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INTERACTION BETWEEN ENERGY INTEGRATION AND CONTROL PERFORMANCE OF HYDRODEALKYLATION PROCESS

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กระบวนการที่มีการเบ็ดเสร็จทางด้านพลังงานเป็นการพัฒนาประสิทธิภาพทางเทอร์โมไดนามิกส์ของกระบวนการ เป็นผลให้เกิดการลดค่าใช้จ่าย วิธีการหนึ่งที่ใช้คือ การติดตั้งเครื่องแลกเปลี่ยนความร้อนเพื่อนำความร้อนจากสายร้อนที่ออกจากหน่วยให้ความร้อนภายในกระบวนการ เช่น ความร้อนจากปฏิกิริยาคายความร้อนภายในเครื่องปฏิกรณ์ มาถ่ายโอนความร้อนให้กับสายเย็นที่กำลังจะเข้าสู่แหล่งความร้อนนั้นเพื่อลดพลังงานที่จะต้องเพิ่มเติมจากแหล่งพลังงานภายนอกกระบวนการ เช่น เตาเผา ที่จะต้องทำหน้าที่เพิ่มพลังงานความร้อนต่อไปให้ได้อุณหภูมิสูงขึ้นถึงที่ต้องการ เครื่องแลกเปลี่ยนความร้อนที่กล่าวมานี้เรียกว่า “feed-effluent heat exchanger” ซึ่งถูกนำมาใช้ในกระบวนการมากมาย เช่น ในกระบวนการไฮโดรดีอัลคีลเลชัน แต่การนำพลังงานกลับมาใช้ใหม่นี้ส่งผลให้เกิดการยากในการควบคุม วัตถุประสงค์ในงานวิจัยนี้ เพื่อที่จะศึกษาระดับของการเบ็ดเสร็จของพลังงานและพลังงานที่วนอยู่ในกระบวนการ (Q3) ต่างๆกันว่ามีผลอย่างไรต่อสมรรถนะการควบคุมในกระบวนการไฮโดรดีอัลคีลเลชัน ซึ่งจะมีการออกแบบให้กระบวนการมีระดับพลังงานวนอยู่ในกระบวนการต่างๆกันในกระบวนการไฮโดรดีอัลคีลเลชันในทางเลือกที่หก โดยได้มีการนำแนวความคิดทางด้านเส้นทางการไหลของความร้อน “heat pathways” เข้ามาช่วยในการวิเคราะห์ จากนั้นจะมีการประเมินสมรรถนะการควบคุมของกระบวนการเหล่านั้นจากโครงสร้างการควบคุมต่างกันสองแบบ “Overall effectiveness” ที่ได้จากการพัฒนาสมการขึ้นใหม่ให้อยู่ในรูปแบบทั่วไปถูกนำมาสัมพันธ์กับระดับพลังงานที่วนอยู่ในกระบวนการ ผลที่ได้คือ สมรรถนะการควบคุมจะแย่ขึ้นไปตามระดับพลังงานที่วนอยู่ในกระบวนการที่มากขึ้น และได้ใช้ค่าต่ำสุดของอัตราส่วนระหว่าง IAE/Q3 เป็นตัวชี้ถึงระดับพลังงานที่ดีที่สุดสำหรับกรณีศึกษาในงานวิจัยนี้ และการมี “feed-effluent heat exchanger” เปรียบเหมือนการมีถังพักที่สามารถลดความรุนแรงของตัวรบกวนระบบที่ผ่านมาได้ ตัวชี้วัดระดับของพลังงานที่วนอยู่ในกระบวนการที่ใช้ (Overall effectiveness) ที่ได้จากการพัฒนาสมการขึ้นใหม่ให้อยู่ในรูปแบบทั่วไปสามารถเป็นตัวแทนได้ดีกว่า สำหรับโครงสร้างการควบคุมที่สองที่มีการใช้ตัวควบคุมสัดส่วนระหว่างสารป้อนไฮโดรเจน/โทลูอีน จะให้แนวโน้มของระดับของพลังงานที่วนอยู่ในกระบวนการที่มีต่อสมรรถนะการควบคุมเช่นเดียวกับโครงสร้างการควบคุมแรก และให้การควบคุมที่ดีกว่าในลูปควบคุมที่มีความเกี่ยวเนื่องกับสารเหล่านั้นโดยตรง

ภาควิชา.......วิศวกรรมเคมี...................ลายมือชื่อนิสิต..........พัชรี คุณสวัสดิ์..........................
สาขาวิชา...... วิศวกรรมเคมี...................ลายมือชื่ออาจารย์ที่ปรึกษา......................................
ปีการศึกษา...........2549..............

##4870399821 : MAJOR CHEMICAL ENGINEERING

KEY WORD: HDA PROCESS / HEAT PATHWAY /
CONTROL PERFORMANCE / ENERGY INTEGRATION

PATCHAREE KUNSAWAD: INTERACTION BETWEEN ENERGY INTEGRATION AND CONTROL PERFORMANCE OF HYDRODEALKYLATION PROCESS. THESIS ADVISOR: ASST. PROF. MONTREE WONGSRI, D.Sc., 147 pp. ISBN 974-14-2942-8.

The use of energy integration is to improve thermodynamic efficiency of a process. This translates into a reduction in utility cost. Thus, it is common practice to install feed-effluent design 2-6 exchangers around reactors and distillation columns as Hydrodealkylation of Toluene (HDA) process (alternative 6). Positive feedback can occur and make the plants more difficult to control. The objective of this research was to study the effect of levels of energy integration and energy maintained within the process on control performance of energy integrated Hydrodealkylation of toluene (HDA) process. The ideas of Luyben's heat pathways were taken into account in order to get insight of the roles of heat pathways and their effects on the control performance. These ideas helped us to design several levels of energy maintained within the process (third pathway, Q3) for HDA process and evaluate the control performance quantitatively. Design Alternative 6 was chosen for our case studies. The performances of those designed processes were evaluated dynamically with two different control structures. The corrected overall effectiveness was used to relate with energy maintained within the process (Q3). Results showed that the designed process maintaining most of energy within the process gave poorer control performance and the lowest ratio of IAE/Q3 was referred to indicate optimum Q3 in this work. Having FEHEs could attenuate the disturbances because it behaved like buffer tanks. The corrected overall effectiveness was used to evaluate the design and control more accurately. When ratio control (CS2) was used to keep hydrogen/toluene constant, gave the same trend of the effect of levels of energy maintained within the process on control performance and also gave the smoother operations in control loop relating to the those reactants.

Department Chemical Engineering Student's signature....Patcharee Kunsawad
Field of study Chemical Engineering Advisor's signature...Montree Wongsri
Academic year 2006

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NOMENCLATURES

ϵ	thermodynamic effectiveness
ϵ_o	overall effectiveness
ϵ_1,ϵ_2,ϵ_3	effectiveness of the third FEHE, the second FEHE and the first FEHE, respectively.
$\epsilon_{ex,1}$,$\epsilon_{ex,2}$,$\epsilon_{ex,3,1}$,$\epsilon_{ex,3,2}$	effectiveness of the steam generator at positive feedback loop, the recycle column reboiler, and the stabilizer and product column reboiler, respectively.
K_R	reactor gain
τ_R	reactor time constant
G_R	reactor transfer function

CHAPTER I

INTRODUCTION

1.1 Importance and reasons for research

Energy conservation has always been important in process design. Use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost. Thus, it was common practice to install feed-effluent exchangers around reactors and distillation columns as Hydrodealkylation of toluene (HDA) process (alternative 6). Positive feedback can occur and makes the plants more difficult to control (Luyben, 1999). There are conflicts between steady-state economics and dynamic controllability. Luyben (1999) has mentioned three different ”heat pathways” and their illustration of HDA process. The first pathway is from inside the process and flows out to the environment through cooler. The second pathway carries heat from utilities into the process and flows out to the environment through three reboilers. The third pathway is internal to the process. Here heat flows back and forth between different unit operations. However, we cannot specify exactly where heat source of dissipated heat to any available heat sinks is. In addition, studies of the effect of levels of energy maintained within the process (Q3) on control performance have not been done. We report the results of the effect of levels of energy integration and energy maintained within the process on control performance in which we evaluated from seven designed case studies and the ideas of heat pathways are taken into account in order to get insight of the roles of heat pathways and their effects on the control performance. These help us to design levels of energy maintained within the process for our case studies.

1.2 Research objectives

To study the effect of levels of energy integration on control performance of energy integrated hydrodealkylation of toluene (HDA) process.

1.3 Scope of research

1. Simulation of hydrodealkylation of toluene (HDA) process of seven case studies is performed using the commercial software, HYSYS.PLANT.
2. The process descriptions of HDA are obtained from Douglas (1988).
3. The designed plants are evaluated dynamically.

1.4 Contribution of Research

The effect of energy integration on control performance of energy integrated hydrodealkylation of toluene (HDA) process.

1.5 Procedure Plan

1. Study plantwide process control and heat pathways theory.
2. Design and model different levels of energy maintained within the process (path 3) of HDA process (alternative6); model HDA process (alternative 1) and HDA process (NO FEHE) in steady state.
3. Study method of tuning parameters for controlling in HYSYS.
4. Continue to dynamic simulation.
5. Assess the performance of the designed processes.
6. Analyze effect of levels of energy integration on control performance and summarize the results.
7. Do full thesis report.

This thesis is divided into seven chapters.

Chapter I is an introduction to this research. This chapter consists of research objective, scope of research, contribution of research, and procedure plan.

Chapter II reviews the work carried out on plantwide control and heat integrated processes.

Chapter III gives some background information about plantwide process control.

Chapter IV gives some background information about heat exchanger and energy management.

Chapter V describes the process description in HDA process.

Chapter VI shows the study of level of energy in the process and describes the effect of level of energy integration on control performance.

Chapter VII presents the conclusion of this research and makes the recommendations for future work.

This is follow by:

References

Appendix A: HDA Process Stream and Equipment Data
Appendix B: Parameter Tuning of Control Structures
Appendix C: Dynamic Responses

CHAPTER II

LITERATURE REVIEW

Plantwide control and Heat-integrated process

Douglas et al. (1962) studied design and control of feed-effluent, exchanger-reactor systems. A dynamic study of the system indicated that the desired steady-state conditions were metastable. However, a feedback proportional controller could be used to stabilize the process. Computations were made to determine the effect of various controller gains, positions of the sensing element, and time lags in the feedback loop. They found that a proportional controller with a fast-acting feedback loop could be used to provide adequate control of a metastable condition. And best control was obtained by locating the sensing element at a position where the reaction rate, rather than the heat transfer rate, was predominant.

Handogo and Luyben (1987) studied design and control of a heat-integrated reactor/column process. An exothermic reactor was the heat source, and a distillation column reboiler was the heat sink. Indirect and direct heat-integration schemes were studied. In the indirect heat-integration system, the reactor was cooled by generating steam, which was then used as the heating medium for the reboiler. In the direct heat-integration system, the reactor liquid was circulated directly through the distillation column reboiler. The indirect heat-integration system was found to have several advantages over the direct heat-integration system in terms of its dynamic performance. Both systems were operable for both large and small temperature differences between the reactor and the column base. Somewhat unexpectedly, the heat-integration system with a small temperature difference was found to be more controllable than a system with a large temperature difference. However, the cost of the heat exchanger increased rapidly as the temperature difference decreased. The minimum economic temperature difference appears to be about 60 ^{O}C. Changing kinetic parameters, such as the activation energy, did not have a drastic effect on the overall dynamic performance of either the indirect or direct heat-integration systems.

Terrill and Douglas (1987a,b,c) developed 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 29-43 % 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. After that Shih-Wen Lina, Cheng-Ching Yub (2004) analyzed the tradeoff between steady-state economics and dynamic controllability for heat-integrated recycle plants. The process consists of one reactor, two distillation columns, and two recycle streams first studied by Tyreus and Luyben which the two distillation columns was heat integrated. Results show that the steady-state controllability deteriorates gradually as the degree of heat integration increases. However, if the recycle plant is optimally designed, acceptable turndown ratio is observed and little tradeoff between steady-state economics and dynamic operability may result. The results reveal that improved control can be achieved for well-designed heat-integrated recycle plants (compared to the plants without energy integration). More importantly, better performance is achieved with up to 40 % energy saving and close to 20 % saving in total annual cost.

Luyben et al. (1997) presented a general heuristic design procedure for plantwide process control. Their nine steps of the proposed procedure center around the undamental principles of plantwide control: 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.

Luyben (1999) discerned three different heat pathways in the process and classified it in the Hydrodealkylation process (alt.6). The first pathway is from inside the process and flows out to the environment through cooler. The second pathway carries heat from utilities into the process and flows out to the environment through three reboilers. The third pathway is internal to the process. Here heat flows back and forth between different unit operations.

Chen and Yu (2000) quantified the relationship between thermal efficiency and dynamic controllability. For a given feed-effluent heat exchanger (FEHE), relationships between the degree of heat recovery and open-loop poles were derived. Since the controllability was characterized by the pole locations. Achievable closed-loop performance of heat integrated systems could also be evaluated. Internal as well as external energy load disrurbances were compared. The results showed that Increased heat integration deteriorated control performance under internal disturbances (source of the disturbances was in the positive feedback loop) but gave better performance for external disturbances (source of the disturbances came from outside).

Qiu et al. (2002) a rigorous model for the hydrodealkylation of toluene (HDA) process was developed using the commercial software, HYSYS.PLANT. After reviewing the reported methods for plant-wide control, a systematic method, namely, Control Configuration Design (CCD) method, was selected for application to the HDA process. The resulting control structures from the application of this method were evaluated and compared through rigorous dynamic simulation. The results showed that the CCD method successfully yields workable base-level regulatory control structures for the HDA process. The control structures obtained by the CCD method were also compared with that reported by Luyben et al. (Plant-wide Process Control, McGraw-Hill, 1999) using their nine-step method.

Kietwarin (2002) presented a comparison among four control structures designed for withstanding disturbances that caused production rate change. The changes have 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 accordingly. The second was modified from the first scheme by added a cooling unit to controlled the outlet temperature from the reactor. In the third scheme, a ratio was introduced to the second control scheme for controlling the ration of hydrogen and toluene within the process. These three control structures were compared with reference control structure on plantwide process control book, Luyben (1999) , and shown better performances.

Chen and Yu (2003) quantified the controllability of a complex heat-integrated reactor. First, a systematic approach was proposed to model the complex heat-integrated reactors. A simple measure, the overall effectiveness, could be derived directly from the flowsheet. Because a loss of controllability came from the positive feedback loop, several design parameters were studied, and design heuristic were proposed to improve the controllability of heat-integration schemes. The results showed that some of the complex heat-integrated reactor were indeed more controllable than the simpler heat-integration schemes.

Thaicharoen (2004) presented the new control structures for the hydrodealkylation of toluene process with energy integration schemes alternative 3. Five control structures had been designed, tested and compared the performance with Luyben's control structure (CS1). The results showed that hydrodealkylation of toluene process with energy integration could reduce energy cost. Furthermore, this process could be operated well by using plantwide methodology to design the control structure. The dynamic responses of the designed control structures and the reference structure were similar. The CS2 had been limited in bypass, so it was able to handle in small disturbance.The CS3 used auxiliary heater instead of bypass valve to control temperature of stabilizer column. The CS4 used reboiler duty of column to control column temperature giving more effective than bottom flow. The CS5 used on-demand structure. The CS6 had been modified from CS2 and CS4 to optimize energy cost.

Hermawan (2005) developed the new heuristic of selection and manipulation heat pathway called heat pathway heuristic (HPH) for plantwide control.

A selective controller i.e. a low override switch (LOS) was employed in order to select an appropriate heat pathway through the process to carry the associated load to a utility unit. In order to evaluate the dynamic performance of the control system, some disturbances were made. The results revealed that the complex energy integration deteriorated the dynamic performances of the process. The new designed plantwide control structure for HDA process was also compared with the earlier work given by Luyben et al. (1999). In general, better responses of the furnace and cooler utility consumptions were achieved compare to the Luyben's control structure. Both furnace and cooler duties could be decreased according to the input disturbance load, since the HPH was applied in the current work. Therefore, the proposed HPH was proven to be useful as in the illustration of the HDA process to achieve DMER.

CHAPTER III

PLANTWIDE PROCESS CONTROL

Most industrial prosesses contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. Recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. They also interconnect separate unit operations and create a path for disturbance propagation. Essentially, the plantwide control problem is how to develop the control loops needed to operate an entire process and achieve its design objectives.

3.1 Integrated Process

Three basic features of integrated chemical process lie at the root of our need to consider the entire plant's control system: (1) the effect of material recycle, (2) the effect of energy integration, and (3) the need to account for chemical component inventories.

3.1.1 Material recycle

Material is recycled for six basic and important reasons.

1. Increase conversion: 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.

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.

3.1.2 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.

we could theoretically introduce considerably more energy integration into the HDA process (Fig. 3.1). This is a good illustration of how units anywhere in the process can be linked together thermally. This highlights why we cannot combine the control systems of individual unit operations in such processes.

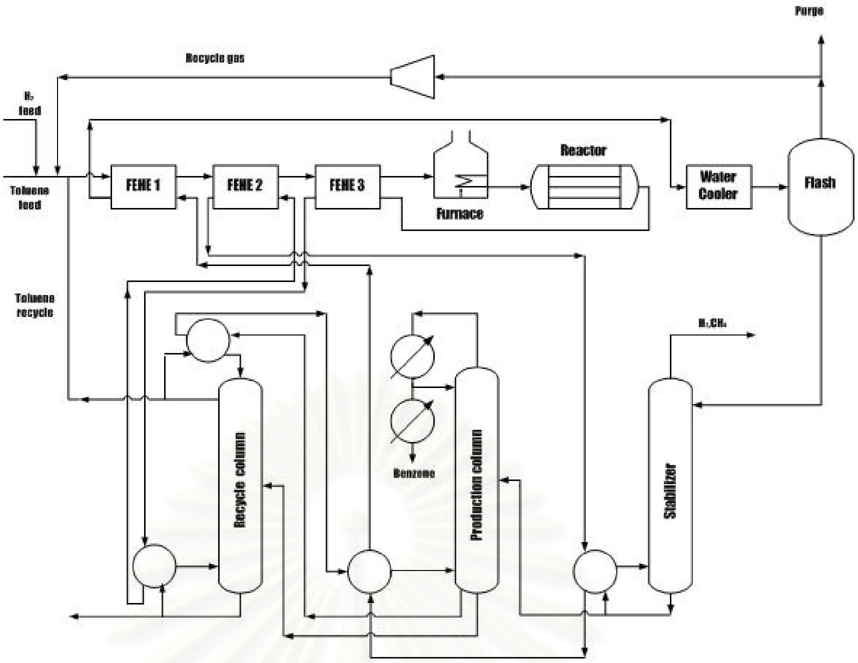


Figure 3.1: HDA process flowsheet with complex heat integration.

3.1.3 Chemical component inventories

We can characterize a plant's chemical species into three types: reactants, products, and inerts. The real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every molecule of reactants fed into the plant must either be consumed or leave as impurity or purge. Because of their value, we want to minimize the loss of reactants exiting the process since this represents a yield penalty. So we prevent reactants from leaving. This means we must ensure that every mole of reactant fed to the process is consumed by the reactions.

3.2 Effects of Recycle

The presence of recycle streams profoundly alters the plant's dynamic and steady-state behavior. In this section it's about two basic effects of recycle: (1) Recycle has an impact on the dynamics of the process. It means that any change in a recycle process can take a long time to line out back to steady state. (2) Recycle leads to the "snowball" effect. That's to say, A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates. These disturbances can lead to even larger dynamic changes in flows, which propagate around the recycle loop. The effective way to prevent the snowball effect is to apply the following plantwide control heuristic:

A stream somewhere in each liquid recycle loop should be flow controlled.

3.3 Partial Control

The term partial control arises because we typically have fewer available manipulators than variables we would like to control. Variables with a large effect are called *dominant*. By controlling the dominant variables in a process, we achieve what is called *partial control*. The setpoints of the partial control loops are then manipulated to hold the important economic objectives in the desired ranges.

Hence a goal of the plantwide control strategy is to handle variability in production rate and in fresh reactant feed compositions while minimizing changes in the feed stream to the separation section.

3.4 Plantwide Control Design Procedure

There is a philosophy that *It is always best to utilize the simplest control system that will achieve the desired objectives.*

The goals for an effective plantwide process control system include

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

3.4.1 Basic Concepts of Plantwide Control

3.4.1.1 Buckley Basic

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

1. Material balance control.

2. Production quality control.

He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loop is established, using the flowrates of liquid and gas process streams. He then proposed establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated as small as possible. The most level controllers should be proportional-only (P) to achieve flow smoothing. The time constants of the liquid level loops are a factor of 10 larger than the product-quality time constants.

