Comp Mole Frac (Toluene)	-	0.02594	0.08387	0.08503	0.02449	0.02594	0.08387	0.08503	0.01968	0.02097
Comp Mole Frac (BiPhenyl)	-	0.00166	0.00001	0.00001	0.00172	0.00166	0.00001	0.00001	0.00136	0.00133

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	gas		liq		grecycle		purge		dicharg	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	45.00000	45.00000	45.00000	45.00000	45.00000	45.00000	45.00000	45.00000	70.38487	69.91251
Pressure [Psia]	476.80000	477.26383	476.80000	477.26383	476.80000	477.26383	476.80000	477.26383	605.00000	603.30262
Molar Flow [kgmole/h]	1815.93439	1842.43247	216.88093	221.76620	1596.29865	1624.63533	219.63574	217.79714	1596.29865	1624.63533
Comp Mole Frac (Hydrogen)	0.41050	0.40130	0.00477	0.00469	0.41050	0.40130	0.41050	0.40130	0.41050	0.40130
Comp Mole Frac (Methane)	0.57828	0.58753	0.04418	0.04497	0.57828	0.58753	0.57828	0.58753	0.57828	0.58753
Comp Mole Frac (Benzene)	0.01007	0.00994	0.71506	0.70355	0.01007	0.00994	0.01007	0.00994	0.01007	0.00994
Comp Mole Frac (Toluene)	0.00116	0.00122	0.21985	0.23134	0.00116	0.00122	0.00116	0.00122	0.00116	0.00122
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.01613	0.01545	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Name	toC1		v2out		d1		b1		v4out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.02915	0.02977	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000
Temperature [oC]	45.25341	45.24750	45.99086	45.96362	51.04137	74.47282	189.39256	189.69911	44.60447	44.58933
Pressure [Psia]	551.60000	550.31886	150.30000	150.08353	150.00000	149.99993	150.54317	150.33968	446.80000	446.80000
Molar Flow [kgmole/h]	167.66566	172.94701	167.66566	172.94701	8.57024	9.45864	159.09542	163.48830	219.63574	217.79714
Comp Mole Frac (Hydrogen)	0.00477	0.00469	0.00477	0.00469	0.09333	0.08571	0.00000	0.00000	0.41050	0.40130
Comp Mole Frac (Methane)	0.04418	0.04497	0.04418	0.04497	0.86434	0.82221	0.00000	0.00000	0.57828	0.58753
Comp Mole Frac (Benzene)	0.71506	0.70355	0.71506	0.70355	0.04200	0.09115	0.75132	0.73898	0.01007	0.00994
Comp Mole Frac (Toluene)	0.21985	0.23134	0.21985	0.23134	0.00033	0.00093	0.23168	0.24467	0.00116	0.00122
Comp Mole Frac (BiPhenyl)	0.01613	0.01545	0.01613	0.01545	0.00000	0.00000	0.01700	0.01634	0.00000	0.00000

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	d2		v2		tov9		v90ut		p2out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	105.55001	105.54866	143.65031	143.32186	143.90473	143.57822	143.93694	143.60707	143.90473	143.57822
Pressure [Psia]	30.00000	29.99995	32.20905	32.16384	95.96762	95.58683	75.75319	76.87491	95.96762	95.58683
Molar Flow [kgmole/h]	119.58017	120.79627	423.65750	426.80919	39.51434	42.68918	39.51434	42.68918	423.65659	426.83202
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.99970	0.99970	0.00095	0.00116	0.00095	0.00116	0.00095	0.00116	0.00095	0.00116
Comp Mole Frac (Toluene)	0.00030	0.00030	0.93077	0.93620	0.93077	0.93619	0.93077	0.93619	0.93077	0.93619
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.06828	0.06265	0.06828	0.06266	0.06828	0.06266	0.06828	0.06266

Name	v12out		toTop3		d3		b3		hCRout	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.01889	0.00805	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	143.02286	143.02286	180.17695	181.05154	180.64937	181.56308	346.88665	347.54321	178.16575	178.13319
Pressure [Psia]	27.20905	27.20905	75.42000	76.73903	75.41960	76.73643	76.43487	77.19769	72.51885	72.51954
Molar Flow [kgmole/h]	0.00091	0.00000	9.98685	9.98685	46.81733	50.01704	2.68386	2.65814	43.50738	50.00990
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00205	0.00205	0.00087	0.00123	0.00099	0.00123	0.00000	0.00000	0.00099	0.00123
Comp Mole Frac (Toluene)	0.99616	0.99616	0.99870	0.99833	0.99861	0.99833	0.00026	0.00027	0.99861	0.99833
Comp Mole Frac (BiPhenyl)	0.00179	0.00179	0.00042	0.00044	0.00041	0.00044	0.99974	0.99973	0.00041	0.00044

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	v15in		v15out		p3out		tov11		Tout2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.01889	0.00805	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	182.40862	181.86269	180.17488	181.05154	182.40862	181.86269	182.40862	181.86269	178.16984	178.15609
Pressure [Psia]	875.00000	769.95696	75.42000	76.73903	875.00000	769.95696	875.00000	769.95696	72.51885	72.51954
Molar Flow [kgmole/h]	9.98685	9.98685	9.98685	9.98685	43.46780	50.01793	33.48095	40.03108	43.46780	50.01793
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00093	0.00123	0.00093	0.00123	0.00093	0.00123	0.00093	0.00123	0.00093	0.00123
Comp Mole Frac (Toluene)	0.99863	0.99833	0.99863	0.99833	0.99863	0.99833	0.99863	0.99833	0.99863	0.99833
Comp Mole Frac (BiPhenyl)	0.00044	0.00044	0.00044	0.00044	0.00044	0.00044	0.00044	0.00044	0.00044	0.00044

Name	v8out		v10out		bp2		hCRin		v16out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.11624	0.11623	0.18475	0.19346	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	80.85283	80.85269	332.80374	332.80333	180.64937	181.56299	180.64937	181.56299	180.32205	181.08893
Pressure [Psia]	15.00006	15.00006	61.43492	61.43492	75.41960	76.73643	75.41960	76.73643	72.51885	72.51954
Molar Flow [kgmole/h]	119.58017	120.79627	2.68386	2.65814	3.30995	0.00799	43.50738	50.00904	3.30995	0.00799
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.99970	0.99970	0.00000	0.00000	0.00099	0.00123	0.00099	0.00123	0.00099	0.00123
Comp Mole Frac (Toluene)	0.00030	0.00030	0.00026	0.00027	0.99861	0.99833	0.99861	0.99833	0.99861	0.99833
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.99974	0.99973	0.00041	0.00044	0.00041	0.00044	0.00041	0.00044

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	vbp1out		mbpout		hHEin		Toltol		Rgas	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.91292	0.91208	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000
Temperature [oC]	64.80321	65.89894	571.29498	573.20771	620.18979	621.11098	65.85703	71.13267	70.38274	69.91251
Pressure [Psia]	543.00000	545.90695	543.00000	545.90695	486.00000	486.90219	605.00000	603.30262	605.00000	603.30262
Molar Flow [kgmole/h]	104.13900	129.30731	1983.60001	2015.37942	2032.81533	2064.19857	164.58522	169.44453	1596.29865	1624.63533
Comp Mole Frac (Hydrogen)	0.43904	0.43001	0.43904	0.43001	0.36721	0.35869	0.00000	0.00000	0.41022	0.40130
Comp Mole Frac (Methane)	0.46895	0.47692	0.46895	0.47692	0.52130	0.52924	0.00000	0.00000	0.57854	0.58753
Comp Mole Frac (Benzene)	0.00813	0.00804	0.00813	0.00804	0.08528	0.08446	0.00018	0.00029	0.01009	0.00994
Comp Mole Frac (Toluene)	0.08387	0.08503	0.08387	0.08503	0.02449	0.02594	0.99974	0.99961	0.00115	0.00122
Comp Mole Frac (BiPhenyl)	0.00001	0.00001	0.00001	0.00001	0.00172	0.00166	0.00009	0.00010	0.00000	0.00000

Name	cHEin		quench		M2out		coolant		toquench	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.91199	0.91119	0.00000	0.00000	1.00000	1.00000	0.89331	0.89257	0.00000	0.00000
Temperature [oC]	65.44733	66.50737	45.46230	45.44923	620.18304	621.11111	45.00000	44.99998	45.25341	45.24750
Pressure [Psia]	605.00000	603.30262	486.00000	487.05487	486.00000	487.05487	476.80000	477.26383	551.60000	550.31886
Molar Flow [kgmole/h]	1879.46101	1886.07211	49.21528	48.81918	2032.81533	2064.19859	2032.81533	2064.19869	49.21528	48.81918
Comp Mole Frac (Hydrogen)	0.43904	0.43001	0.00477	0.00469	0.36721	0.35869	0.36721	0.35869	0.00477	0.00469
Comp Mole Frac (Methane)	0.46895	0.47692	0.04418	0.04497	0.52130	0.52924	0.52130	0.52924	0.04418	0.04497
Comp Mole Frac (Benzene)	0.00813	0.00804	0.71506	0.70355	0.08524	0.08446	0.08528	0.08446	0.71506	0.70355
Comp Mole Frac (Toluene)	0.08387	0.08503	0.21985	0.23134	0.02453	0.02594	0.02449	0.02594	0.21985	0.23134
Comp Mole Frac (BiPhenyl)	0.00001	0.00001	0.01613	0.01545	0.00172	0.00166	0.00172	0.00166	0.01613	0.01545

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	v3out		p1out		v6out		v7out		boil2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.00000	0.00000	1.00000	1.00000	0.44966	0.45005	0.88837	0.89418
Temperature [oC]	45.46230	45.44923	45.25341	45.24750	50.14428	73.52086	115.39876	115.72673	165.55556	164.02629
Pressure [Psia]	486.00000	487.05487	551.60000	550.31886	120.00000	120.00000	31.04000	31.00942	32.26000	32.17249
Molar Flow [kgmole/h]	49.21528	48.81918	216.88093	221.76620	8.57024	9.45864	159.09542	163.48830	384.14225	384.29872
Comp Mole Frac (Hydrogen)	0.00477	0.00469	0.00477	0.00469	0.09333	0.08571	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.04418	0.04497	0.04418	0.04497	0.86434	0.82221	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.71506	0.70355	0.71506	0.70355	0.04200	0.09115	0.75132	0.73898	0.00108	0.00116
Comp Mole Frac (Toluene)	0.21985	0.23134	0.21985	0.23134	0.00033	0.00093	0.23168	0.24467	0.93066	0.93661
Comp Mole Frac (BiPhenyl)	0.01613	0.01545	0.01613	0.01545	0.00000	0.00000	0.01700	0.01634	0.06826	0.06223