3.4.1.2 Douglas doctrines

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Douglas points out that in the typical chemical plant the costs of raw materials and the value of the products are usually much greater than the costs of capital and energy. This leads to two Douglas doctrines.

1. Minimize losses of reactants and products.

2. Maximize flowrates through gas recycle systems.

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

The control structure implication is that we do not attempt to regulate the gas recycle flow and we do not worry about what we control with its manipulation. We simply maximize its flow. This removes one control degree of freedom and simplifies the control problem.

3.4.1.3 Downs drill

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

3.4.1.4 Luyben laws

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

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

3. If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). Even if steady-state economics favor a liquid feed stream, the profitability of an operating plant with a product leaving the bottom of a column may be much better if the feed to column is vaporized.

3.4.1.5 Richardson rule

Bob Richardson 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.

3.3.1.6 Shinskey schemes

Greg Shinskey (1988) has produced a number of "advanced control" structures that permit improvements in dynamic performance.

3.4.1.7 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:

$$K_{ZN} = K_u/2.2 \qquad \tau_{ZN} = P_u/1.2$$
$$K_{TL} = K_u/3.2 \qquad \tau_{TL} = 2.2P_u$$

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

3.4.2 Step of Plantwide Process Control Design Procedure

Step1: Establish control objectives

Assess the steady-state design and dynamic control objects for the process. This is probably the most important aspect of the problem because different control objectives lead to different control structures.

Step 2: Determine control degrees of freedom

Count the number of control valves available.

This is the number of degrees of freedom for control, i.e., the number of variables that can be controlled to setpoint.

Most of these valves will be used to achieve basic regulatory control of the process: (1) set production rate, (2) maintain gas and liquid inventories, (3) control product qualities, and (4) avoid safety and environmental constraints. Any valve that remain after these vital tasks have been accomplished can be utilized to enhance steady-state economic objectives or dynamic controllability (e.g. minimize energy consumption, maximize yield, or reject disturbances).

We may find that we lack suitable manipulators to achieve the desired economic control objectives. Then we must change the process design to obtain additional handles.

Step 3: Establish energy management system

Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system.

We use the term energy management to describe two function

1. We must provide a control system that removes exothermic heats of reaction from the process. If heat is not removed to utilities directly at the reactor, then it can be used elsewhere in the process by other unit operations. This heat, however, must ultimately be dissipated to utilities.

2. If heat integration does occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensure 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 transfer between process streams can create significant interaction. In the case of reactor feed/effluent heat exchangers it can lead to positive feedback and even instability.

Heat integration of a distillation column with other columns or with reactors is widely used in chemical plants to reduce energy consumption. While these designs look great in terms of steady-state economics, they can lead to complex dynamic behavior and poor performance due to recycling of disturbances. If not already included in the design, trim heater/cooler or heat exchanger bypass line 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, we must increase overall reaction rates. This can be accomplished by raising temperature, increasing reactant concentrations, increasing reactor holdup, or increasing reactor pressure. The variable we select must be dominant for the reactor.

Once we identify the dominant variables, we must also identify the manipulators (control valve) that are most suitable to control them.

We often want to select 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.

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.

We should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and deadtimes and large steady-state gains.

It should be note that, since product quality considerations have become more important, so it should be establish the product-quality loops first, before the material balance control structure.

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

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

In most process 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 the recycle loop are controlled by level.

From a dynamic viewpoint, whenever all flows in a recycle loop are set by level controllers, wide dynamic excursions can occur in these flows because the total system inventory is not regulated.

We have to determine what valve should be used to control each inventory variable. Inventories include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should be controlled with the manipulate variable that has the largest effect on it within that unit (Richardson rule).

Gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields (Douglas doctrine).

Step 7: Check component balances

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

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

Hence we are limited to the use of two methods: consuming the reactants by reaction or adjusting their fresh feed flow. The purge rate is adjusted to control the inert composition 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

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

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

CHAPTER IV

HEAT EXCHANGER AND ENERGY MANAGEMENT

The energy would not be an issue if all the processing steps operated at the same constant temperature. Furthermore, since raw materials and products are stored at roughly the same temperature, the net energy requirement for heating and cooling equals the heat losses from the process. We therefore realize that most of the energy required for heating certain streams within the process is matched by a similar amount required for cooling other streams. Heat recovered 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).

4.1 Heat-exchanger networks

The energy integration analysis is the calculation of the minimum heating and cooling requirements for a heat-exchanger network.

Any important rule of thumbs:

1. Do not transfer heat across the pinch.

   If we transfer an amount of heat across the pinch, we must put this additional heat into the process from a hot utility somewhere in the network. Furthermore, we must also reject this amount of heat to a cold utility.

2. Add heat only above the pinch.

3. Cool only below the pinch.

4.2 Feed-Effluent Heat Exchangers (FEHEs)

In an adiabatic reactor, the heat of the exothermic reactions can be recovered by preheating the feed, as shown in Figure 4.1. The reactor outlet stream (T_{out}) is used to heat the feed stream (T_f) to the reaction temperature (T_{in}). The

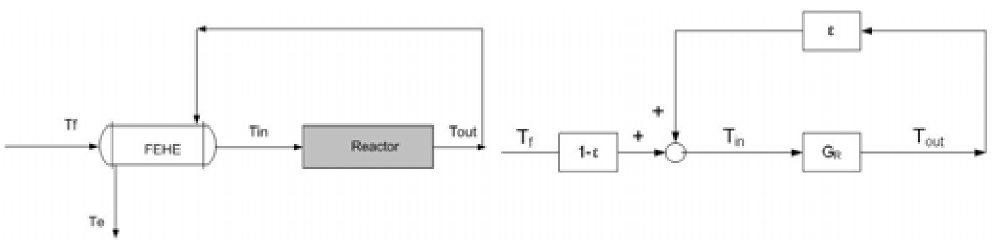


Figure 4.1: Heat-integrated systems with a single FEHE and block diagram.

positive feedback nature resulting from the heat recovery makes the simple FEHE scheme difficult to control as shown below.

The reactor inlet temperature (T_{in}) is related to the feed temperature and the reactor outlet temperature by the following equation:

$$T_{in} = (1-\epsilon)T_f + \epsilon T_{out} \tag{4.1}$$

The reactor is assumed to be a simple open-loop stable system with a time constant τ_R and a reactor gain K_R.

$$G_R = \frac{T_{out}}{T_{in}} = \frac{K_R}{\tau_R s + 1} \tag{4.2}$$

Combining Eq. (4.1) Eq. (4.2) gives:

$$\frac{T_{in}}{T_f} = \frac{1-\epsilon}{1-\epsilon G_R} = \frac{(1-\epsilon/1-\epsilon K_R)(\tau_R s+1)}{(\tau_R/1-\epsilon K_R)s+1} \tag{4.3}$$

The coupled open-loop system has a pole at s=(ϵK_R-1)/τ_R

Observation can be made that the open-loop pole moves to the right-half-plane as percent of energy recovery increases (i.e. as ϵ increases).

4.2.1 Modeling

The thermodynamic effectiveness (ϵ) of a heat exchanger was proposed as an important parameter by Kays and London in the 1940s. The heat exchanger effectiveness is defined as:

$$\epsilon = \left(\frac{actual\ \ heat\ \ transfer}{maximum\ \ possible\ \ heat\ \ transfer}\right) \tag{4.4}$$

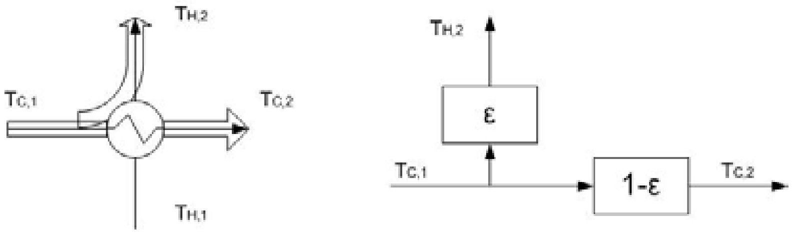


Figure 4.2: Heat exchanger block diagram representation.

The 'maximum possible heat transfer' is attained if one of the fluids experienced a temperature change equal to the maximum temperature difference present in the exchanger:

$$\Delta T_{max} = T_{hi} - T_{ci} \tag{4.5}$$

The fluid to which this happens must have the lower capacity rate, otherwise the temperature change of the other fluid would be larger than this maximum temperature difference, which is clearly impossible.

The maximum possible heat transfer is then

$$Q = (\dot{m}C_p)_{min}(T_{hi} - T_{ci}) \tag{4.6}$$

giving the following expression for the effectiveness of the heat exchanger

$$\epsilon = \frac{(\dot{m}C_p)_H(T_{hi} - T_{ho})}{(\dot{m}C_p)_{min}(T_{hi} - T_{ci})} = \frac{(\dot{m}C_p)_C(T_{co} - T_{ci})}{(\dot{m}C_p)_{min}(T_{hi} - T_{ci})} \tag{4.7}$$

If the hot fluid has the minimum capacity rate

$$\epsilon = \frac{(T_{hi} - T_{ho})}{(T_{hi} - T_{ci})} \tag{4.8}$$

and if the cold fluid has the minimum capacity rate

$$\epsilon = \frac{(T_{co} - T_{ci})}{(T_{hi} - T_{ci})} \tag{4.9}$$

If we know effectiveness, the heat transfer can also be determined,

$$Q = \epsilon(\dot{m}C_p)_{min}(T_{hi} - T_{ci}) \tag{4.10}$$

For a heat exchanger (Fig. 4.2), the effectiveness is defined as

$$\epsilon = \frac{(\dot{m}C_p)_H(T_{H1} - T_{H2})}{(\dot{m}C_p)_{min}(T_{H1} - T_{C1})} = \frac{(\dot{m}C_p)_C(T_{C2} - T_{C1})}{(\dot{m}C_p)_{min}(T_{H1} - T_{C1})} \tag{4.11}$$

Where $(\dot{m}C_p)_H$, $(\dot{m}C_p)_C$, and $(\dot{m}C_p)_{min}$ are the capacity flow rates for the hot stream, the cold stream, and the smaller of the two, respectively. Depending on the heat transfer area,ϵ ranges from 0 (no heat exchangers) to 1 (infinite heat-transfer area). Assuming that the heat capacities of the hot and cold stream are the same, i.e.,C_{pH}=C_{pC} , and because the mass flow rates of the hot and cold streams are identical in an FEHE, equation (4.11) can be rearranged to give

$$T_{C,2} = (1 - \epsilon)T_{C,1} + \epsilon T_{H,1} \tag{4.12}$$

$$T_{H,2} = (1 - \epsilon)T_{H,1} + \epsilon T_{C,1} \tag{4.13}$$

Equations (4.12) and (4.13) describe the propagation of the temperature disturbance as the inlet temperature changes, (Figure 4.2) and they serve as the basic formula for the construction of more complex schemes as shown in chapter 6.

4.3 Heat pathways

There are three different "heat pathways" in the process (Luyben, 1999). See Fig. 4.3 for an illustration.

The first pathway is from inside the process and flows out. It is of course possible to convert some of the heat to work as it is removed from high temperatures in the process.

The second pathway carries heat from utilities into the process. Mechanical work is extracted from the heat as it flows from a high supply temperature to the lower temperature of the environment.

The third pathway is internal to the process. Here heat flows back and forth between different unit operations. 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.

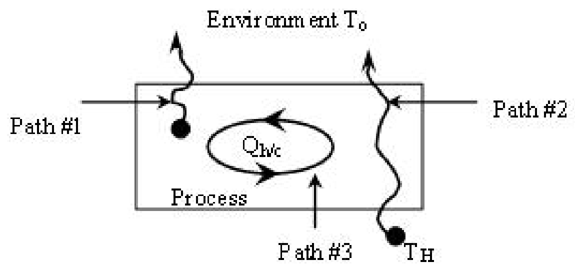


Figure 4.3: Heat pathways.

4.3.1 Identification the three heat pathways in HDA process

Path 1 is intended to carry heat from exothermic reactions that must be dissipated from the process. This path, shown in Fig. 4.4, goes through all three distillation column reboilers as well as the three preheaters before it terminates in the water cooler.

Path 2, shown in Fig. 4.5, conveys heat to the distillation columns. This heat covers the thermodynamic work requirement for the separations. In Alternative 6 for the HDA process all the heat needed to run the process is supplied by the furnace. Heat intended for the columns must travel through the reactor and the preheaters before it reaches its destinations in the three condensers.

Path 3, shown in Fig. 4.6, is the heating and cooling circuit that starts from the reactor exit and goes through the preheaters and column reboilers. In the preheaters the hot streams give up most of their enthalpy to the incoming cold feed streams that travel back to the reactor. The third path also connects the reactor to the separation section thus creating the potential for interaction.

4.4 Control of utility exchangers

The purpose of unit operation controls is to regulate the amount of energy supplied or removed. This is typically done by measuring a temperature in the process and manipulating the flowrate of utility. A PI-controller is adequate in most instances. The location of the temperature measurement depends upon the

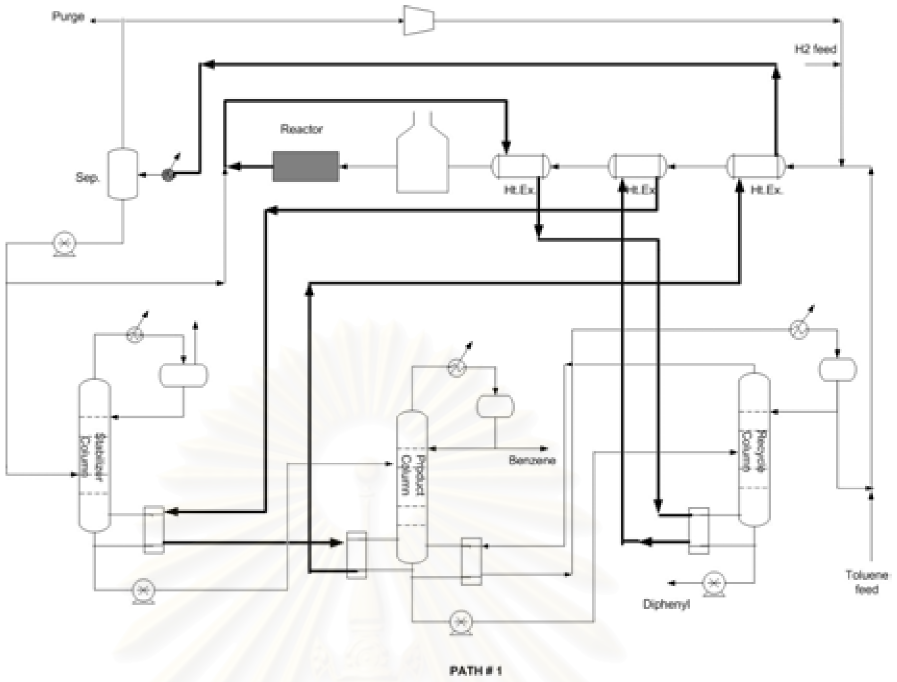


Figure 4.4: HDA process path of exothermic reaction heat.

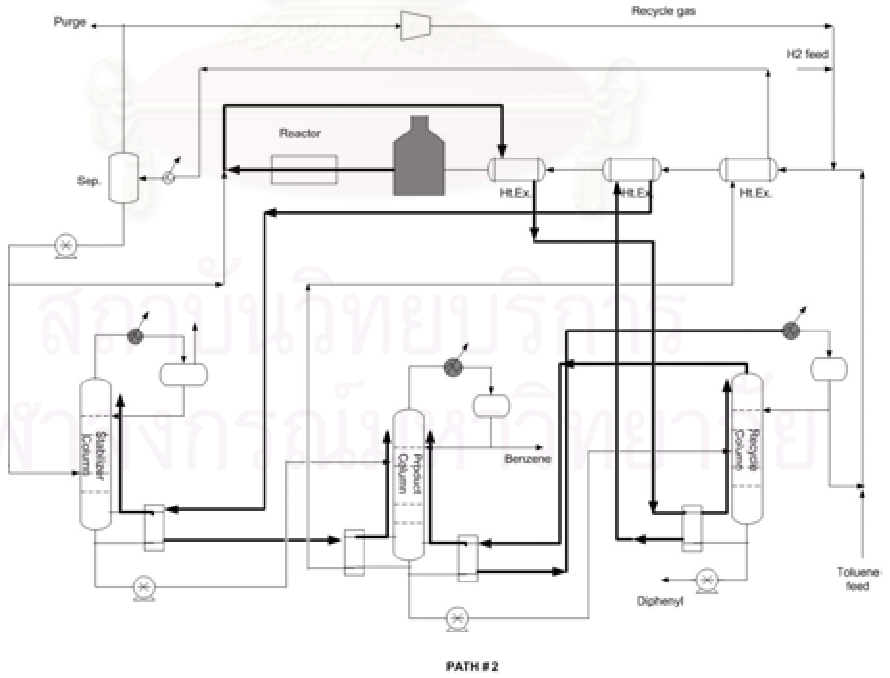


Figure 4.5: HDA process path of heat supply to distillation columns.

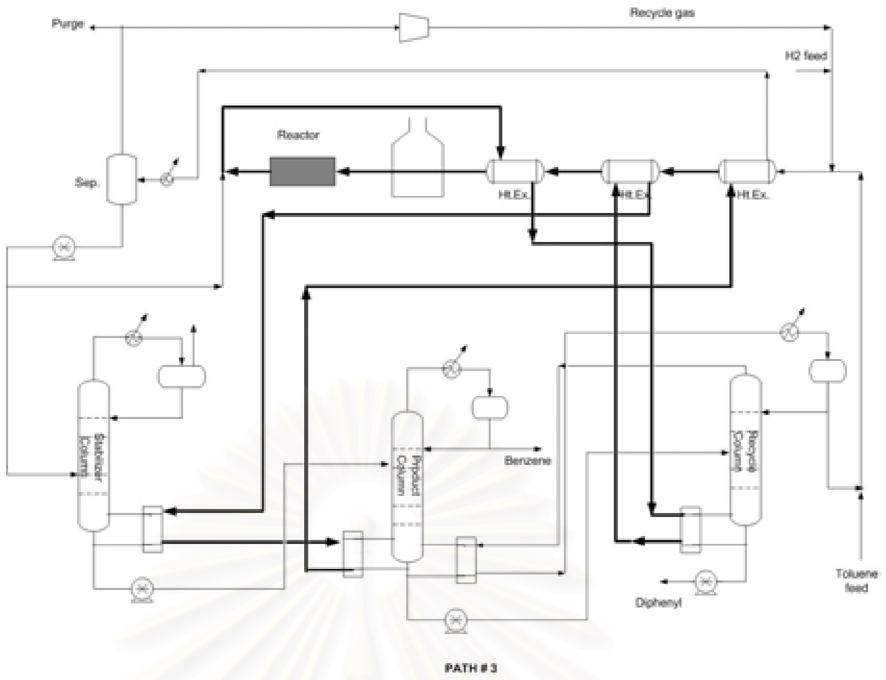


Figure 4.6: HDA process path of heat used internally for stream heating and cooling.

purpose of the heat exchange. The control point should be located where the effects of the added energy are felt the most.

4.5 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provided we can independently manipulate the two inlet flowrates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom for temperature control. We can restore one of these degrees of freedom fairly easily. It is possible to oversize the P/P exchanger and provide a controlled bypass around it as in Fig. 4.7 a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig 4.7 b.

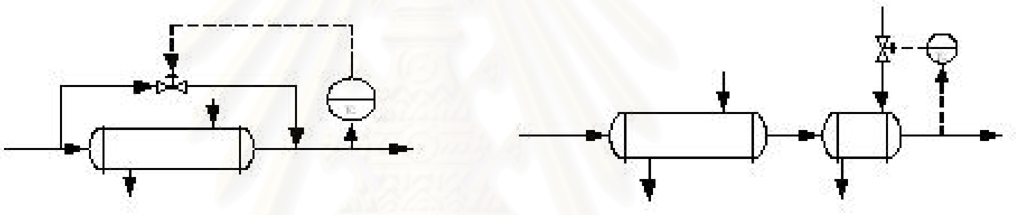


Figure 4.7: Control of P/P heat exchangers (a) Use of bypass; (b) use of auxiliary utility exchanger.