Name	cCRin		tankout		vtb2		coldout2		v13out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.00000	0.00000	1.00000	1.00000	0.00000	0.00000	0.08217	0.09586
Temperature [oC]	143.90473	143.57822	143.65031	143.32328	143.65031	143.32328	159.62708	161.80618	147.65246	147.77379
Pressure [Psia]	95.96762	95.58683	32.20905	32.16384	32.20905	32.16384	93.06687	92.65595	35.09687	35.39529
Molar Flow [kgmole/h]	384.14225	384.14285	423.65659	426.83202	0.00091	0.00000	384.14225	384.14288	384.14225	384.14288
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00095	0.00116	0.00095	0.00116	0.00205	0.00249	0.00095	0.00116	0.00095	0.00116
Comp Mole Frac (Toluene)	0.93077	0.93619	0.93077	0.93619	0.99616	0.99587	0.93077	0.93618	0.93077	0.93618
Comp Mole Frac (BiPhenyl)	0.06828	0.06266	0.06828	0.06266	0.00179	0.00164	0.06828	0.06266	0.06828	0.06266

Table A.2.1 Process data of HDA plant alternative 2 (cont)

Name	boil2out		vtb3		v14out		retol		m4out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.88831	0.89373	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.07154	0.00000
Temperature [oC]	165.55556	164.23459	178.16984	178.15609	177.60242	177.60242	182.60269	181.97799	178.16984	178.15579
Pressure [Psia]	32.26000	32.17249	72.51885	72.51954	67.51885	67.51885	605.00000	603.30262	72.51885	72.51954
Molar Flow [kgmole/h]	384.14225	384.29872	3.34953	0.00000	3.34953	0.00000	33.48095	40.03108	46.81733	50.01789
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00095	0.00116	0.00169	0.00224	0.00169	0.00169	0.00093	0.00123	0.00099	0.00123
Comp Mole Frac (Toluene)	0.93077	0.93574	0.99829	0.99774	0.99829	0.99829	0.99863	0.99833	0.99861	0.99833
Comp Mole Frac (BiPhenyl)	0.06828	0.06311	0.00002	0.00002	0.00002	0.00002	0.00044	0.00044	0.00041	0.00044

Name	m1out		bp1	
	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.91199	0.91119	0.91199	0.91119
Temperature [oC]	65.44733	66.50737	65.44733	66.50737
Pressure [Psia]	605.00000	603.30262	605.00000	603.30262
Molar Flow [kgmole/h]	1983.60001	2015.37942	104.13900	129.30731
Comp Mole Frac (Hydrogen)	0.43904	0.43001	0.43904	0.43001
Comp Mole Frac (Methane)	0.46895	0.47692	0.46895	0.47692
Comp Mole Frac (Benzene)	0.00813	0.00804	0.00813	0.00804
Comp Mole Frac (Toluene)	0.08387	0.08503	0.08387	0.08503
Comp Mole Frac (BiPhenyl)	0.00001	0.00001	0.00001	0.00001

Table A.2.2 Energy stream data of HDA plant alternative 2

Name	qfur		qcooler		wkcomp		wkp1		qc1	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	1835.54932	1808.63718	3665.89480	3701.56981	378.19653	378.19653	3.90333	3.90333	172.12705	158.42355

Name	qr1		qc2		wkp2		qr3		qar2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	1217.41769	1244.89686	3993.76802	4009.80564	8.70598	8.70598	525.02436	559.62515	3058.00936	2998.18203

Name	wkp3	
	steady state	dynamic
Heat Flow (kw)	11.65052	11.65052

Table A.3.1 Process data of HDA plant alternative 3

Name	FFH2		v1out		Toltol		m1out		Regas	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.90653	0.90819	1.00000	1.00000
Temperature [oC]	30.00000	30.00000	29.99646	29.99646	52.77907	67.37977	59.33677	62.90240	65.58062	65.18959
Pressure [Psia]	605.00000	604.99999	575.00000	574.99999	575.00000	574.99999	575.00000	574.99999	575.00000	574.99999
Molar Flow [kgmole/h]	252.80412	228.26750	252.80412	228.26750	169.49594	169.44706	1959.10956	1965.61806	1536.80950	1567.90350
Comp Mole Frac (Hydrogen)	0.97000	0.97000	0.97000	0.97000	0.00000	0.00000	0.43933	0.43259	0.40048	0.40110
Comp Mole Frac (Methane)	0.03000	0.03000	0.03000	0.03000	0.00000	0.00000	0.46476	0.47214	0.58753	0.58753
Comp Mole Frac (Benzene)	0.00000	0.00000	0.00000	0.00000	0.00009	0.00023	0.00889	0.00821	0.01132	0.01026
Comp Mole Frac (Toluene)	0.00000	0.00000	0.00000	0.00000	0.99987	0.99968	0.08702	0.08706	0.00066	0.00110
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.00004	0.00009	0.00000	0.00001	0.00000	0.00000

Name	Rout		m2out		quench		coolout		gas	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.88897	0.88971	1.00000	1.00000
Temperature [oC]	670.74469	667.04725	621.03590	621.10998	45.44134	45.44628	45.00000	45.00000	45.00002	45.00000
Pressure [Psia]	487.68420	489.26321	487.68420	489.26321	487.68420	489.26321	473.43142	475.21786	473.43142	475.21786
Molar Flow [kgmole/h]	1959.10973	1965.61849	2012.89352	2015.62741	53.78379	50.00892	2012.89345	2015.62774	1789.39245	1793.32756
Comp Mole Frac (Hydrogen)	0.36618	0.36635	0.35652	0.35738	0.00450	0.00463	0.35652	0.35738	0.40048	0.40110
Comp Mole Frac (Methane)	0.54046	0.53995	0.52720	0.52766	0.04415	0.04469	0.52720	0.52766	0.58753	0.58753
Comp Mole Frac (Benzene)	0.07948	0.07287	0.09868	0.08904	0.79809	0.72457	0.09868	0.08904	0.01132	0.01026
Comp Mole Frac (Toluene)	0.01132	0.01924	0.01432	0.02393	0.12372	0.20806	0.01432	0.02393	0.00066	0.00110
Comp Mole Frac (BiPhenyl)	0.00256	0.00158	0.00328	0.00199	0.02955	0.01804	0.00328	0.00199	0.00000	0.00000

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	discharge		v4out		p1out		toquench		toC1	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	65.58062	65.18959	44.63814	44.61604	45.25150	45.25319	45.25150	45.25319	45.25150	45.25319
Pressure [Psia]	575.00000	574.99999	446.79340	446.79340	548.44149	550.06052	548.44149	550.06052	548.44149	550.06052
Molar Flow [kgmole/h]	1536.80950	1567.90350	252.58294	225.42406	223.50097	222.30023	53.78379	50.00892	169.71718	172.29130
Comp Mole Frac (Hydrogen)	0.40048	0.40110	0.40048	0.40110	0.00450	0.00463	0.00450	0.00463	0.00450	0.00463
Comp Mole Frac (Methane)	0.58753	0.58753	0.58753	0.58753	0.04415	0.04469	0.04415	0.04469	0.04415	0.04469
Comp Mole Frac (Benzene)	0.01132	0.01026	0.01132	0.01026	0.79809	0.72457	0.79809	0.72457	0.79809	0.72457
Comp Mole Frac (Toluene)	0.00066	0.00110	0.00066	0.00110	0.12372	0.20806	0.12372	0.20806	0.12372	0.20806
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.00000	0.00000	0.02955	0.01804	0.02955	0.01804	0.02955	0.01804

Name	b1		v6out		v7out		d2		b2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	1.00000	1.00000	0.45023	0.45008	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	187.03214	189.07839	41.80405	46.92007	113.20313	115.05776	105.37727	105.34431	149.51235	143.97461
Pressure [Psia]	150.43885	150.51544	120.00000	119.99997	30.95484	30.95177	30.00000	30.00000	32.06274	32.05581
Molar Flow [kgmole/h]	341.78479	344.04806	8.52008	8.83079	161.19729	163.46232	135.20573	124.50724	410.12798	423.09744
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.08956	0.09045	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00002	0.00002	0.87910	0.87186	0.00002	0.00002	0.00002	0.00002	0.00000	0.00000
Comp Mole Frac (Benzene)	0.83862	0.76168	0.03121	0.03741	0.83862	0.76168	0.99973	0.99968	0.00058	0.00099
Comp Mole Frac (Toluene)	0.13025	0.21929	0.00012	0.00028	0.13025	0.21929	0.00025	0.00030	0.80648	0.91918
Comp Mole Frac (BiPhenyl)	0.03111	0.01902	0.00000	0.00000	0.03111	0.01901	0.00000	0.00000	0.19293	0.07983

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	d3		b3		p4out		v10out		boil2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.16025	0.18095	0.77378	0.87606
Temperature [oC]	179.44893	180.54011	345.00744	346.59623	184.62835	182.62059	332.77950	332.80200	186.95745	167.69967
Pressure [Psia]	73.73291	75.21811	74.34169	76.10418	1325.04581	918.66423	61.43492	61.43492	32.06868	32.06176
Molar Flow [kgmole/h]	30.97078	45.84688	5.00875	3.09475	30.97001	45.84656	5.00875	3.09475	384.14353	384.14053
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00072	0.00108	0.00000	0.00000	0.00072	0.00108	0.00000	0.00000	0.00058	0.00099
Comp Mole Frac (Toluene)	0.99892	0.99849	0.00034	0.00026	0.99892	0.99849	0.00034	0.00026	0.80648	0.91918
Comp Mole Frac (BiPhenyl)	0.00036	0.00043	0.99966	0.99974	0.00036	0.00043	0.99966	0.99974	0.19294	0.07983

Name	cCRin		t2out		boil1		vtb1		tank1out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.00000	0.00000	0.89404	0.92633	1.00000	1.00000	0.00000	0.00000
Temperature [oC]	149.72711	144.22570	149.72711	144.22570	202.56024	202.61629	187.03153	189.07722	187.03154	189.07722
Pressure [Psia]	95.26970	95.92602	95.26970	95.92602	150.47273	150.58498	150.43885	150.51544	150.43885	150.51544
Molar Flow [kgmole/h]	384.14237	384.14327	25.99166	38.95439	180.58827	180.58625	0.00000	0.00000	341.78808	344.05384
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00001	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00002	0.00002	0.00064	0.00067	0.00002	0.00002
Comp Mole Frac (Benzene)	0.00058	0.00099	0.00058	0.00099	0.83862	0.76168	0.91470	0.85365	0.83862	0.76168
Comp Mole Frac (Toluene)	0.80648	0.91918	0.80648	0.91918	0.13025	0.21929	0.08354	0.14494	0.13025	0.21929
Comp Mole Frac (BiPhenyl)	0.19293	0.07983	0.19293	0.07983	0.03111	0.01902	0.00112	0.00073	0.03111	0.01901