CHAPTER V

HYDRODEALKYLATION PROCESS

5.1 Process Description

Figure 5.1 shows the nine basic unit operations of the hydrodealkylation of toluene (HDA) process as described in Douglas (1988): 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

$$\text{Toluene} + \text{H}_2 \rightarrow \text{Benzene} + \text{CH}_4$$
$$2\text{Benzene} \leftrightarrow \text{Diphenyl} + \text{H}_2$$

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:

$$r_1 = 3.6858 \times 10^6 exp(\frac{-25616}{T}) p_T p_H^{1/2} \tag{5.1}$$

$$r_2 = 5.987 \times 10^4 exp(\frac{-25616}{T}) p_B^2 - 2.553 \times 10^5 exp(\frac{-25616}{T}) p_D p_H \tag{5.2}$$

Where r_1 and r_2 have units of lb*mol/(min*ft3) and T is the absolute temperature in Kelvin. The heats of reaction given by Douglas (1988) are -21500 Btu/lb*mol of toluene for 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.

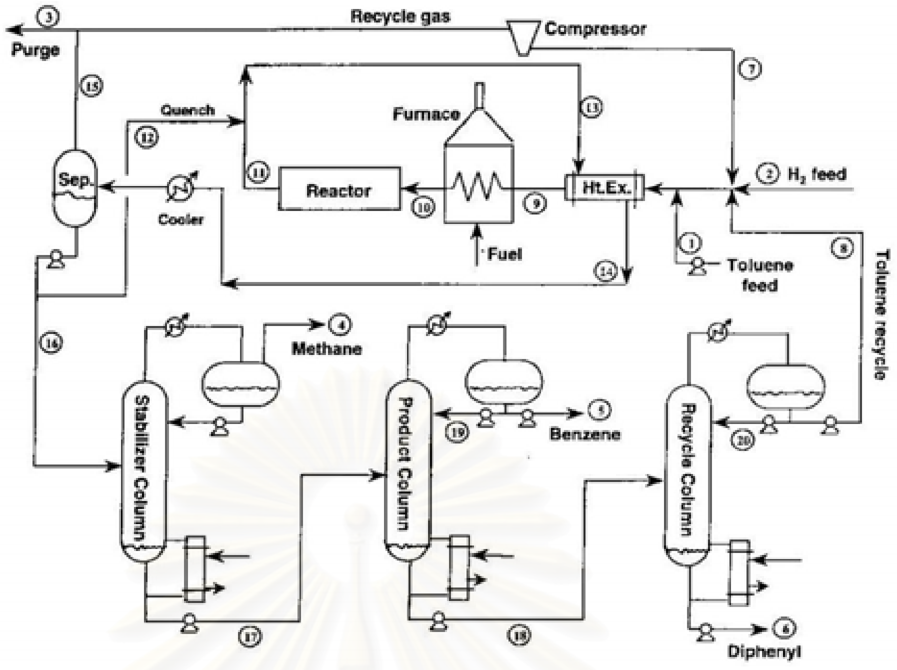


Figure 5.1: Hydrodealkylation of toluene (HDA) process flowsheet.

The liquid stream from the separator (after part is taken for the quench) is fed to the stabilizer column, which has a partial condenser components. 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.

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

Table 5.1 Equipment data and specifications of HDA process

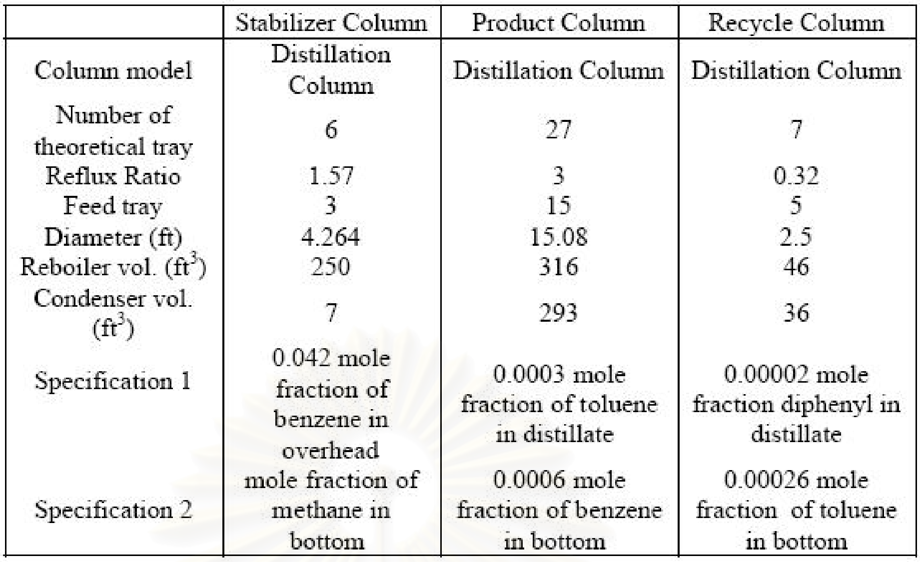
Reactor	Diameter (ft) Length (ft) Number of tubes	9.53 57 1	Exchanger (E1)	Shell volume (ft^3) Tube volume (ft^3)	500 500
Exchanger (E2)	Shell volume (ft^3) Tube volume (ft^3)	500 500	Exchanger (E3)	Shell volume (ft^3) Tube volume (ft^3)	500 500
Heater (E4)	Tube volume (ft^3)	60	Exchanger (E5)	Shell volume (ft^3) Tube volume (ft^3)	100 100
Cooler	Tube volume (ft^3)	300	Furnace	Tube volume (ft^3)	300
Separator	Volume (ft^3)	80	Aux	Tube volume (ft^3)	30

5.2 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 5.1 presents the data and specifications for the equipment employed other than the three columns. For our simulation, Peng-Robinson model is selected for physical property calculations because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions. The reaction kinetics of both reactions are modeled with standard Arrhenius kinetic expressions available in HYSYS.PLANT, and the kinetic data are taken from Luyben et al. (1998). Since there are four material recycles, four RECYCLE operations are inserted in the streams, Hot-In, Gas-Recycle, Quench, and Stabilizer-Feed (Fig.5.1). 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

Table 5.2 Column specifications of HDA process



	Stabilizer Column	Product Column	Recycle Column
Column model	Distillation Column	Distillation Column	Distillation Column
Number of theoretical tray	6	27	7
Reflux Ratio	1.57	3	0.32
Feed tray	3	15	5
Diameter (ft)	4.264	15.08	2.5
Reboiler vol. (ft^3)	250	316	46
Condenser vol. (ft^3)	7	293	36
Specification 1	0.042 mole fraction of benzene in overhead	0.0003 mole fraction of toluene in distillate	0.00002 mole fraction diphenyl in distillate
Specification 2	mole fraction of methane in bottom	0.0006 mole fraction of benzene in bottom	0.00026 mole fraction of toluene in bottom

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 5.2 This table also includes details of trays, which are required for dynamic modeling. The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on Glitsch design parameters for valve trays. Though the tray diameter and spacing, and weir length and height are not required in steady-state modeling, they are required for dynamic simulation.

Results from steady-state simulation are found to be consistent with those in Luyben et al. (1998) However, there are also some differences: for example, flow rates of reflux stream in product columns in our case is smaller than those in Luyben et al. (1998) and flow rates of reflux stream in recycle columns is larger than those in the earlier study. The possible reasons for these differences may be that: in Luyben et al. (1998), vapor-liquid equilibrium behavior was assumed to be ideal and the stabilizer column was modeled as a component splitter and tank; but our simulation employs Peng-Robinson equation of state and the stabilizer column is modeled rigorously. The operating pressure for this column is chosen as more than the design information in Luyben (1998). Thus the pressures for the streams around stabilizer column are different.

CHAPTER VI

THE EFFECT OF LEVELS OF ENERGY INTEGRATION ON CONTROL PERFORMANCE

6.1 Steady state study of level of energy

6.1.1 Pinch temperature analysis

The energy integration analysis is the calculation of the minimum heating and cooling requirements for a heat-exchanger network. The Problem Table Method is applied to find pinch temperature and reach maximum energy recovery (MER).

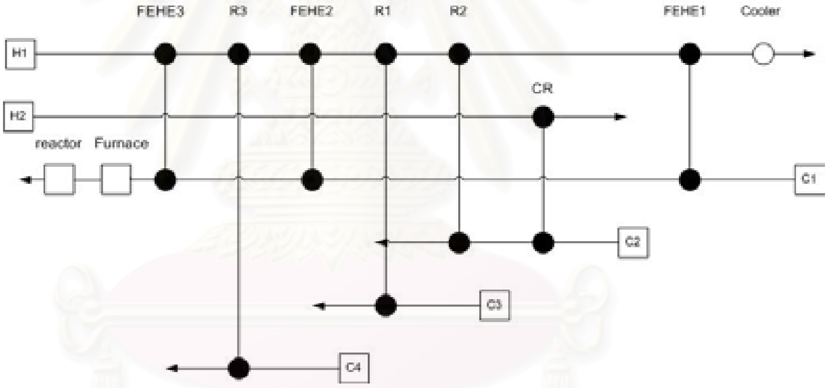
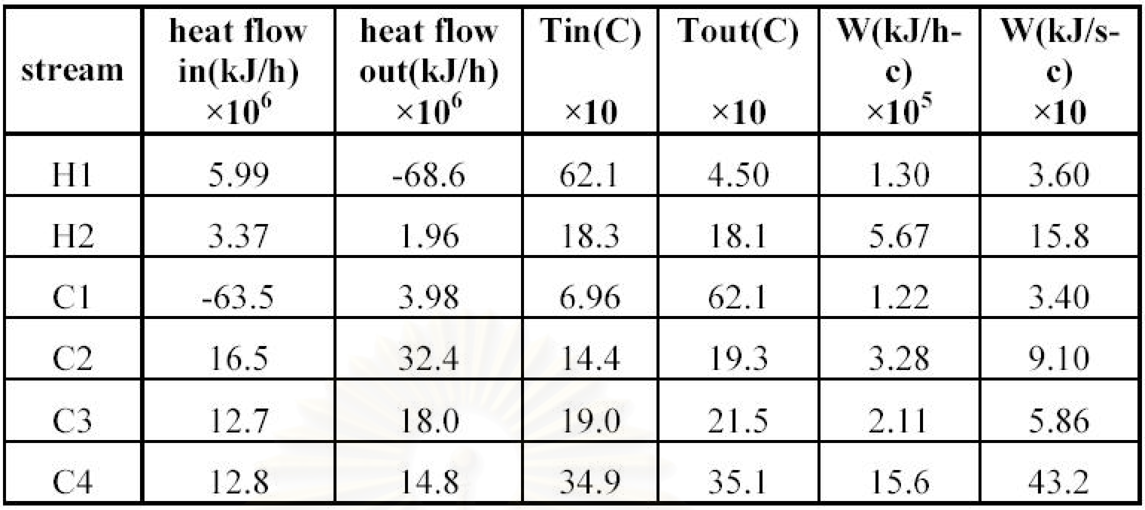


Figure 6.1: Heat Pathways through HEN with multiple FEHEs in energy-integrated design the alternative 6 of the HDA process. (Hermawan , 2004).

In Fig. 6.1, H1 is the quenched reactor product stream, and H2 is the hot-side stream from the top tray of the recycle column. C1 is the reactor feed stream prior to the furnace. C2, C3, and C4 are the cold-side streams coming from the bottoms of product, stabilizer, and recycle columns, respectively.

In Table 6.1, inlet and outlet heat flow and temperature are obtained from HYSYS run. W is calculated by heat flow difference divided by temperature difference, i.e., $\dot{m}C_p$. Data in this table are used to find pinch temperature in problem table in Table 6.2.

Table 6.1 Data for using in problem table (obtained from HYSYS run)



stream	heat flow in(kJ/h) $\times 10^6$	heat flow out(kJ/h) $\times 10^6$	Tin(C) ×10	Tout(C) ×10	W(kJ/h-c) $\times 10^5$	W(kJ/s-c) ×10
H1	5.99	-68.6	62.1	4.50	1.30	3.60
H2	3.37	1.96	18.3	18.1	5.67	15.8
C1	-63.5	3.98	6.96	62.1	1.22	3.40
C2	16.5	32.4	14.4	19.3	3.28	9.10
C3	12.7	18.0	19.0	21.5	2.11	5.86
C4	12.8	14.8	34.9	35.1	15.6	43.2

The pinch calculation result and various position temperatures are presented in Fig. 6.2 showing that heat is added only above the pinch and removed only below the pinch following up the rule of thumbs. So the furnace and the cooler in HDA process already have been located properly.

Pinch temperature can be found by using Problem table method as shown in Table 6.2. The result is 149 ^{o}C.

Table 6.2 Problem table for HDA process (Alt. 6)

W						T hot °C	T cold °C	ΔT	sum W(kW)	Interval	sum interval	Require	Cascade
H1	H2	C1	C2	C3	C4								
0.00	0.00	0.00	0.00	0.00	0.00	631.11	621.11						5459.92
0.00	0.00	33.97	0.00	0.00	0.00	620.84	610.84	10.27	-33.97	**-348.84**	-348.84	**5459.92**	5111.08
35.99	0.00	33.97	0.00	0.00	0.00	360.70	350.70	260.14	2.02	**525.87**	177.04	5111.08	5636.95
35.99	0.00	33.97	0.00	0.00	431.98	359.43	349.43	1.27	-429.96	**-546.04**	-369.01	5636.95	5090.91
35.99	0.00	33.97	0.00	0.00	0.00	225.00	215.00	134.43	2.02	**271.75**	-97.26	5090.91	5362.66
35.99	0.00	33.97	0.00	58.59	0.00	203.00	193.00	22.00	-56.57	**-1244.46**	-1341.72	5362.66	4118.20
35.99	0.00	33.97	90.98	58.59	0.00	199.90	189.90	3.10	-147.55	**-457.40**	-1799.12	4118.20	3660.80
35.99	0.00	33.97	90.98	0.00	0.00	183.29	173.29	16.61	-88.96	**-1477.65**	-3276.77	3660.80	2183.15
35.99	157.54	33.97	90.98	0.00	0.00	180.80	170.80	2.49	68.58	**170.76**	-3106.00	2183.15	2353.92
35.99	0.00	33.97	90.98	0.00	0.00	**154.34**	**144.34**	26.46	-88.96	**-2353.92**	**-5459.92**	2353.92	**0.00**
35.99	0.00	33.97	0.00	0.00	0.00	79.62	69.62	74.72	2.02	**151.05**	-5308.87	**0.00**	151.05
35.99	0.00	0.00	0.00	0.00	0.00	45.00	35.00	34.62	35.99	**1245.84**	-4063.03	151.05	1396.89

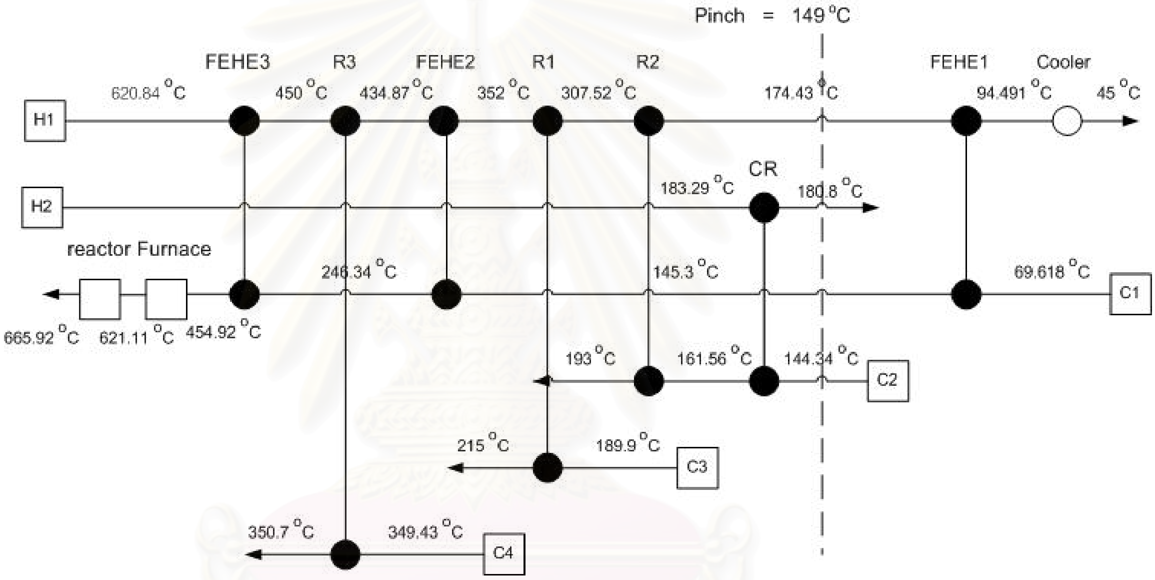


Figure 6.2: Heat Pathways through HEN with multiple FEHEs and pinch temperature.

6.1.2 Optimum reactor inlet temperature

In this section, optimum reactor inlet temperature is found in order to maximize product yield and minimize furnace duty by varying reactor inlet temperature from original value.

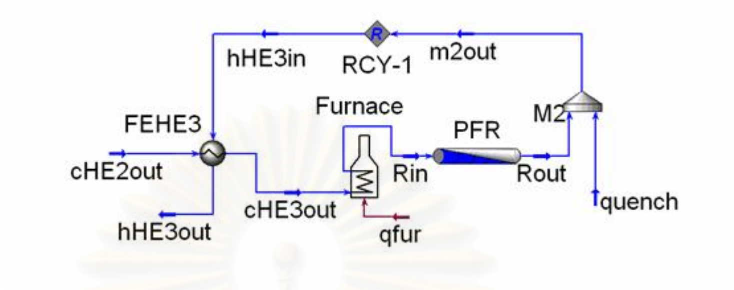


Figure 6.3: Reaction section with a single FEHE of HDA flowsheet.

Reaction in HDA process, two raw materials, hydrogen and toluene, are converted into the benzene product, with methane and diphenyl produced as by-products.

Reaction 1 $\text{Toluene} + H_2 \rightarrow \text{Benzene} + CH_4$

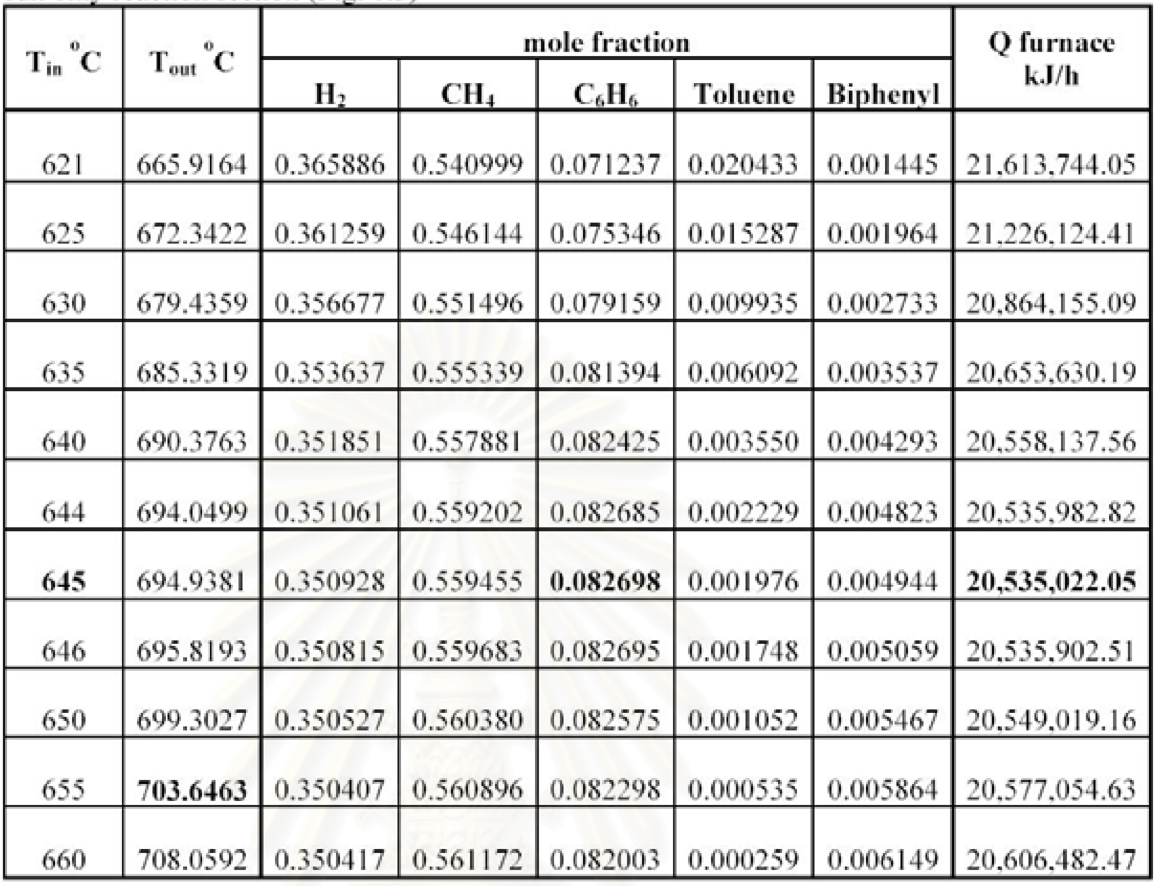
Reaction 2 $2\text{Benzene} \leftrightarrow \text{Diphenyl} + H_2$

The reaction type is exothermic so temperature out of the reactor increases due to the exothermic heat of reaction which heat recovered through FEHE3 as shown in Fig. 6.3. That causes to reduce furnace duty. But we are constrained by the upper reactor outlet temperature limit of 704.44 ^oC. The original reactor inlet temperature is 621.11 ^oC. We will find the reactor inlet temperature that maximizes benzene product and minimizes furnace duty. We try to vary reactor inlet temperature from original value and the results present in table 6.3.

In Table 6.3, Analysis of optimum reactor inlet temperature is made only reaction section with a single FEHE. The result shows that the yield of benzene is highest and the furnace duty is minimum at T = 645 ^oC.

Next, analysis of optimum reactor inlet temperature is made on throughout the plant. The result in Table 6.4 shows that they are different from run only reaction section because of recycle effect, but they are still satisfied because we

Table 6.3 Results of operating at different reactor inlet temperatures from HYSYS run only reaction section (Fig. 6.3)



T_{in} °C	T_{out} °C	mole fraction					Q furnace kJ/h
		H_2	CH_4	C_6H_6	Toluene	Biphenyl	
621	665.9164	0.365886	0.540999	0.071237	0.020433	0.001445	21,613,744.05
625	672.3422	0.361259	0.546144	0.075346	0.015287	0.001964	21,226,124.41
630	679.4359	0.356677	0.551496	0.079159	0.009935	0.002733	20,864,155.09
635	685.3319	0.353637	0.555339	0.081394	0.006092	0.003537	20,653,630.19
640	690.3763	0.351851	0.557881	0.082425	0.003550	0.004293	20,558,137.56
644	694.0499	0.351061	0.559202	0.082685	0.002229	0.004823	20,535,982.82
645	694.9381	0.350928	0.559455	**0.082698**	0.001976	0.004944	**20,535,022.05**
646	695.8193	0.350815	0.559683	0.082695	0.001748	0.005059	20,535,902.51
650	699.3027	0.350527	0.560380	0.082575	0.001052	0.005467	20,549,019.16
655	**703.6463**	0.350407	0.560896	0.082298	0.000535	0.005864	20,577,054.63
660	708.0592	0.350417	0.561172	0.082003	0.000259	0.006149	20,606,482.47

also get most yield of benzene and small furnace and cooler duties at 645 ^oC.

The reason why the furnace and cooler duties decrease is an increase of energy maintained within the process (Q in path3) as shown later.

Table 6.4 Results of operating at different reactor inlet temperatures from HYSYS run throughout the plant.

T_{in} ^{o}C	**T_{out} ^{o}C**	**mole fraction**				
		H_2	**CH_4**	**C_6H_6**	**Toluene**	**Biphenyl**
621	665.9164	0.365886	0.540999	0.071237	0.020433	0.001445
630	676.2170	0.355194	0.557521375	0.073901	0.010435	0.002949
640	686.6205	0.359261	0.557381715	0.075464	0.003919	0.003974
645	690.8786	0.357643	0.560193168	**0.075534**	0.00236	0.00427
650	695.0631	0.360323	0.558735486	0.075146	0.001324	0.004472
655	699.7555	0.359992	0.559367825	0.075176	0.000691	0.004773
660	**704.3971**	0.359873	0.559716374	0.075065	0.000342	0.005003

T_{in} ^{o}C	**T_{out} ^{o}C**	**Q furnace kJ/h**	**Q cooler kJ/h**		
			Path 1	**Path 2**	**sum**
621	665.9164	21,613,744.05	6,989,807.11	19,532,324.70	26,522,131.81
630	676.2170	21,682,046.49	10,152,375.90	16,580,565.54	26,732,941.44
640	686.6205	21,563,297.11	15,263,932.67	11,322,559.72	26,586,492.38
645	690.8786	**21,499,203.33**	15,882,329.67	10,577,209.65	**26,459,539.32**
650	695.0631	21,372,596.04	16,390,959.34	9,768,609.12	26,159,568.46
655	699.7555	21,402,216.88	16,380,540.49	9,768,169.91	26,148,710.41
660	**704.3971**	21,390,787.48	16,380,521.83	9,768,172.36	26,148,694.19

Hint : 1. Q cooler in path1 comes from cooler before separator. (Fig 4.4)

2. Q cooler in path2 are included for condenser at stabilizer and product columns. (Fig. 4.5)

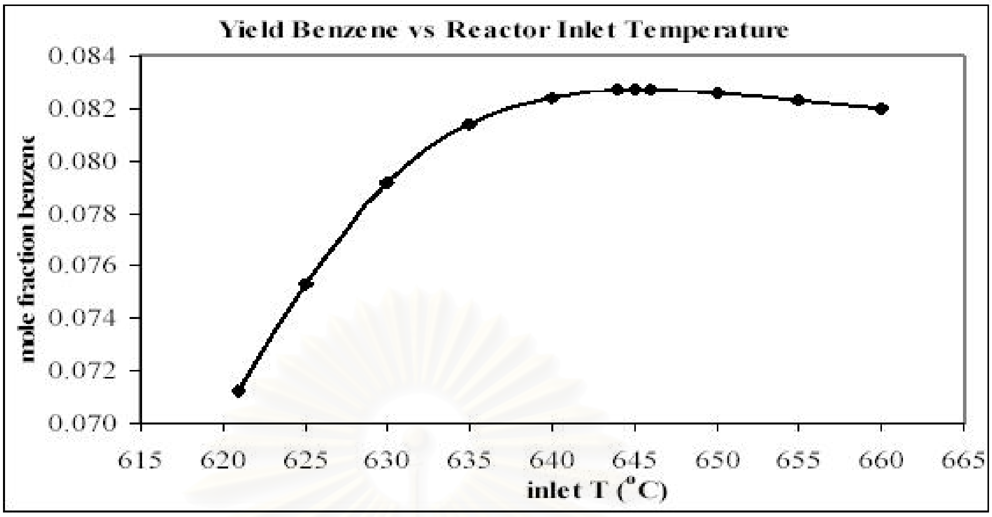


Figure 6.4: Yield benzene versus reactor inlet temperature diagram (data from table 6.3).

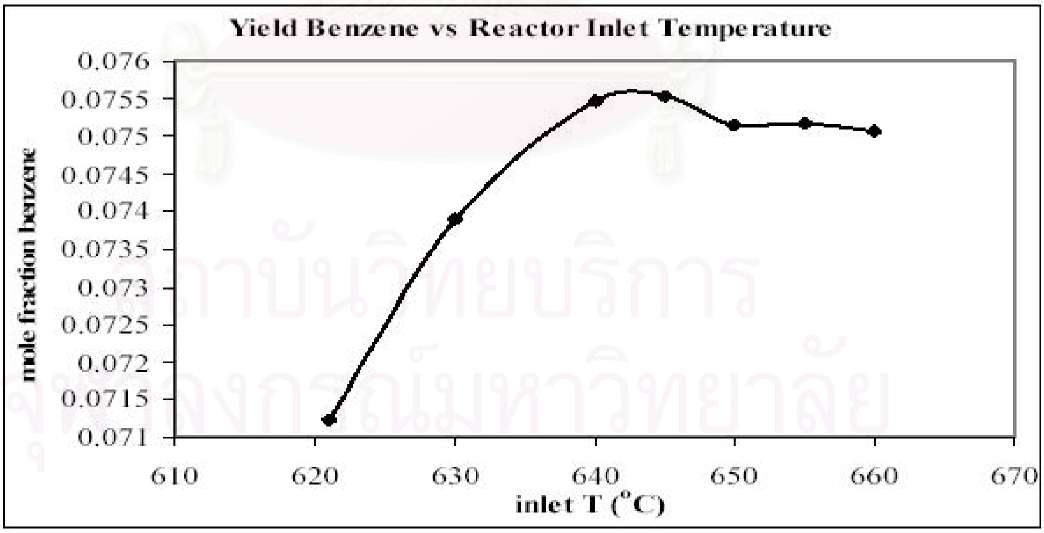


Figure 6.5: Yield benzene versus reactor inlet temperature diagram (data from table 6.4)

6.1.3 Energy maintained within the process (Q in path3)

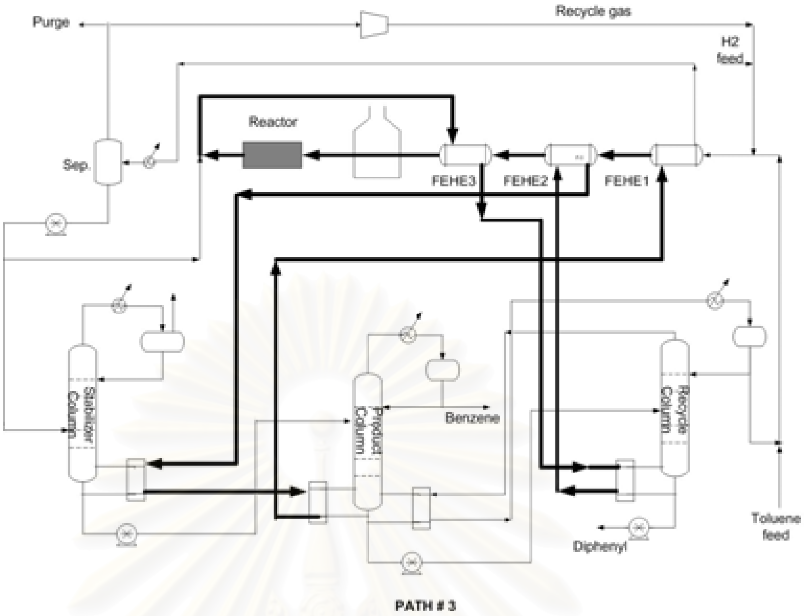


Figure 6.6: HDA process path of heat used internally for stream heating and cooling.

Energy maintained within the process (Q in path3) is calculated from summation of heat flow difference across FEHE1, FEHE2 and FEHE3.

The result in table 6.5 shows that energy maintained within the process (Q in path3) increases when reactor inlet temperature increases. This is reason why furnace and cooler duties decrease when reactor inlet temperature increases previously because of an increase of energy maintained within the process.

Table 6.5 Energy maintained within the process (Q in path3) at different reactor inlet temperatures

FEHE	Energy maintained within the process (Q in path3) kJ/h ($\times 10^7$)						
	621 °C	630 °C	640 °C	645 °C	650 °C	655 °C	660 °C
1	1.164	1.107	1.082	1.083	1.087	1.087	1.087
2	1.042	1.032	1.018	1.017	1.013	1.013	1.013
3	2.376	2.479	2.577	2.628	2.671	2.735	2.803
sum Q	4.582	4.618	4.677	4.729	4.771	4.835	4.903

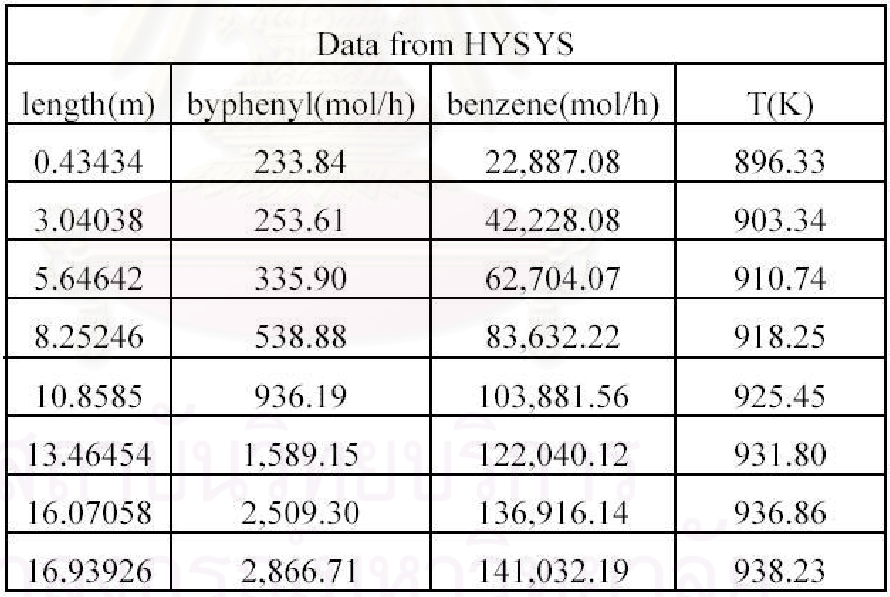
6.1.4 Heat of reaction

In HDA process, the reactor type is the adiabatic exothermic plug-flow reactor, so there is no enthalpy change across the reactor, but the temperature out of the reactor increases due to the exothermic heat of reaction. Some of heat of reaction can be used within the process. Calculation of exothermic heat of reaction is shown below.

Reaction 1 Toluene + H2 → Benzene + CH4
Reaction 2 2Benzene ↔ Diphenyl + H2

CASE 1 : Reactor inlet temperature = 621^oC (original)

Table 6.6 Data of plug flow reactor operation obtained from HYSYS run (case1)



Data from HYSYS			
length(m)	byphenyl(mol/h)	benzene(mol/h)	T(K)
0.43434	233.84	22,887.08	896.33
3.04038	253.61	42,228.08	903.34
5.64642	335.90	62,704.07	910.74
8.25246	538.88	83,632.22	918.25
10.8585	936.19	103,881.56	925.45
13.46454	1,589.15	122,040.12	931.80
16.07058	2,509.30	136,916.14	936.86
16.93926	2,866.71	141,032.19	938.23

Biphenyl is used instead of Diphenyl because Diphenyl doesn't exist in HYSYS's component library.

Mole flow of components in each reaction can be calculated stoichiometrically using data in table 6.6 as presented in table 6.7.

Table 6.7 Mole flow of components in each reactions

PFR length(m)	mole flow of each components in reaction 1 follow to stoichiometry				mole flow of each components in reaction 2 follow to stoichiometry		
	toluene(mol/h)	hydrogen(mol/h)	benzene(mol/h)	methane(mol/h)	biphenyl(mol/h)	benzene(mol/h)	hydrogen(mol/h)
0.43434	23,354.76	23,354.76	23,354.76	23,354.76	233.84	467.68	233.84
3.04038	42,735.31	42,735.31	42,735.31	42,735.31	253.61	507.23	253.61
5.64642	63,375.86	63,375.86	63,375.86	63,375.86	335.90	671.79	335.90
8.25246	84,709.98	84,709.98	84,709.98	84,709.98	538.88	1,077.76	538.88
10.8585	105,753.93	105,753.93	105,753.93	105,753.93	936.19	1,872.37	936.19
13.46454	125,218.42	125,218.42	125,218.42	125,218.42	1,589.15	3,178.30	1,589.15
16.07058	141,934.74	141,934.74	141,934.74	141,934.74	2,509.30	5,018.61	2,509.30
16.93926	146,765.61	146,765.61	146,765.61	146,765.61	2,866.71	5,733.42	2,866.71

Table 6.8 Calculation of heat of reaction from heat of formation by assuming heat of reaction 2 = 0 kJ/mol tol (very small).

length(m)	T(K)	Heat of formation kJ/mol					Heat of reaction	
		$H_f H_2$	$H_f C_7H_8$	$H_f C_6H_6$	$H_f CH_4$	$H_f C_{12}H_{10}$	**$H_{rx,1}$(kJ/h)**	**H_{rx}(kJ/mol tol)**
0.43434	896.33	0	2.60E+01	6.32E+01	-8.85E+01	1.55E+02	**- 1,198,912.96**	**-51.33483487**
3.04038	903.34	0	2.60E+01	6.31E+01	-8.85E+01	1.55E+02	**- 2,197,989.07**	**-51.43262787**
5.64642	910.74	0	2.59E+01	6.30E+01	-8.86E+01	1.55E+02	**- 3,266,099.10**	**-51.53538446**
8.25246	918.25	0	2.58E+01	6.29E+01	-8.87E+01	1.55E+02	**- 4,374,376.54**	**-51.63944811**
10.8585	925.45	0	2.57E+01	6.28E+01	-8.88E+01	1.55E+02	**- 5,471,581.77**	**-51.73880357**
13.46454	931.80	0	2.57E+01	6.27E+01	-8.89E+01	1.55E+02	**- 6,489,593.00**	**-51.82618572**
16.07058	936.86	0	2.56E+01	6.27E+01	-8.89E+01	1.55E+02	**- 7,365,796.33**	**-51.89565395**
16.93926	938.23	0	2.56E+01	6.27E+01	-8.89E+01	1.55E+02	**- 7,619,238.21**	**-51.9143285**
							avg.	**-51.64502528**

From literature data given by Douglas (1988)

Heat of reaction 1 = -50.009 kJ/mol tol

Heat of reaction 2 = 0 kJ/mol tol

Table 6.9 Summary table of heat of reaction related with reactor inlet temperatures

reactor inlet temperature (°C)	heat of reaction (kJ/mol tol)
621 (original)	-51.645
645 (optimum)	-52.088

Increment of heat of reaction can make energy maintained within the process (Q in path 3) larger as presented in Table 6.5.

6.2 Classification of heat pathways

Three different "heat pathways" of HDA process were proposed by Luyben (1999) see Fig. 6.7 - 6.9. The first pathway is from inside the process (heat of reaction) and flows out to the environment through cooler. Heat of reaction inherits from reactor design. The second pathway carries heat from utilities (furnace) into the process and flows out to the environment through three reboilers. Before moving to reactor, process stream is supplied missing heat by furnace. The third pathway is internal to the process. Here heat flows back and forth between different unit operations. We can get insight where energy source, energy sink and paths of energy in the process is from the idea of managing Luyben's heat pathways. Moreover, these helped us to design several levels of energy within the process. However we cannot specify exactly where heat sources of dissipated heat to any available heat sinks is. So we combined path 1 and 2 for convenient sake. They are shown in Fig. 6.10 and Fig. 6.11. For clear picture, Heat pathways through HEN for this plant are presented in Fig. 6.1. H1 stream represents hot stream travelling throughout the process starts from FEHE3 inlet and ends up at cooler. All of its heat is dissipated to three FEHEs, reboilers and cooler. So we defined three heat pathways as follows: The first and second pathway (Q1+Q2) is heat taken away from positive feedback loop through three reboilers and cooler. The third pathway (Q3) is heat brought back in positive feedback loop through three FEHEs. The quantities of two heat pathways were evaluated for next four case studies from data obtained from dynamic simulation.