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	toboil1		cHE2out		hHE2out		hR2out		toP2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.89404	0.92633	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000
Temperature [oC]	202.56025	202.61619	591.51419	585.38869	265.67695	241.45874	226.89651	210.23067	187.03170	189.07712
Pressure [Psia]	150.47273	150.58498	514.18346	515.81887	480.70272	482.30611	478.64928	480.35638	150.43885	150.51544
Molar Flow [kgmole/h]	180.58827	180.58625	1896.05853	1965.61836	2012.89360	2015.62735	2012.89349	2015.62736	180.59079	180.59152
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.43933	0.43259	0.35652	0.35738	0.35652	0.35738	0.00000	0.00000
Comp Mole Frac (Methane)	0.00002	0.00002	0.46476	0.47214	0.52720	0.52766	0.52720	0.52766	0.00002	0.00002
Comp Mole Frac (Benzene)	0.83862	0.76168	0.00889	0.00821	0.09868	0.08904	0.09868	0.08904	0.83862	0.76168
Comp Mole Frac (Toluene)	0.13025	0.21929	0.08702	0.08706	0.01432	0.02393	0.01432	0.02393	0.13025	0.21929
Comp Mole Frac (BiPhenyl)	0.03111	0.01902	0.00000	0.00001	0.00328	0.00199	0.00328	0.00199	0.03111	0.01901

Name	cCRout		vtb3		Tout3		v17in		toR4	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	159.44182	160.55456	178.17516	178.16264	178.17516	178.16264	184.62835	182.62064	184.62835	182.62064
Pressure [Psia]	91.97794	92.98075	72.51878	72.51878	72.51878	72.51878	1325.04581	918.66423	1325.04581	918.66423
Molar Flow [kgmole/h]	384.14222	384.14210	0.00000	0.00000	30.97001	45.84656	9.98684	9.98685	20.98316	35.85971
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00058	0.00099	0.00131	0.00195	0.00072	0.00108	0.00072	0.00108	0.00072	0.00108
Comp Mole Frac (Toluene)	0.80648	0.91918	0.99867	0.99803	0.99892	0.99849	0.99892	0.99849	0.99892	0.99849
Comp Mole Frac (BiPhenyl)	0.19293	0.07983	0.00002	0.00002	0.00036	0.00043	0.00036	0.00043	0.00036	0.00043

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	bp4		vbp4out		hCRout		bp1		cHEin	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	0.00000	0.00000	0.90653	0.90819	0.90653	0.90819
Temperature [oC]	179.44850	180.54009	179.31080	180.23539	162.50450	170.37906	59.33677	62.90240	59.33677	62.90240
Pressure [Psia]	73.73291	75.21811	72.51878	72.51878	72.51878	72.51878	575.00000	574.99999	575.00000	574.99999
Molar Flow [kgmole/h]	3.06812	2.38436	3.06812	2.38436	27.90223	43.46232	52.09451	150.62936	1907.01505	1814.98870
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.43933	0.43259	0.43933	0.43259
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.46476	0.47214	0.46476	0.47214
Comp Mole Frac (Benzene)	0.00072	0.00108	0.00072	0.00108	0.00072	0.00108	0.00889	0.00821	0.00889	0.00821
Comp Mole Frac (Toluene)	0.99892	0.99849	0.99892	0.99849	0.99892	0.99849	0.08702	0.08706	0.08702	0.08706
Comp Mole Frac (BiPhenyl)	0.00036	0.00043	0.00036	0.00043	0.00036	0.00043	0.00000	0.00001	0.00000	0.00001

Name	bp2		cHE2in		vbp2out		m5out		hHEin	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	177.77622	161.16830	177.77622	161.16830	177.48190	585.38879	579.89169	585.38869	226.89651	210.23067
Pressure [Psia]	543.50458	546.02564	543.50458	546.02564	514.18346	515.81887	514.18346	515.81887	478.64928	480.35638
Molar Flow [kgmole/h]	63.05112	0.00000	1896.05853	1965.61834	63.05112	0.00000	1959.10966	1965.61836	2012.89349	2015.62736
Comp Mole Frac (Hydrogen)	0.43933	0.43259	0.43933	0.43259	0.43933	0.43258	0.43933	0.43259	0.35652	0.35738
Comp Mole Frac (Methane)	0.46476	0.47214	0.46476	0.47214	0.46476	0.47215	0.46476	0.47214	0.52720	0.52766
Comp Mole Frac (Benzene)	0.00889	0.00821	0.00889	0.00821	0.00889	0.00821	0.00889	0.00821	0.09868	0.08904
Comp Mole Frac (Toluene)	0.08702	0.08706	0.08702	0.08706	0.08702	0.08706	0.08702	0.08706	0.01432	0.02393
Comp Mole Frac (BiPhenyl)	0.00000	0.00001	0.00000	0.00001	0.00000	0.00001	0.00000	0.00001	0.00328	0.00199