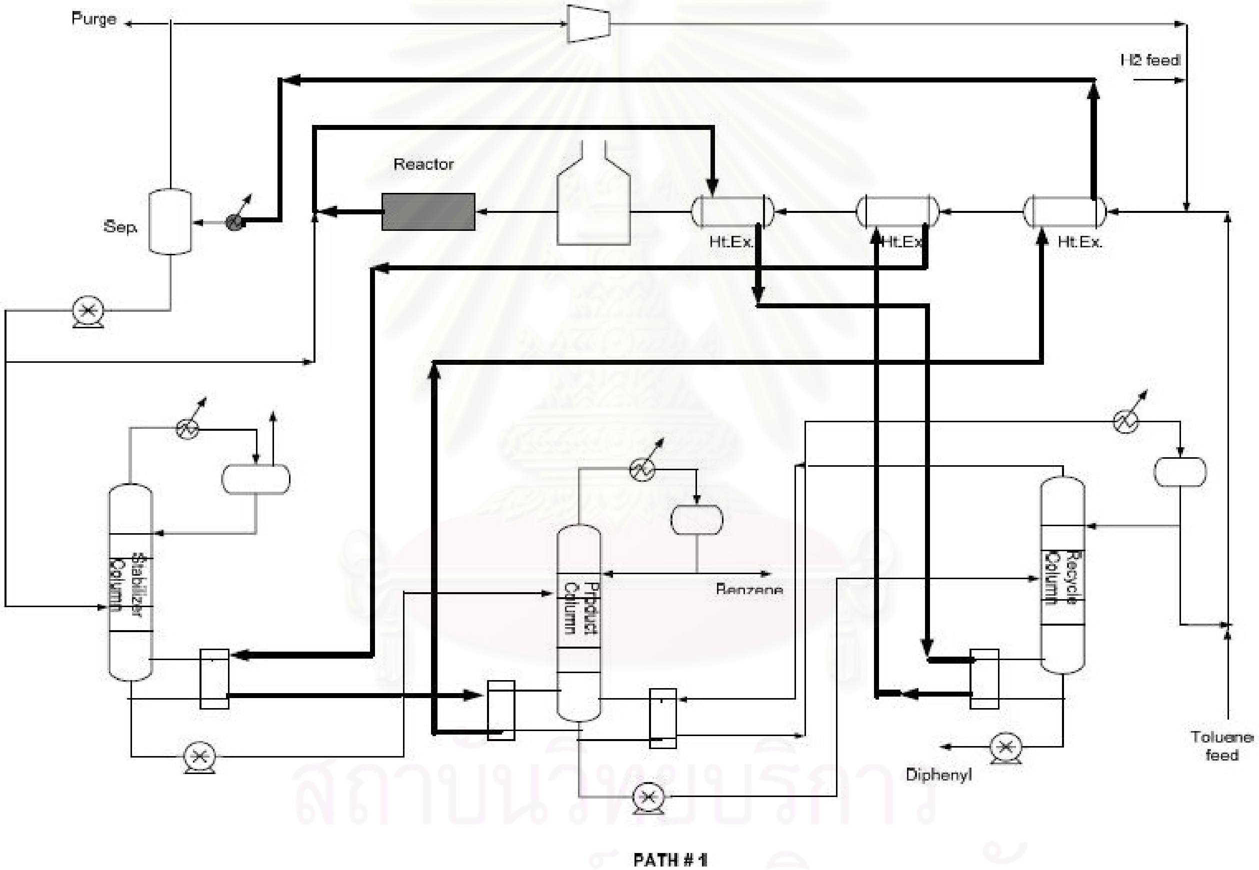


Figure 6.7: HDA process path of exothermic reaction heat. (Luyben, 1999)

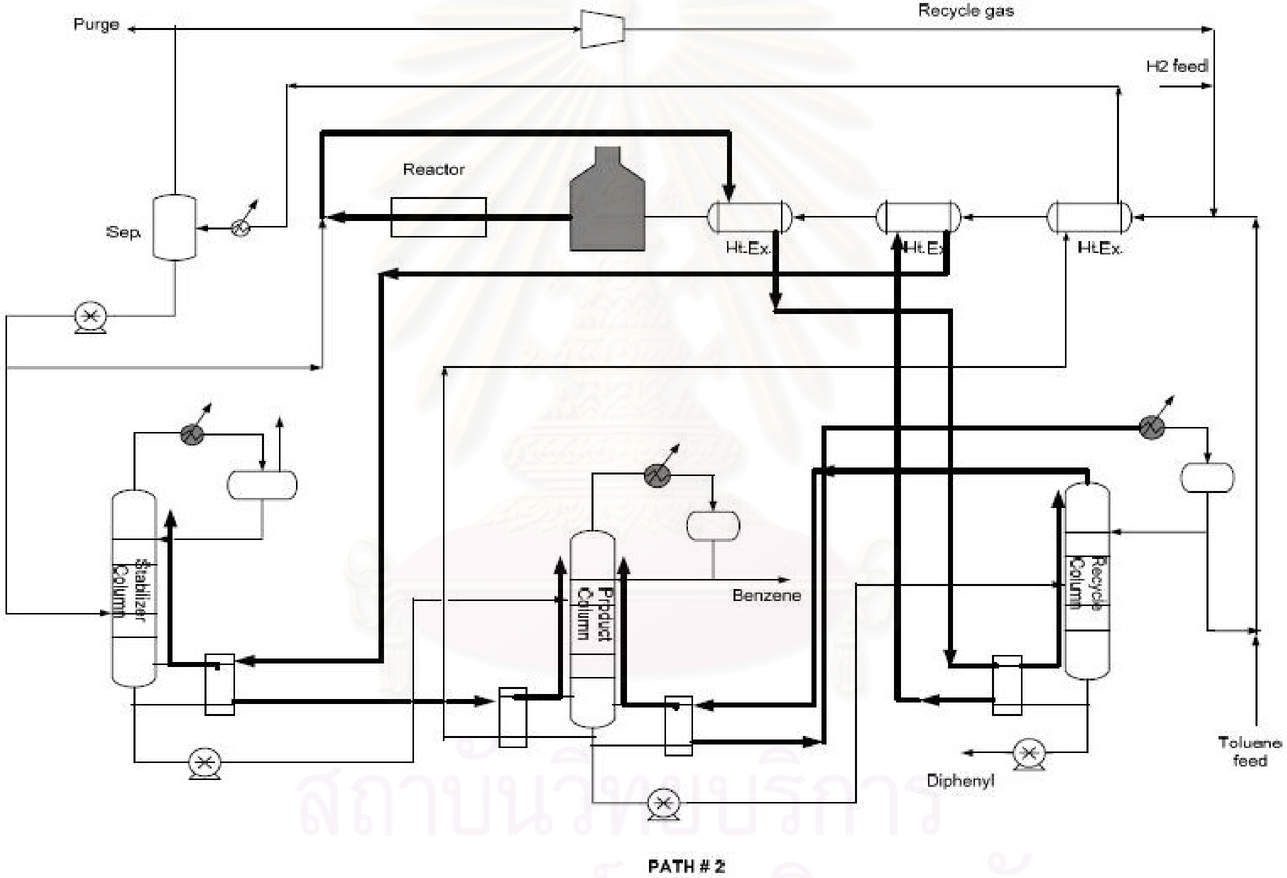
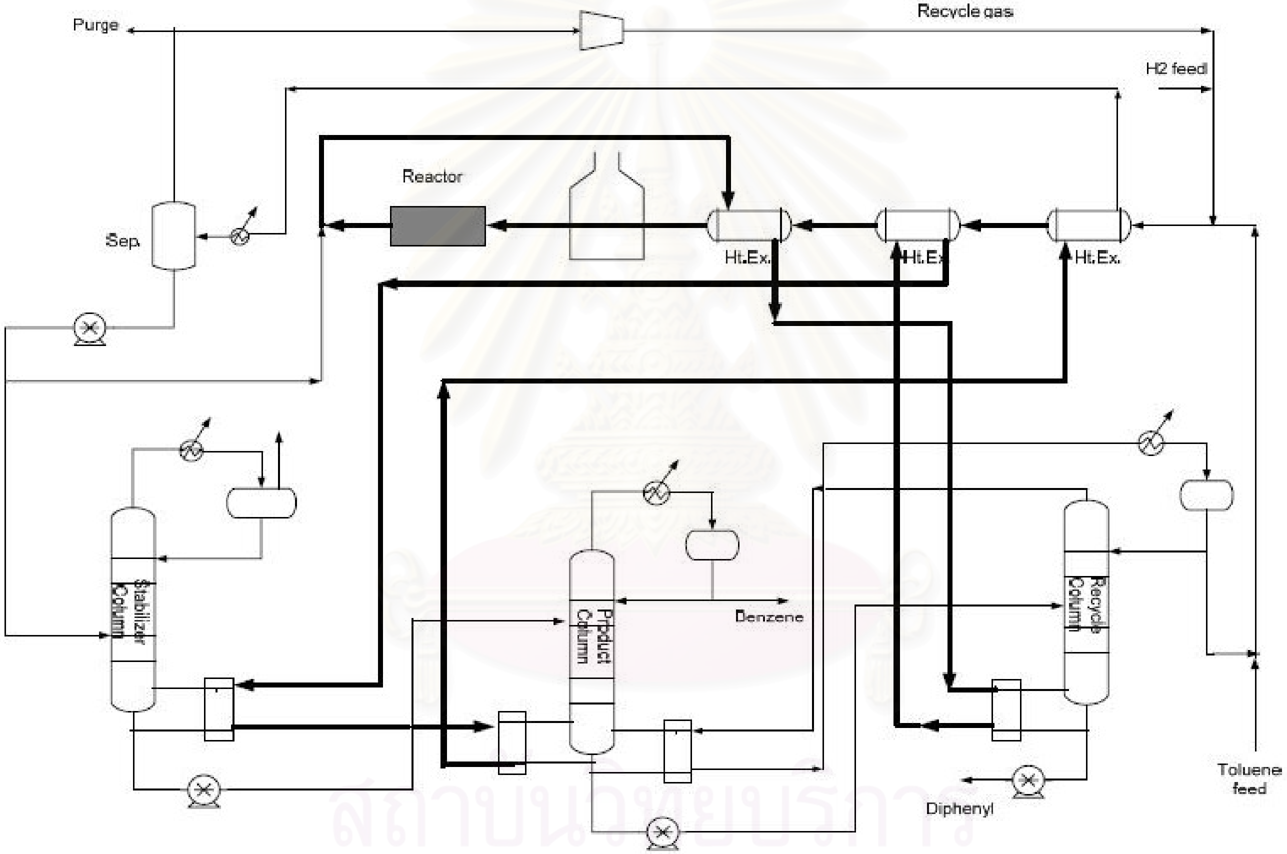


Figure 6.8: HDA process path of heat supply to distillation columns. (Luyben, 1999)



PATH # 3

Figure 6.9: HDA process path of heat used internally for stream heating and cooling. (Luyben, 1999)

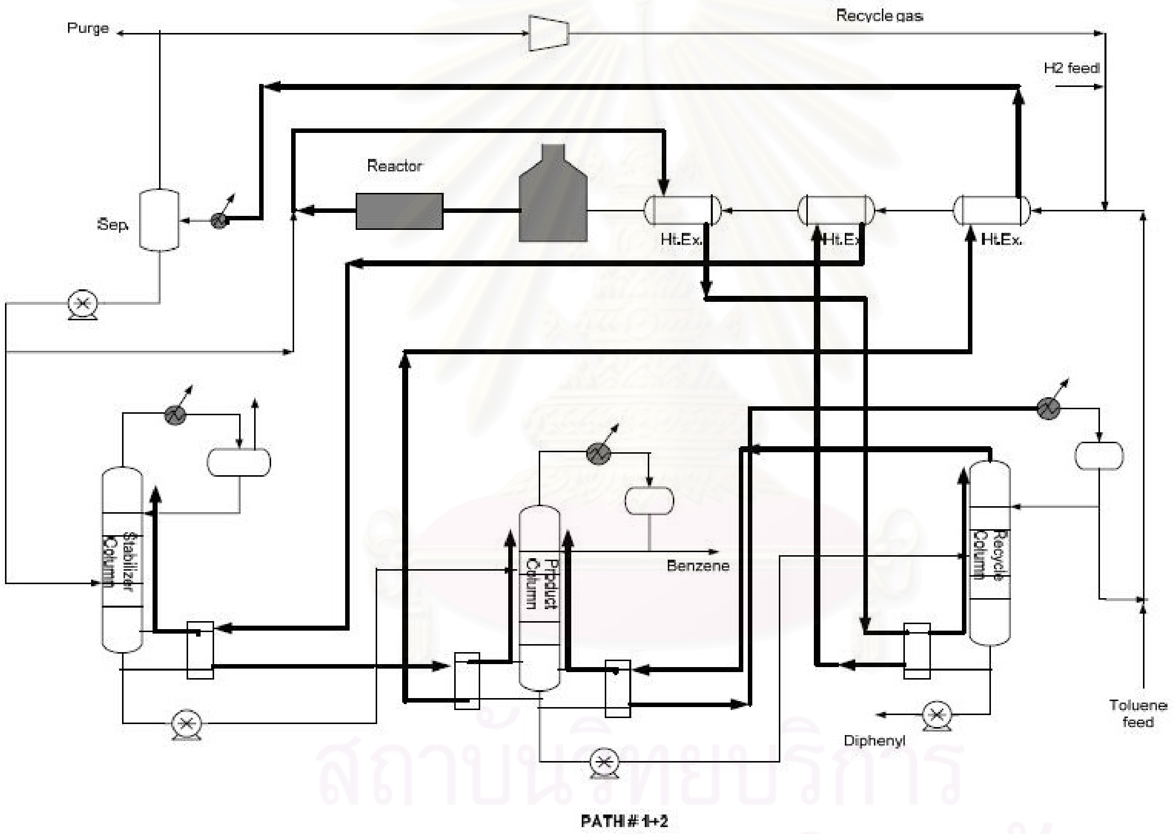
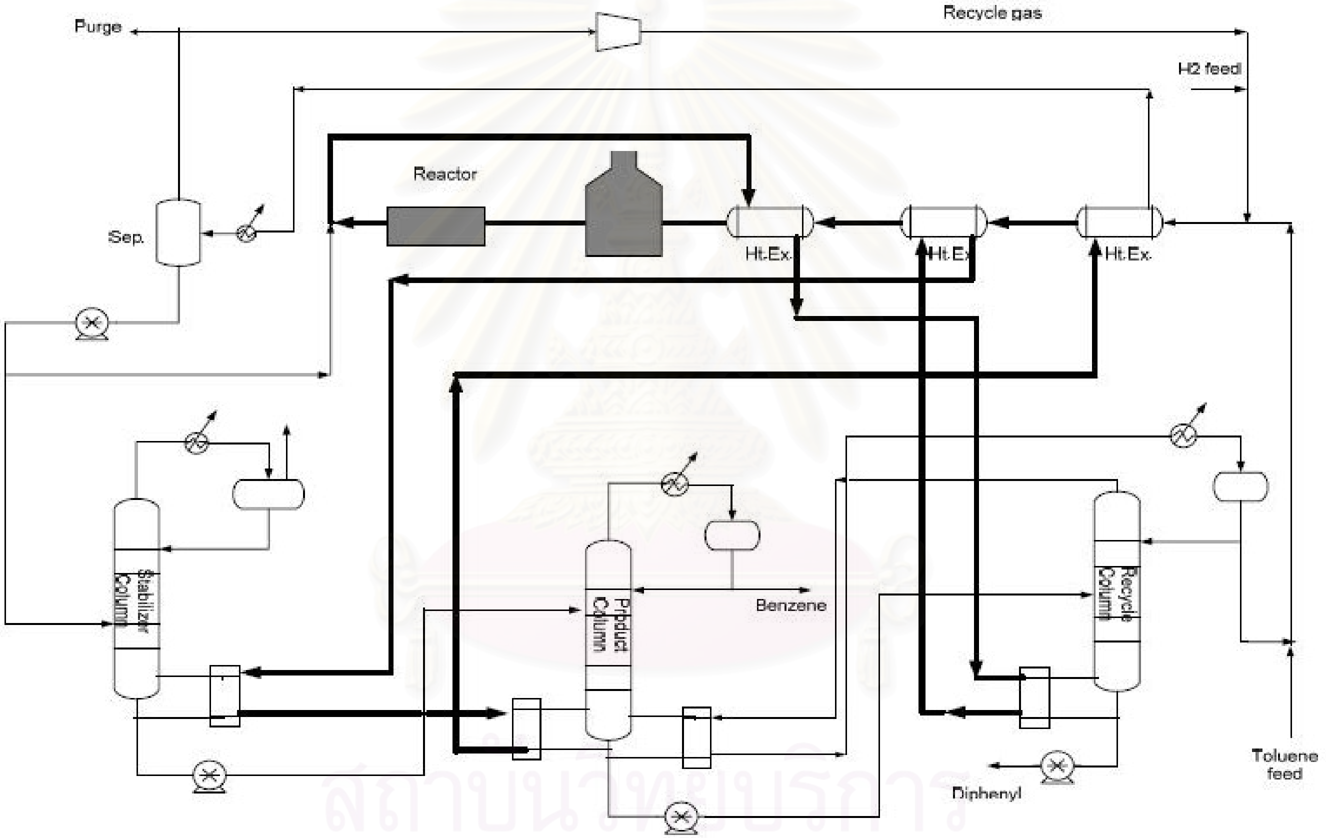


Figure 6.10: HDA process path of heat taken away from positive feedback loop through three reboilers and cooler.



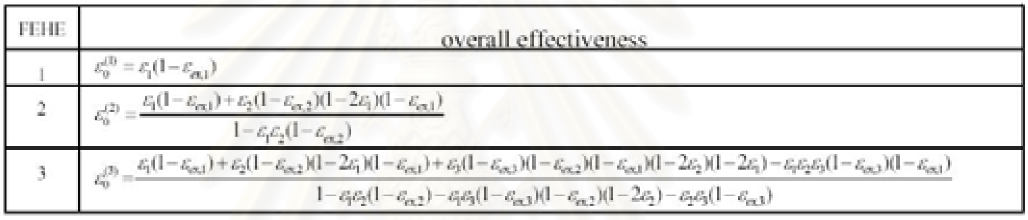
PATH # 3

Figure 6.11: HDA process path of heat brought back in positive feedback loop.

6.3 Overall Effectiveness

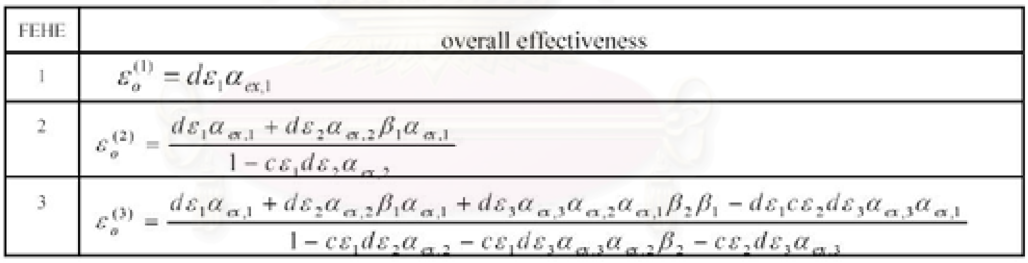
The overall effectiveness factors for the cases of one, two, and three FEHEs (ϵ_o(i) , i = 1,2,3) are shown in table 6.10 (Chen and Yu, 2003). Their equations include an assumption that the heat capacities of the hot and cold streams are the same, i.e., $C_{P,H} = C_{P,C}$, and the mass flow rates of the hot and cold streams are identical and the stability can be assessed by evaluating the overall effectiveness. In this research, those equations were modified in general form without assumption m$C_{P,H}$ = m$C_{P,C}$ as shown in table 6.11 because the capacity flow rates of the hot and cold streams inlet are not practically equal. Overall effectiveness were evaluated for our case studies from data obtained from dynamic simulation.

Table 6.10 Structure Effect on Overall Effectiveness



FEHE	overall effectiveness
1	$\varepsilon_0^{(1)} = \varepsilon_1(1-\varepsilon_{ex1})$
2	$\varepsilon_0^{(2)} = \dfrac{\varepsilon_1(1-\varepsilon_{ex1})+\varepsilon_2(1-\varepsilon_{ex2})(1-2\varepsilon_1)(1-\varepsilon_{ex1})}{1-\varepsilon_1\varepsilon_2(1-\varepsilon_{ex2})}$
3	$\varepsilon_0^{(3)} = \dfrac{\varepsilon_1(1-\varepsilon_{ex1})+\varepsilon_2(1-\varepsilon_{ex2})(1-2\varepsilon_1)(1-\varepsilon_{ex1})+\varepsilon_3(1-\varepsilon_{ex3})(1-\varepsilon_{ex2})(1-\varepsilon_{ex1})(1-2\varepsilon_2)(1-2\varepsilon_1)-\varepsilon_1\varepsilon_2\varepsilon_3(1-\varepsilon_{ex3})(1-\varepsilon_{ex1})}{1-\varepsilon_1\varepsilon_2(1-\varepsilon_{ex2})-\varepsilon_1\varepsilon_3(1-\varepsilon_{ex3})(1-\varepsilon_{ex2})(1-2\varepsilon_2)-\varepsilon_2\varepsilon_3(1-\varepsilon_{ex3})}$

Table 6.11 Structure effect on overall effectiveness (general form)



FEHE	overall effectiveness
1	$\varepsilon_o^{(1)} = d\varepsilon_1\alpha_{ex,1}$
2	$\varepsilon_o^{(2)} = \dfrac{d\varepsilon_1\alpha_{ex,1} + d\varepsilon_2\alpha_{ex,2}\beta_1\alpha_{ex,1}}{1 - c\varepsilon_1 d\varepsilon_2\alpha_{ex,2}}$
3	$\varepsilon_o^{(3)} = \dfrac{d\varepsilon_1\alpha_{ex,1} + d\varepsilon_2\alpha_{ex,2}\beta_1\alpha_{ex,1} + d\varepsilon_3\alpha_{ex,3}\alpha_{ex,2}\alpha_{ex,1}\beta_2\beta_1 - d\varepsilon_1 c\varepsilon_2 d\varepsilon_3\alpha_{ex,3}\alpha_{ex,1}}{1 - c\varepsilon_1 d\varepsilon_2\alpha_{ex,2} - c\varepsilon_1 d\varepsilon_3\alpha_{ex,3}\alpha_{ex,2}\beta_2 - c\varepsilon_2 d\varepsilon_3\alpha_{ex,3}}$

where

α_i =1-cϵ_i and β_i=1-(c+d)ϵ_i

c=$(\dot{m}C_p)_{min}/(\dot{m}C_p)_H$ and d=$(\dot{m}C_p)_{min}/(\dot{m}C_p)_C$ of each heat exchanger multiplied by each ϵ_i in equations

ϵ_o= overall effectiveness

ϵ_1,ϵ_2,ϵ_3= effectiveness of the third FEHE, the second FEHE and the first FEHE, respectively.

$\epsilon_{ex,1}$,$\epsilon_{ex,2}$,$\epsilon_{ex,3,1}$,$\epsilon_{ex,3,2}$= effectiveness of the steam generator at positive feedback loop, the recycle column reboiler and the stabilizer and product column reboiler, respectively.

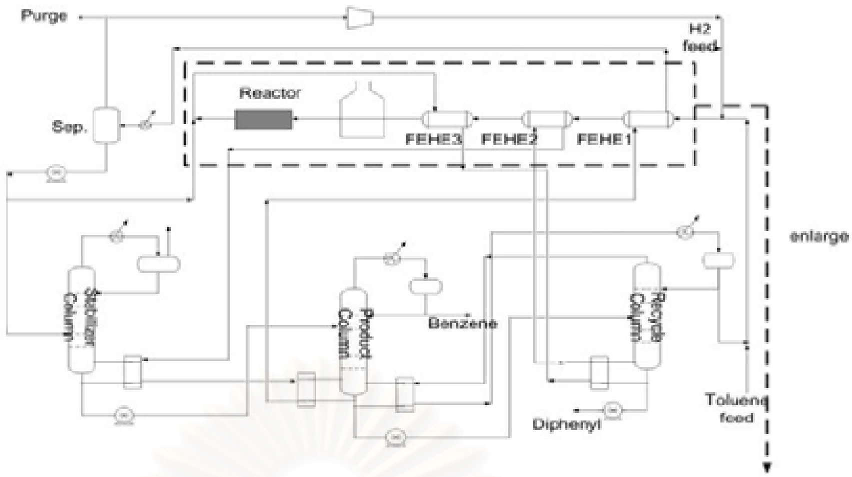
6.4 Control Performance vs. Energy Integration

6.4.1 Case Studies

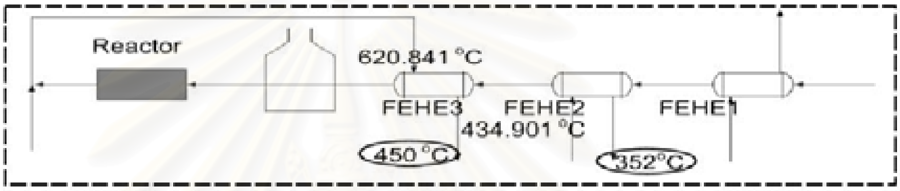
6.4.1.1 Steady-state modeling

Steady-state model was built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Douglas (12988); Luyben et al. (1998). Peng-Robinson model was 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 were modelled with standard Arrhenius kinetic expressions available in HYSYS.PLANT, and the kinetic data were taken from Luyben et al. (1998).

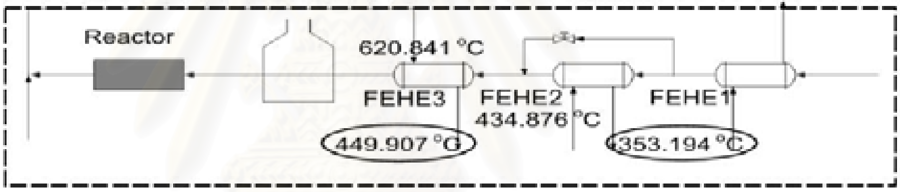
The levels of energy maintained within the process (Q3) was perturbed by bypassing small portion of the cold stream around Feed-Effluent Heat Exchangers(FEHEs). This translated into reduction of the heat transfer area of FEHEs in dynamic models. In this research, seven case studies were modeled. Five different levels of energy in path 3 were different FEHEs as shown in Fig. 6.12 for Case Study 1-5. The temperatures out of each FEHEs were different in each cases which indicated the levels of energy maintained within the process. HDA process (alt.1) and HDA process (NO FEHE) were chosen as Case Study 6 and 7, respectively, in order to consider the effect of energy integration only in reaction section and without energy integration on control performance. See Fig. 6.13, 6.14.



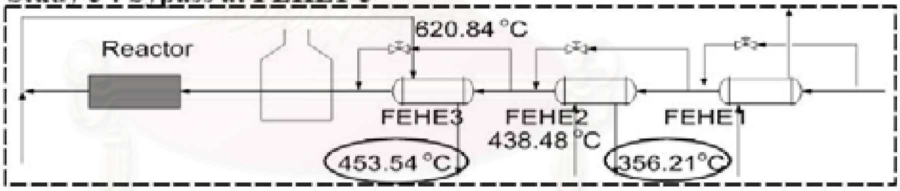
Case Study 1 : no bypass



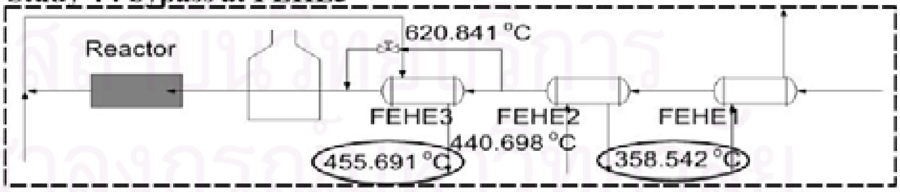
Case Study 2 : bypass at FEHE2



Case Study 3 : bypass at FEHE1-3



Case Study 4 : bypass at FEHE3



Case Study 5 : bypass at FEHE2 and FEHE3

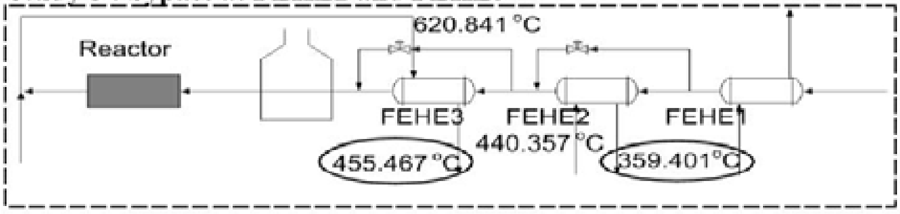


Figure 6.12: The flowsheet of HDA process (alt.6) used in steady state simulation for Case Study 1-5

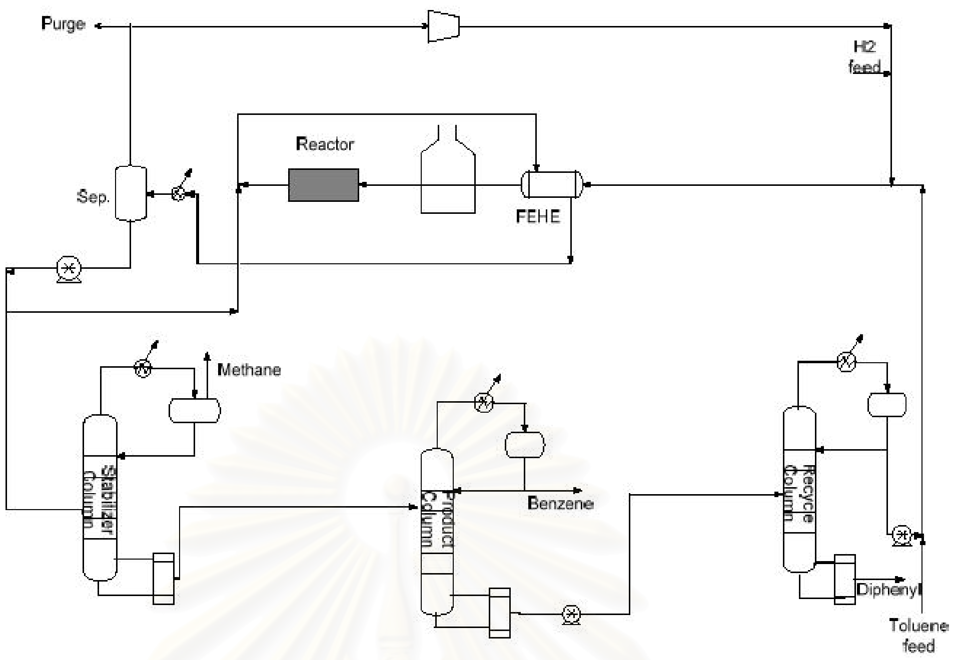


Figure 6.13: The flowsheet of HDA process (alt.1) used in steady- state simulation for Case Study 6.

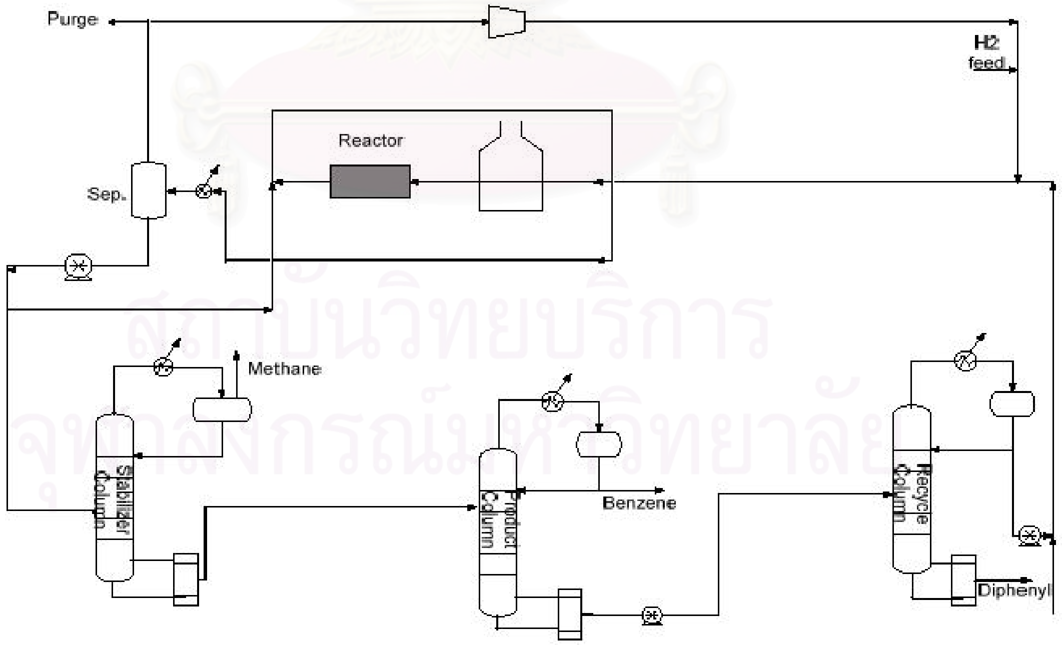


Figure 6.14: The flowsheet of HDA process (NO FEHE) used in steady- state simulation for Case Study 7.

6.4.1.2 Dynamic modeling

In the integrated steady state and dynamic simulation environment provided by HYSYS.PLANT, the dynamic model shares the same physical property packages and flowsheet topology as the steady-state model. Thus it is easy to switch from steady-state to dynamic mode. All flowsheet information from the steady-state simulation case transfers easily to the dynamic simulation environment.

Since hot outlet streams of FEHE 2,3 travel to separation section, temperature control loops were positioned at hot side stream by manipulating bypass valves across FEHEs. But FEHE1 was left without temperature controller because hot stream going out of FEHE1 runs to cooler, and it is good to give up most of its heat to incoming cold stream that can reduce cooler duty. Their set points were different for each of Case Study 1-5 which received from steady state simulation shown in Fig. 6.12. And then seven case studies were evaluated control performances using integral absolute error (IAE) by two different control structures.

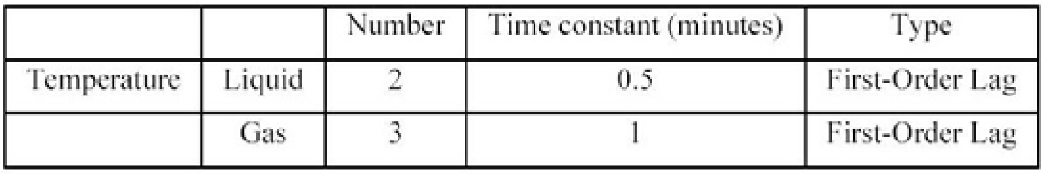
6.4.2 Plant Control Structures

Two control structures, CS1 and CS2, were considered for evaluating the interaction of energy integration and control performance. In CS1, pressure of recycle gas stream is controlled by manipulating fresh feed hydrogen because pressure of recycle gas stream relates to the amount of recycled hydrogen to the process. In CS2, the proportion of hydrogen/toluene is controlled by measuring total toluene feed flow rate to calculate set-point of fresh feed hydrogen flow rate. This loop also controls indirectly the pressure of recycle gas stream. The control configuration of the two control structures are illustrated in Fig. 6.15 - 6.18.

6.4.2.1 Tuning Parameter

In this research, heuristic tuning (Luyben, 2002) was used in flow, level and pressure loops. A value of $\tau_I = 0.3$ minutes works in most flow controllers and the value of controller gain should be kept modest because flow measurement signals are sometime noisy due to the turbulent flow through the orifice plate. A

Table 6.12 Typical measurement lags



		Number	Time constant (minutes)	Type
Temperature	Liquid	2	0.5	First-Order Lag
	Gas	3	1	First-Order Lag

value of controller gain of $K_C = 0.5$ is often used. Derivative action should not be used. In a real plant application, filtering of the flow signal is also recommended because of the noise. So filter was put at flow controller output signal and a good number to use for a flow loop is $\tau_F = 0.1$ minute. Recommended tuning of a level controller is $K_C = 2$. Typical pressure controller tuning constants for columns and tanks are $K_C = 2$ and $\tau_I = 10$ minutes. The relay-feedback test is a tool that serves tuning parameter for temperature loops. The results of the test are the ultimate gain and the ultimate frequency. This information is usually sufficient to permit us to calculate some reasonable controller tuning constants. Relay feedback testing can be done in HYSYS. It simply click the Tuning botton on the controller faceplate, select Autotuning and click the Start Autotuning button. The loop will start to oscilate. After several cycles, the tuning is stopped and some recommended settings for a PID controller are suggested. The temperature loops have significant dynamic lags and/or deadtimes. Realistic dynamic simulations require that we explicitly include lags and/or dead times in these loops. In this plant, we included lags at temperature loops of TCQ, TCR, TC2 and TC3. Some lags are recommended in table 6.12 (Luyben, 2002).

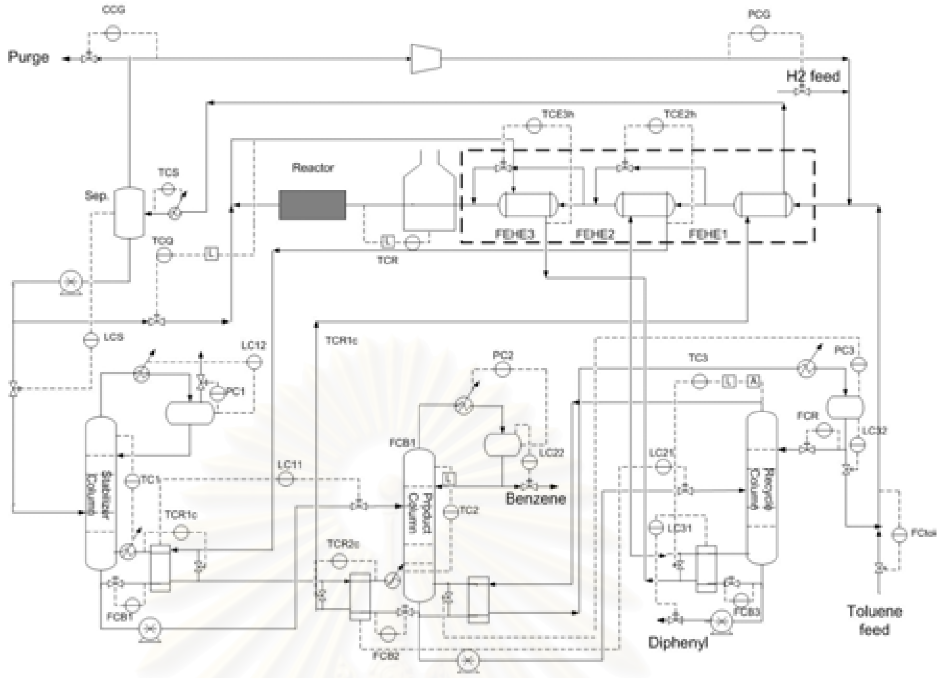


Figure 6.15: The control configuration of HDA process (alt.6) used in dynamic simulation for Case Study 1-5 with control scheme (CS1).

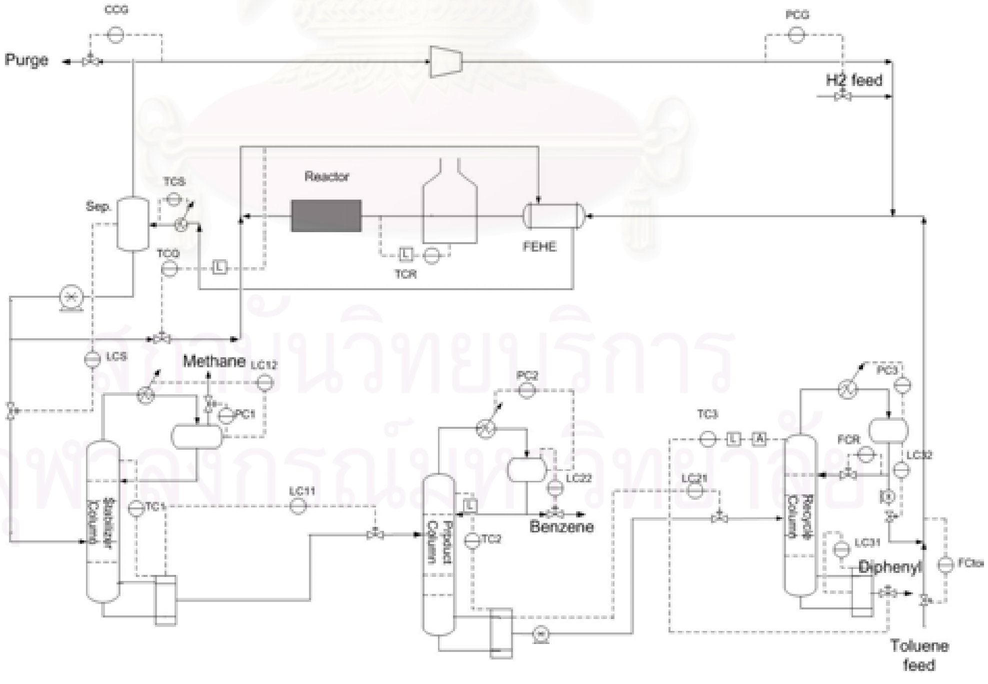


Figure 6.16: The control configuration of HDA process (alt.1) used in dynamic simulation for Case Study 6 with control scheme (CS1).

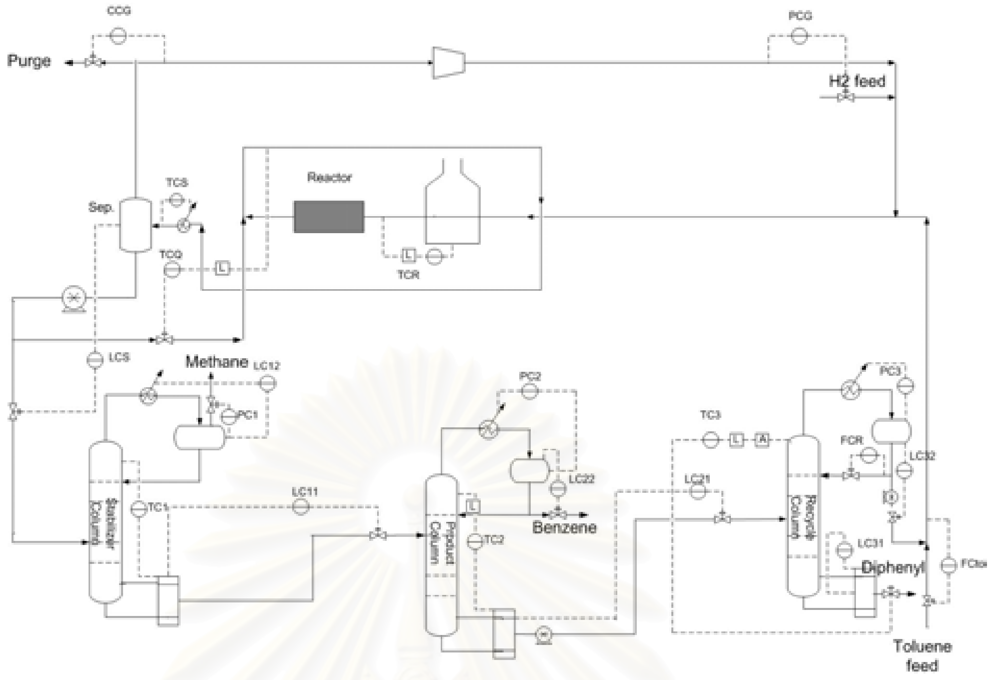


Figure 6.17: The control configuration of HDA process (NO FEHE) used in dynamic simulation for Case Study 7 with control scheme (CS1).