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	hHE2in		hHE1out		Rin		liq		Purge	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.93807	0.93831	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000
Temperature [oC]	621.03114	621.11111	99.99812	101.12829	621.11003	621.11110	45.00002	45.00000	45.00002	45.00000
Pressure [Psia]	482.71748	484.31374	476.65159	478.43655	504.46899	505.97634	473.43142	475.21786	473.43142	475.21786
Molar Flow [kgmole/h]	2012.89352	2015.62741	2012.89338	2015.62766	1959.10965	1965.61841	223.50097	222.30023	252.58294	225.42406
Comp Mole Frac (Hydrogen)	0.35652	0.35738	0.35652	0.35738	0.43933	0.43259	0.00450	0.00463	0.40048	0.40110
Comp Mole Frac (Methane)	0.52720	0.52766	0.52720	0.52766	0.46476	0.47214	0.04415	0.04469	0.58753	0.58753
Comp Mole Frac (Benzene)	0.09868	0.08904	0.09868	0.08904	0.00889	0.00821	0.79809	0.72457	0.01132	0.01026
Comp Mole Frac (Toluene)	0.01432	0.02393	0.01432	0.02393	0.08702	0.08706	0.12372	0.20806	0.00066	0.00110
Comp Mole Frac (BiPhenyl)	0.00328	0.00199	0.00328	0.00199	0.00000	0.00001	0.02955	0.01804	0.00000	0.00000

Name	gasre		v3out		v5out		d1		p3out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.00000	0.00000	0.02900	0.02948	1.00000	1.00000	0.00000	0.00000
Temperature [oC]	45.00002	45.00000	45.44134	45.44628	45.93626	45.96547	42.71143	47.82184	149.72711	144.22458
Pressure [Psia]	473.43142	475.21786	487.68420	489.26321	150.21204	150.23163	149.99995	150.00327	95.26970	95.92602
Molar Flow [kgmole/h]	1536.80950	1567.90350	53.78379	50.00892	169.71718	172.29130	8.52008	8.83079	410.13404	423.09765
Comp Mole Frac (Hydrogen)	0.40048	0.40110	0.00450	0.00463	0.00450	0.00463	0.08956	0.09045	0.00000	0.00000
Comp Mole Frac (Methane)	0.58753	0.58753	0.04415	0.04469	0.04415	0.04469	0.87910	0.87186	0.00000	0.00000
Comp Mole Frac (Benzene)	0.01132	0.01026	0.79809	0.72457	0.79809	0.72457	0.03121	0.03741	0.00058	0.00099
Comp Mole Frac (Toluene)	0.00066	0.00110	0.12372	0.20806	0.12372	0.20806	0.00012	0.00028	0.80648	0.91918
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.02955	0.01804	0.02955	0.01804	0.00000	0.00000	0.19293	0.07983

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	v8out		v9out		vtb2		tank20out		v14out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.11545	0.11529	0.00000	0.00000	1.00000	1.00000	0.00000	0.00000	1.00000	1.00000
Temperature [oC]	80.84612	80.84600	149.76252	144.25857	149.51195	143.97386	149.51195	143.97386	143.12887	143.12887
Pressure [Psia]	15.00000	15.00006	73.90549	75.47361	32.06274	32.05581	32.06274	32.05581	27.26000	27.26000
Molar Flow [kgmole/h]	135.20573	124.50724	25.99166	38.95439	0.00000	0.00000	410.13404	423.09765	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00002	0.00002	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.99973	0.99968	0.00058	0.00099	0.00142	0.00217	0.00058	0.00099	0.00227	0.00227
Comp Mole Frac (Toluene)	0.00025	0.00030	0.80648	0.91918	0.99271	0.99571	0.80648	0.91918	0.99590	0.99590
Comp Mole Frac (BiPhenyl)	0.00000	0.00000	0.19293	0.07983	0.00587	0.00212	0.19293	0.07983	0.00182	0.00182

Name	v12out		v13out		tov7		p2out		toTop3	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.04590	0.02169
Temperature [oC]	188.91285	188.91285	187.26999	189.31520	187.03170	189.07712	187.30145	189.35207	179.02559	180.03246
Pressure [Psia]	145.54000	145.54000	158.36722	158.38085	150.43885	150.51544	191.64002	191.21287	73.73595	75.22121
Molar Flow [kgmole/h]	0.00000	0.00000	180.59079	180.59152	161.19729	163.46232	180.59079	180.59152	9.98684	9.98685
Comp Mole Frac (Hydrogen)	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00069	0.00069	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00000	0.00000
Comp Mole Frac (Benzene)	0.84341	0.84341	0.83862	0.76168	0.83862	0.76168	0.83862	0.76168	0.00072	0.00108
Comp Mole Frac (Toluene)	0.15522	0.15522	0.13025	0.21929	0.13025	0.21929	0.13025	0.21929	0.99892	0.99849
Comp Mole Frac (BiPhenyl)	0.00068	0.00068	0.03111	0.01901	0.03111	0.01901	0.03111	0.01901	0.00036	0.00043

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	hotout5		v17out		v16out		v11out		V2out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	0.04590	0.02169	1.00000	1.00000	0.00000	0.00000	0.00000	0.00000
Temperature [oC]	178.17558	178.16253	179.02559	180.03246	177.59344	177.59344	185.23387	182.86651	30.22984	30.22984
Pressure [Psia]	72.51878	72.51878	73.73595	75.22121	67.51885	67.51885	575.00000	574.99999	575.00000	574.99999
Molar Flow [kgmole/h]	30.97035	45.84668	9.98684	9.98685	0.00000	0.00000	20.98316	35.85971	148.51277	133.58735
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Benzene)	0.00072	0.00108	0.00072	0.00108	0.00204	0.00204	0.00072	0.00108	0.00000	0.00000
Comp Mole Frac (Toluene)	0.99892	0.99849	0.99892	0.99849	0.99794	0.99794	0.99892	0.99849	1.00000	1.00000
Comp Mole Frac (BiPhenyl)	0.00036	0.00043	0.00036	0.00043	0.00002	0.00002	0.00036	0.00043	0.00000	0.00000

Name	Retol		hCRint		vbp1out		cHE1out		m4out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	0.00000	0.00000	1.00000	1.00000	0.90699	0.90863	1.00000	1.00000	1.00000	1.00000
Temperature [oC]	184.62835	182.62064	179.44850	180.54009	59.03084	62.60502	182.37923	173.57443	177.77622	161.16830
Pressure [Psia]	1325.04581	918.66423	73.73291	75.21811	543.50458	546.02564	543.50458	546.02564	543.50458	546.02564
Molar Flow [kgmole/h]	20.98316	35.85971	27.90266	43.46252	52.09451	150.62936	1907.01515	1814.98898	1959.10966	1965.61834
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.43933	0.43259	0.43933	0.43259	0.43933	0.43259
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.46476	0.47214	0.46476	0.47214	0.46476	0.47214
Comp Mole Frac (Benzene)	0.00072	0.00108	0.00072	0.00108	0.00889	0.00821	0.00889	0.00821	0.00889	0.00821
Comp Mole Frac (Toluene)	0.99892	0.99849	0.99892	0.99849	0.08702	0.08706	0.08702	0.08706	0.08702	0.08706
Comp Mole Frac (BiPhenyl)	0.00036	0.00043	0.00036	0.00043	0.00000	0.00001	0.00000	0.00001	0.00000	0.00001

Table A.3.1 Process data of HDA plant alternative 3 (cont)

Name	toX1		v15out		boil2out		v3out	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Vapour Fraction	1.00000	1.00000	0.05302	0.08780	0.77379	0.87606	0.86847	0.71504
Temperature [oC]	621.03590	621.10998	152.75341	147.93188	186.95826	167.69970	200.66904	194.74614
Pressure [Psia]	487.68420	489.26321	34.04714	34.82847	32.06868	32.06176	151.60530	151.50803
Molar Flow [kgmole/h]	2012.89352	2015.62741	384.14222	384.14210	384.14353	384.14053	180.58956	180.58885
Comp Mole Frac (Hydrogen)	0.35652	0.35738	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.52720	0.52766	0.00000	0.00000	0.00000	0.00000	0.00002	0.00002
Comp Mole Frac (Benzene)	0.09868	0.08904	0.00058	0.00099	0.00058	0.00099	0.83862	0.76168
Comp Mole Frac (Toluene)	0.01432	0.02393	0.80648	0.91918	0.80648	0.91918	0.13025	0.21929
Comp Mole Frac (BiPhenyl)	0.00328	0.00199	0.19293	0.07983	0.19294	0.07983	0.03111	0.01901

Table A.3.2 Energy stream data of HDA plant alternative 3

Name	qfur		qcooler		wkcomp		wkp1		qc1	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	3226.60825	3196.856	1544.07701	1316.234	3.96507	3.97539	466.85956	466.86151	4282.62984	4280.668

Name	qc2		wkp3		qr3		wkp4		wkp2	
	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	3.99249	3.99861	0.96088	0.95807	325.2676	722.00380	381.368	845.13	315.36413	278.21422

Name	qar2		qar1	
	steady state	dynamic	steady state	dynamic
Heat Flow (kw)	103.58299	105.667	9.02037	9.08662

APPENDIX B

HDA Process Equipment Data

Table B.1.1 Column specifications of HDA plant alternative 1

Detail	Stabilizer column		Product column		Recycle column	
	steady state	dynamic	steady state	dynamic	steady state	dynamic
Inlet stream	v5out	v5out	v7out	v7out	v9out	v9out
Top Pressure [psia]	150.00000	150.00000	30.00000	30.00000	30.00000	30.00000
Bottom Pressure [psia]	153.00000	150.55504	33.00000	32.25611	33.00000	32.25611
Top Temperature [C]	48.88889	48.88889	106.66667	106.66667	139.44444	139.44444
Bottom Temperature [C]	193.33333	193.33333	147.77778	147.77778	292.70000	293.33333
Condenser Duty (kW)	179.97338	176.92956	4004.06811	4066.96295	425.10275	329.77434
Reboiler Duty (kW)	1259.36518	1228.63573	3413.32958	3479.53942	469.40104	390.75457
Specification	Benzene mole fraction in overhead = 0.042		Toluene mole fraction in overhead = 0.0003		Diphenyl mole fraction in overhead = 0.00002	
	Methane mole fraction in bottoms = 0.000001		Benzene mole fraction in bottoms = 0.0006		Toluene mole fraction in bottoms = 0.00026	
Column model	Distillation	Distillation	Distillation	Distillation	Distillation	Distillation
Number of tray	Column	Column	Column	Column	Column	Column
Feed tray	6.00000	6.00000	27.00000	27.00000	7.00000	7.00000
Diameter (m)	3.00000	3.00000	15.00000	15.00000	5.00000	5.00000
Weir length (m)	1.06680	1.06680	1.82900	1.82900	0.76200	0.76200
Weir height (m)	0.88420	0.88420	1.26500	1.26500	0.51810	0.51810
Tray spacing (m)	0.05080	0.05080	0.05080	0.05080	0.05080	0.05080
Tray type	0.60960	0.60960	0.60960	0.60960	0.60960	0.60960
Reboiler vol. (m3)	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve
Condenser vol. (m3)	7.07900	9.36194	9.06139	11.98420	1.41584	1.87178
	0.28317	0.37454	8.49505	11.23534	2.83168	3.74749