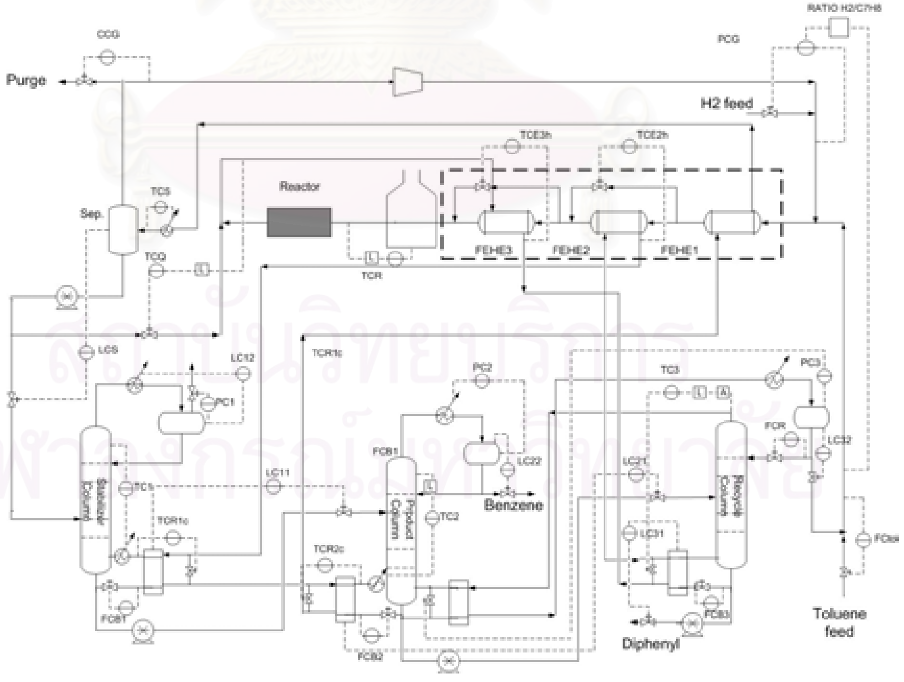


Figure 6.18: The control configuration of HDA process (alt.6) used in dynamic simulation for Case Study 1-5 with control scheme (CS2).

Ratio control was introduced in CS2 for all Case Studies. So control scheme of CS2 for Case Study 6, 7 are not shown.

The hysys flowsheets of the control configurations of seven case studies are illustrated in Fig. 6.19-6.22.

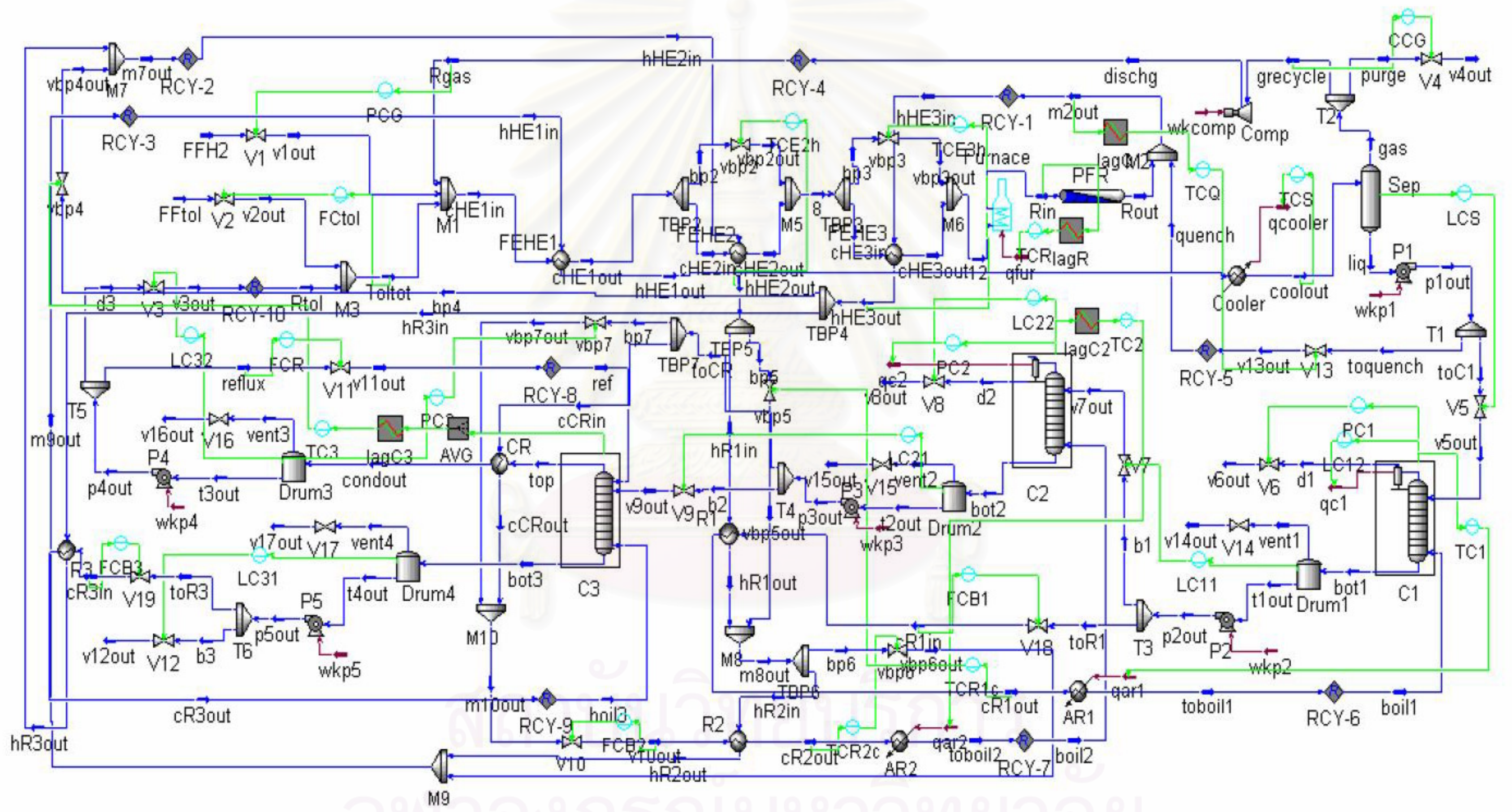


Figure 6.19: The hysys flowsheet of HDA process (alt.6) used in dynamic simulation for Case Study 1-5 with control scheme (CS1).

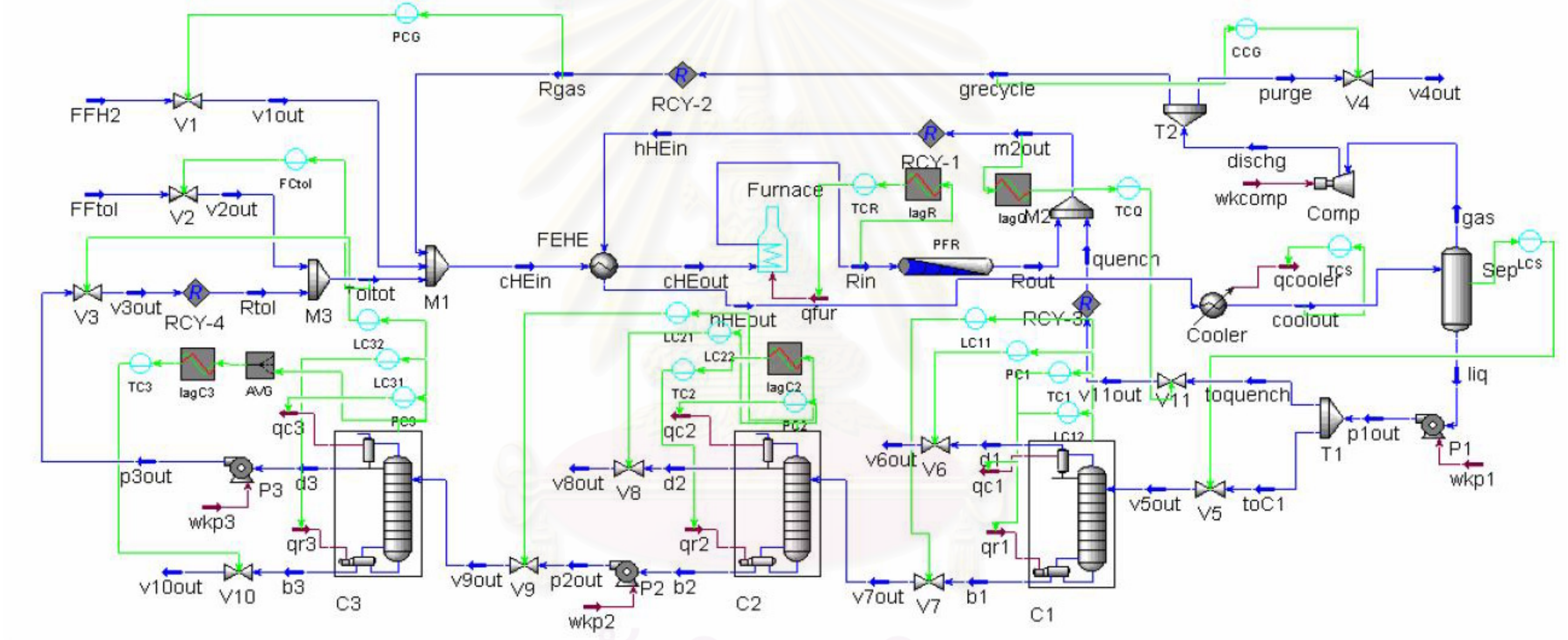


Figure 6.20: The hysys flowsheet of HDA process (alt.1) used in dynamic simulation for Case Study 6 with control scheme (CS1).

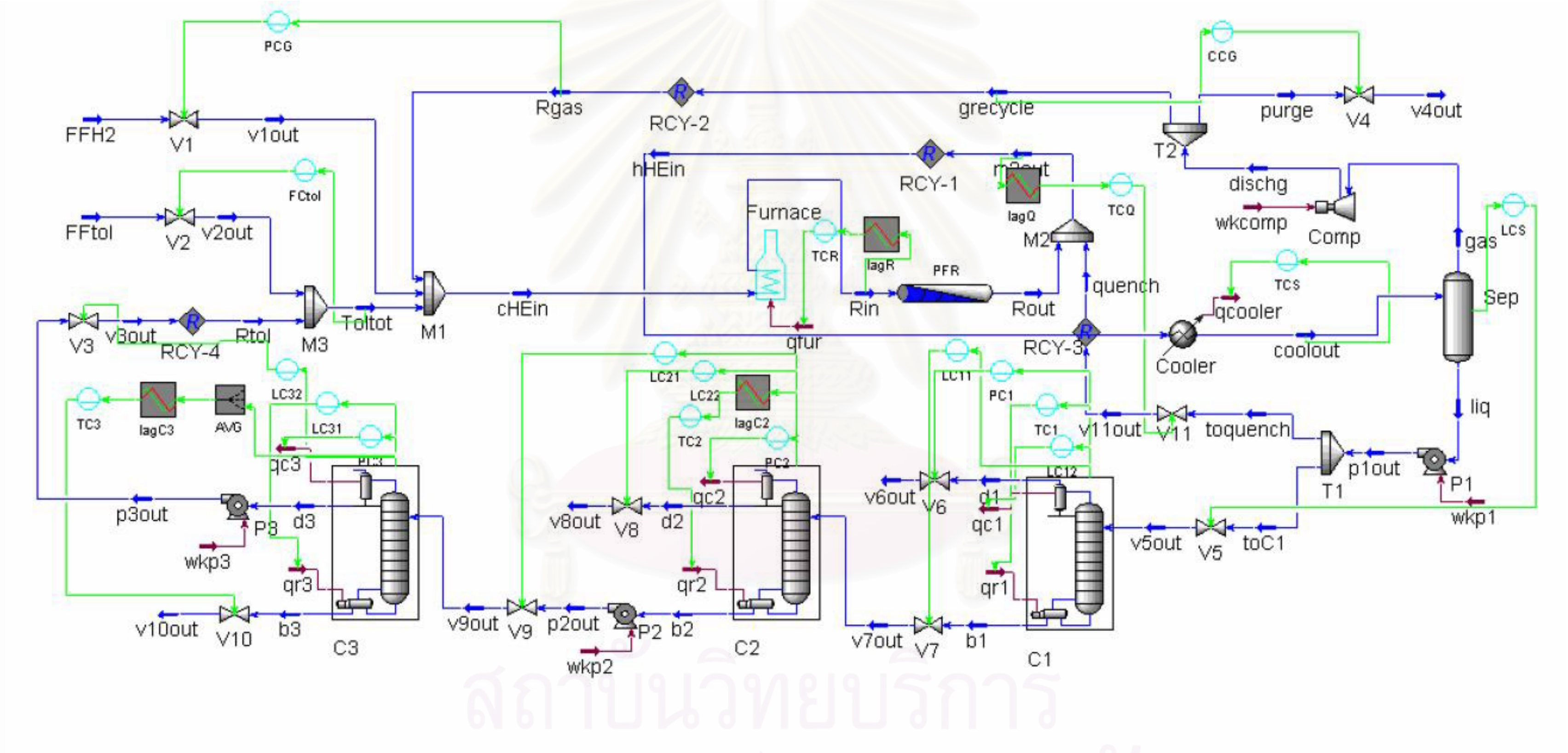


Figure 6.21: The hysys flowsheet of HDA process (NO FEHE) used in dynamic simulation for Case Study 7 with control scheme (CS1).

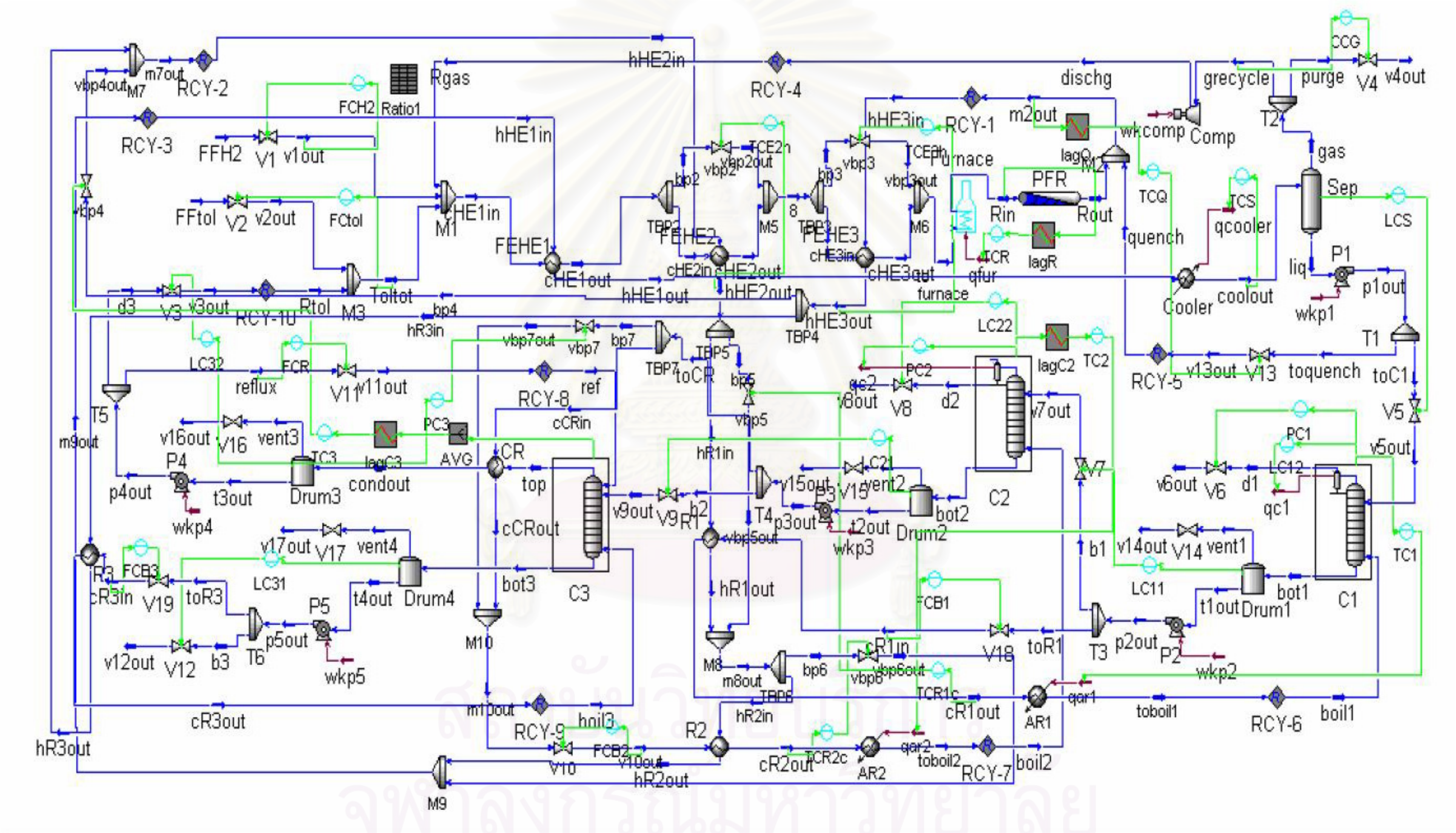


Figure 6.22: The hysys flowsheet of HDA process (alt.6) used in dynamic simulation for Case Study 1-5 with control scheme (CS2).

6.4.3 Interaction Evaluate

We adopted two types of test:
(i) set-point change : total toluene feed is adjusted for production rate (Qiu, 2003).
(ii) load disturbances : toluene feed temperature represent fluctuations in fresh feed streams caused by environmental effect (Qiu, 2003).

The IAEs of control loops of product qualities, i.e. quench temperature (TCQ), reactor inlet temperature(TCR), separator inlet temperature(TCS), temperature control loop of the three distillation columns(TC1-3) and total toluene feed flow rate(FCtol), were assessed for seven case studies. Since IAE of TC3 is 10-100 time higher than the other and the column products are toluene which is recycled and diphenyl, bottom product, which is the by-product. So we do not include its IAE in our study. Anyway their IAEs are shown for reference in Fig. 6.23, 6.25 and 6.27.

6.4.3.1 Control Structure 1 (CS1)

The relationship between heat recovery and control performance from testing set-point change and load disturbance of seven case studies are shown in Fig. 6.23. Since there is no energy integration in the separation section in Case Study 6, 7, Less amount of heat is recovered in Case Study 6 and heat is not recovered at all in Case Study 7. That makes the control loops in the separation section easy to control because the disturbance does not propagate to this section through heat-integrated heat exchangers, i.e., reboiler of distillation columns. So the IAEs of Case Study 6 is the lowest but the IAEs (NO TC3) of Case Study 7 is high because this case does not have FEHEs that behaves like buffer tanks to attenuate the disturbances. So we can see that IAEs of TCQ, TCR loops are much higher from both testings as shown in Fig. 6.24. Next, We consider the relationship between energy maintained within process (Q3) and IAEs curves in the cases having heat recovery in the separation section (Case Study 1-5) since control performances of Case Study 6, 7 have explained above with no effects of energy integration in the separation section.