Table B.1.2 Plug Flow Reactor specification of HDA plant alternative 1

Detail	PFR	
	steady state	dynamic
Pressure Drop [Psia]	17.00000	17.00014
Total Volume [m^3]	115.13183	115.13183
Length [m]	17.37360	17.37360
Diameter [m]	2.90474	2.90474

Table B.1.3 Heat Exchanger specification of HDA plant alternative 1

Detail	FEHE1	
	steady state	dynamic
Shell Inlet Temperature [C]	621.06708	621.11096
Shell Outlet Temperature [C]	119.43767	123.55475
Shell Side Pressure Drop [Psia]	6.00000	6.00000
Tube Inlet Temperature [C]	63.51789	61.10720
Tube Outlet Temperature [C]	609.99576	610.32853
Tube Side Pressure Drop [Psi]	62.00000	62.00001
LMTD [C]	33.88057	33.88057
UA [kJ/C-h]	1859165	10900000
Duty [kW]	17493.84800	17419.17216
Shell Side Volume [m^3]	14.15842	16.28219
Tube Side Volume [m^3]	14.15842	16.28219

Table B.1.4 Separator specification of HDA plant alternative 1

Detail	Sep	
	steady state	dynamic
Vessel Temperature [C]	45.00000	45.00003
Vessel Pressure [Psia]	476.80011	475.85867
Liquid Molar Flow [kgmole/h]	220.99188	222.56534
Liquid Volume [m^3]	-	1.13270
vessel Volume [m^3]	2.26535	2.60475

Table B.1.5 Furnace and Heater specification of HDA plant alternative 1

Detail	Furnace		X1	
	steady state	dynamic	steady state	dynamic
Feed Temperature [C]	584.02005	579.24956	-	621.11111
Product Temperature [C]	621.11111	621.11113	-	621.11111
Duty [kW]	1388.74257	1566.52153	-	0.00000
Volumn [m^3]	8.49505	11.23471	-	14.15842

Table B.1.6 Cooler specification of HDA plant alternative 1

Detail	Cooler	
	steady state	dynamic
Feed Temperature [C]	119.43767	123.55570
Product Temperature [C]	45.00000	45.00002
Duty [kW]	3189.62956	3434.08680
Volumn [m^3]	8.50000	8.50000

Table B.1.7 Parameter tuning of HDA plant alternative 1

Name	FCTol	PCG	CCG
controlled variable	total toluene flow rate : 168.62 kgmole/hr	gas recycle pressure : 605 Psia	methane in gas recycle : 0.5894 molefrac
output target object	valve : V2	valve : V1	valve : V4
OP [%]	50.2202	49.99795081	49.9890205
Gain	0.2000	1.9	0.2
Ti	18	6	1020
Control Action	Reverse	Reverse	Direct
Name	TCR	TCS	TCE1c
controlled variable	reactor inlet temperature : 621.1 °C	separator temperature : 45 °C	furnace inlet temperature : 584 °C
output target object	furnace duty (qfur)	cooler duty (qcooler)	valve : VBP1
OP [%]	17.74562391	28.67168308	51.20399692
Gain	0.14869318	0.124104479	0.399
Ti	12.79256197	12.86656302	5.88
Control Action	Reverse	Direct	Direct
Name	LCS	PC1	TC1
controlled variable	separator liquid level : 50 % level	column C1 pressure : 150 Psia	column C1 tray-6 temp : 153.9 °C
output target object	valve : V5	valve : V6	reboiler duty (qr1)
OP [%]	50.00022643	50.00592924	48.60364592
Gain	2	1	2
Ti	-	600	720
Control Action	Direct	Direct	Reverse

Table B.1.7 Parameter tuning of HDA plant alternative 1 (cont)

Name	LC12	PC2	TC2
controlled variable	column C1 reflux drum level 50 % level	column C2 pressure : 30 Psia	column C2 tray-12 temp : 120.5 $_{o}$C
output target object	column C1 condenser duty (qc1)	column C2 condenser duty (qc2)	column C2 reboiler duty (qr2)
OP [%]	30.71522343	52.32830556	50.76094552
Gain	2	1	2
Ti	-	600	480
Control Action	Reverse	Direct	Reverse
Name	LC22	PC3	TC3
controlled variable	column C2 reflux drum level 50 % level	column C3pressure : 30 Psia	avg. C3-tray 1,2,3,4 temp : 228.7 ^{o}C
output target object	valve : V8	column C3 condenser duty (qc3)	valve : V10
OP [%]	49.99754213	8.472953025	49.98528444
Gain	2	1	0.618474697
Ti	-	900	1200
Control Action	Direct	Direct	Direct
Name	LC32	TCQ	TC3
controlled variable	column C3eflux drum level 50 % level	quenched temperature : 621.1 ^{o}C	cooler inlet temperature : 119.6 ^{o}C
output target object	valve : V3	valve : V11	valve : V10
OP [%]	50.08618066	49.99869442	53.0997
Gain	2	0.213366624	0.8700
Ti	-	12.60467805	63.0000
Control Action	Direct	Direct	Direct

Table B.1.7 Parameter tuning of HDA plant alternative 1 (cont)

Name	LC11	LC21	LC31
controlled variable	column C1 base level : 50 % level	column C2base level : 50 % level	column C3base level : 50 % level
output target object	valve : V7	valve : V9	column C3 reboiler duty (qr3)
OP [%]	50.00044091	50.00792184	29.74775984
Gain	2	2	3
Ti	-	-	-
Control Action	Direct	Direct	Direct