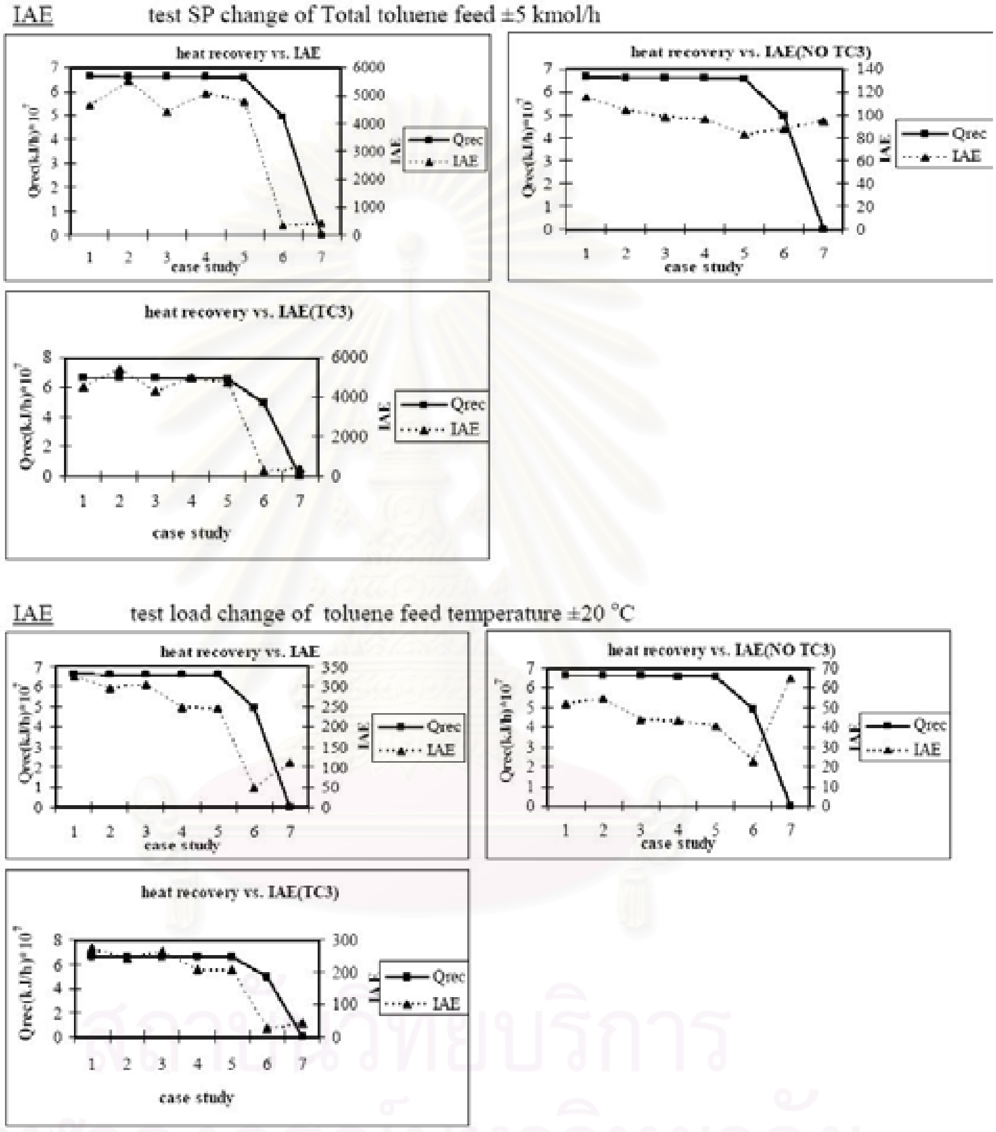
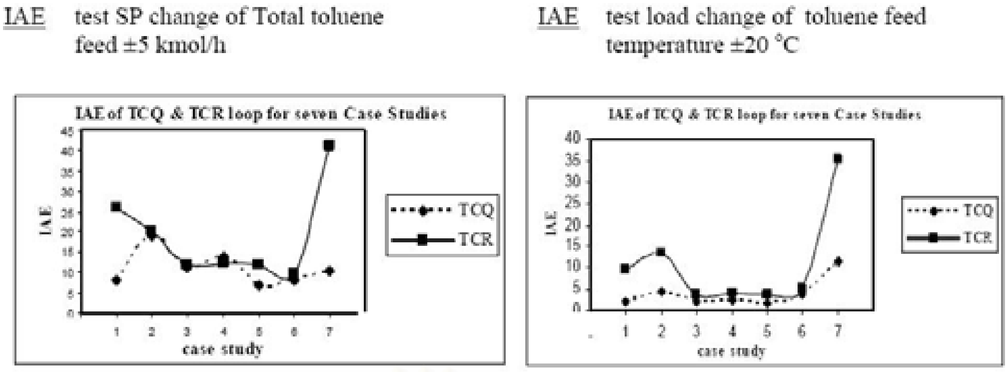


Figure 6.23: Relationship between heat recovery and control performance from testing set-point change and load disturbance of seven case studies. (CS1).



IAE test SP change of Total toluene feed ±5 kmol/h

IAE test load change of toluene feed temperature ±20 °C

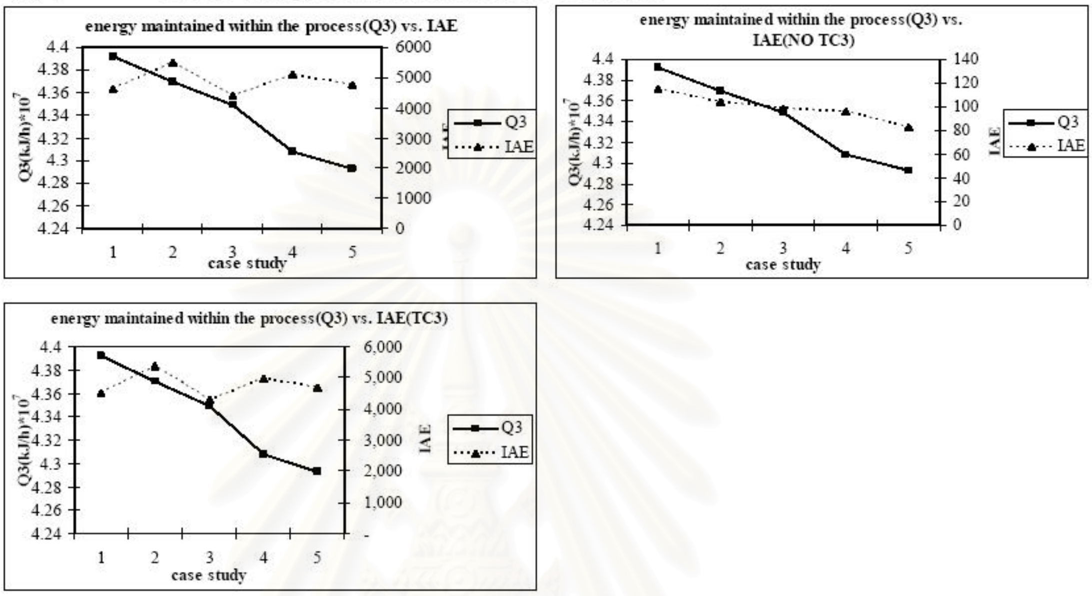
Figure 6.24: Comparison of IAEs of TCQ, TCR loops for seven case studies in both testings.

The relationship between energy maintained within process (Q3) and control performance from testing set-point change and load disturbance of five case studies are shown in Fig. 6.25. We see that, among the Case Studies 1-5, the case with less energy maintained within the process (Q3), i.e., more amount of heat is required from utility, has lower IAEs in most of each control loops because the process containing big furnace (large heat to the furnace) can handle more disturbances load, i.e., available desired outlet temperature. See fig. 6.26 for furnace duty in each cases. We also notice from IAEs of TCQ and TCR loops in Fig. 6.24 that the Case Study 3, 4 and 5 containing large furnace have better control performance in these loops (smaller IAEs). That can also affect to separation section to be easier to control because of not much fluctuation in outlet substances from reaction and fluctuation in temperature coming from quenching.

If considering summation of IAE values, we will see that Case Study 1 and 3 in testing set-point change of total toluene feed give smallest values. Since the temperature profile of the recycle column (TC3) is very sharp due to the large difference in boiling points between toluene and diphenyl, it is difficult to control. The IAE of this loop is higher than other loops studied by the order of 10-100. So the IAE of the recycle column dominate the outcomes. Case study 1 and 3 has smallest summation of IAEs as shown in Fig. 6.25.

If we consider that the recycle column separates Toluene and Diphenyl. Toluene is recycled back to the process and Diphenyl is the by-product, we can ignore its IAEs in our evaluation. The results are shown in Fig. 6.25 which the irregularity is removed.

IAE test SP change of Total toluene feed ±5 kmol/h



IAE test load change of toluene feed temperature ±20 °C

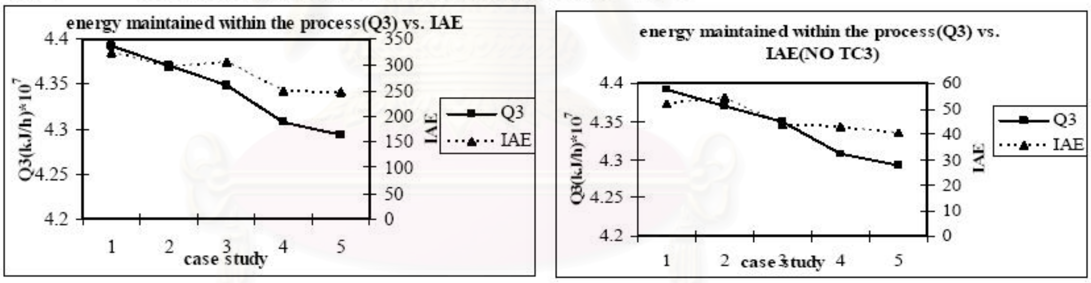


Figure 6.25: Relationship between energy maintained within the process (Q3) and control performance from testing set-point change and load disturbance of five case studies. (CS1).

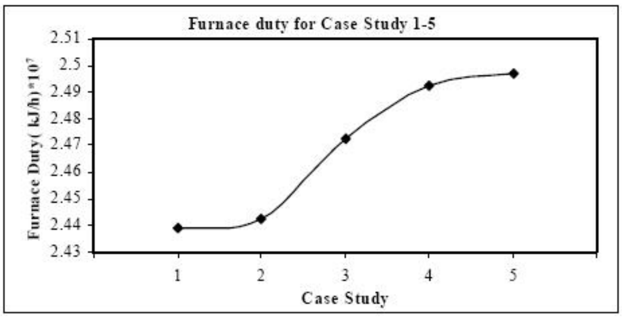


Figure 6.26: Furnace duty for Case Study 1-5.

6.4.3.2 Control Structure 2 (CS2)

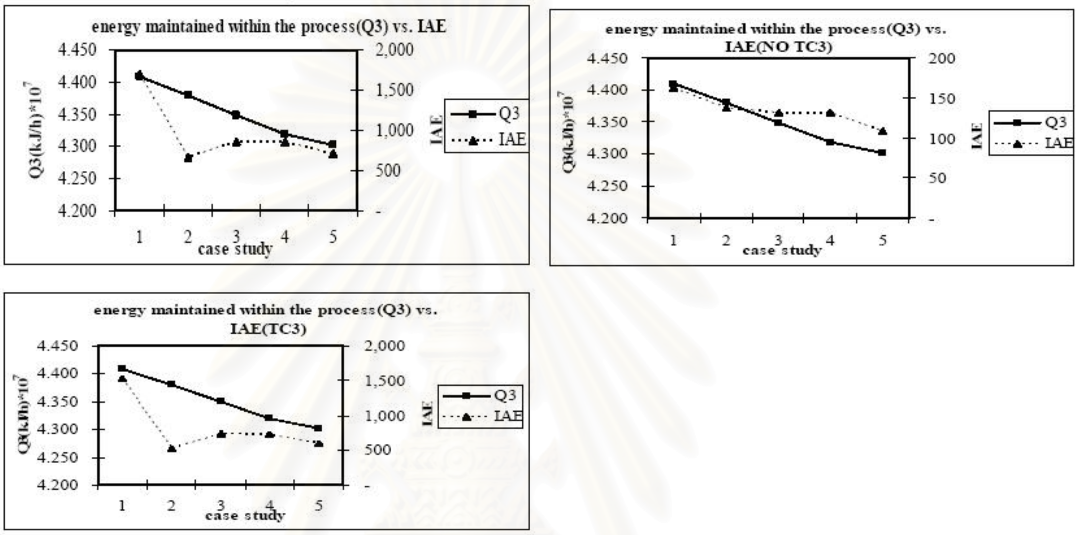
The relationship between energy maintained within the process (Q3) and control performance from testing set-point change and load disturbance of five case studies are shown in Fig. 6.27. The pattern of changes of Q3 of five case studies are similar as in the CS1 except summation of IAE values in set-point change of total toluene feed. Since the IAE of temperature control loop of recycle column is dominating and it has lowest IAE in Case Study 2, the total IAE values is lowest here. The result is shown in Fig. 6.27.

Note that IAE of the temperature control loop of recycle column (TC3) in CS2 is much less than in CS1, especially for the set-point change of total toluene feed rate. See Fig. 6.28 and 6.29. Since the fresh feed hydrogen molar flow is inverse response process and toluene and hydrogen which are the reactants, They affects the reaction resulting in fluctuation of toluene molar flow out of the reactor and toluene molar flow into recycle column. Hence the controlled temperature of the recycle column is oscillated around its set point in the way that decreasing when toluene molar flow into recycle column increases and vice versa.

The inverse response phenomena occurring in CS1 can be explained as follow. When total toluene flow rate decreases, the pressure of recycle gas stream decreases at first and then fresh feed hydrogen control loop will open control valve more. This makes the pressure of recycle gas stream increases.

In CS2, the ratio control is used. Toluene molar flow at those positions does not much fluctuate because proportion of hydrogen/toluene is kept almost constant.

IAE test SP change of Total toluene feed ±5 kmol/h



IAE test load change of toluene feed temperature ±20 °C

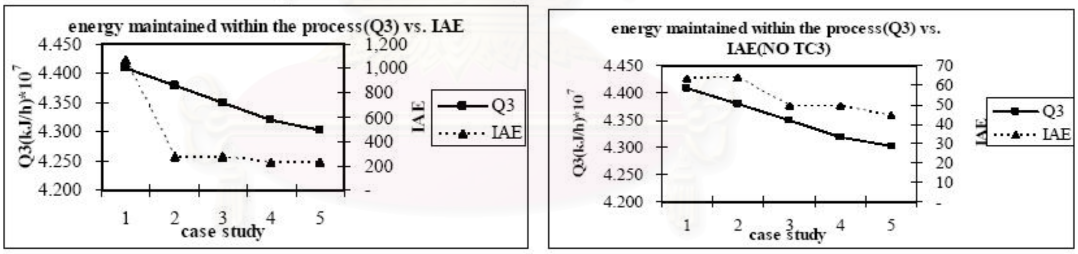


Figure 6.27: Relationship between energy maintained within the process (Q3) and control performance from testing set-point change and load disturbance of five case studies. (CS2).

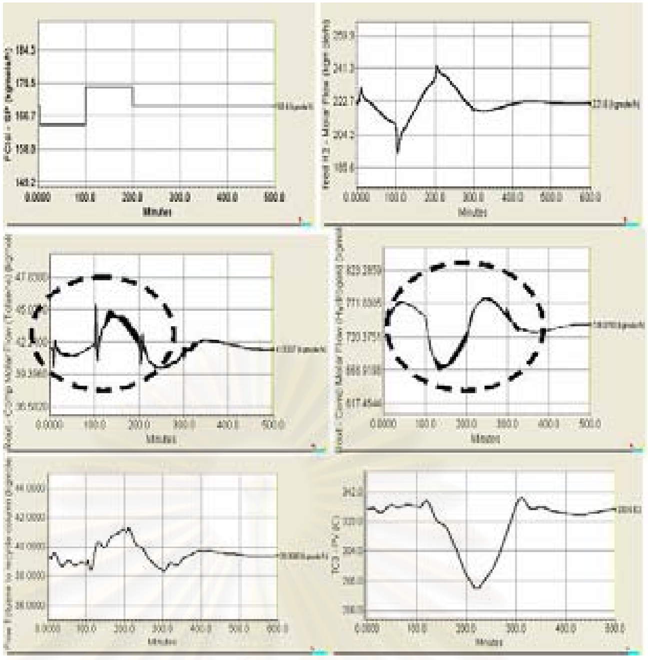


Figure 6.28: Dynamic responses of process variables to a ±5 kmol/h set-point change in total toluene feed rate for CS1.

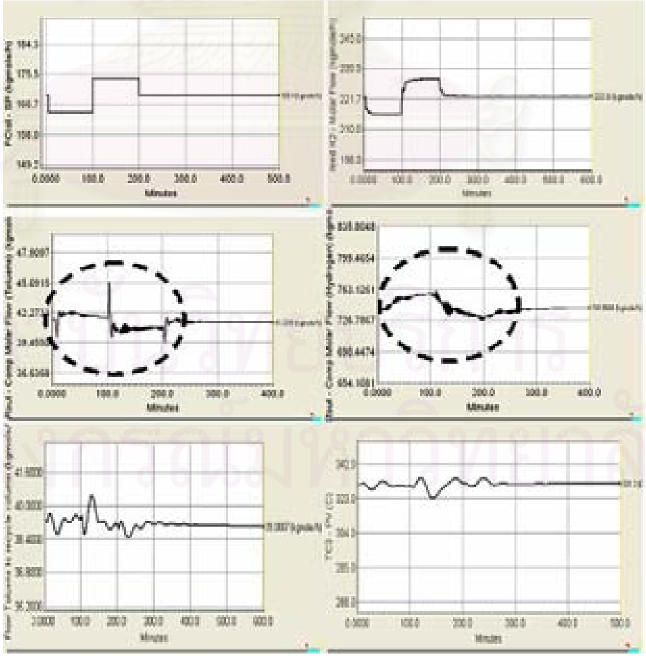
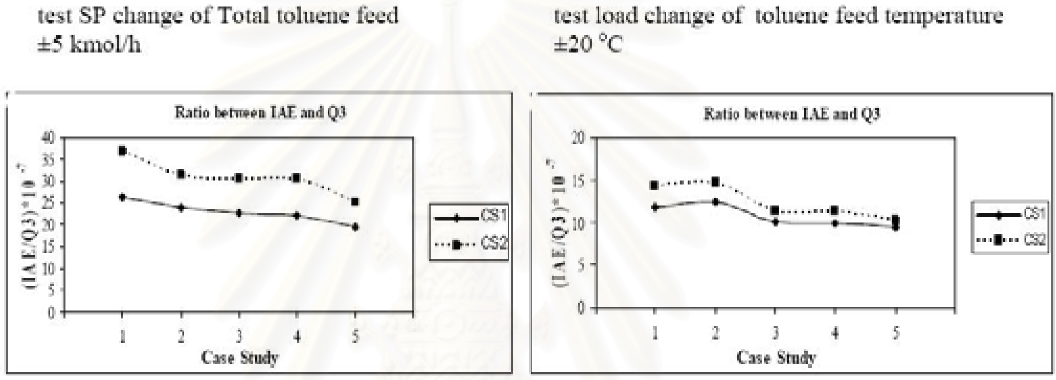


Figure 6.29: Dynamic responses of process variables to a ±5 kmol/h set-point change in total toluene feed rate for CS2.

6.4.3.3 Optimum energy maintained within the process (Q3)

In our five case studies, we usually desire to get a lot of energy maintained in the process (Q3) and also get better control performance, i.e., lower IAE. Trade-off between Q3 and IAE (no TC3) are needed. We provide a ratio of IAE/Q3 in each case studies as shown in Fig. 6.30, and then we need the lowest one from reasons mentioned above.

The result shows that the ratio of IAE/Q3 is decreasing from Case Study 1 to 5 for both two control structures and gives lowest in Case Study 5, so optimum energy maintained within the process (Q3) lies on Case Study 5.


test SP change of Total toluene feed ±5 kmol/h

test load change of toluene feed temperature ±20 °C

Figure 6.30: Trade-off between Q3 and IAE (no TC3) through the ratio of IAE/Q3 in each case studies for both two control structures.

6.5 The relationship between effectiveness of energy utilization and the energy maintained within the process (Q3)

Considering the effectiveness of energy utilization, i.e. the equations in table 6.10, and 6.11, this shows that larger $\epsilon_{ex,i}$'s (i.e., recovery of a large amount of heat at the reboiler) leads to a smaller overall effectiveness, ϵ_o , in other words, less heat is used internally for process stream heating and cooling. Next, consider the three heat pathways point of view, Path 1+2, shown in Fig. 6.10, conveys portion of heat through the distillation columns and reaches its destinations in the condensers. More heat recovered via the reboiler means more heat flowed out of the process to the environment, i.e., Q1+Q2. Hence, less heat is maintained within the process (Q3), as shown in Fig. 6.11.

Moreover, this can also be seen that the effect of $\epsilon_{2,3}$ on the overall effectiveness is decreased by a factor of (1-$\epsilon_{ex,i}$), which is always less than 1 (Chen and Yu, 2003), whereas ϵ_1 still has its original direct effect on ϵ_o . The large the portion of heat recovered via the third FEHE (large ϵ_1) has more effect on increasing of heat used in process internally (large ϵ_o). In our study, the hot stream entering the third FEHE inlet has highest temperature and should transfer most of its heat to incoming cold stream here.

Small amount of heat is recovered via the reboilers of the stabilizer column (R1) and the product column (R2) in Case Study 1, 2 because most heat is utilized in the three FEHEs, resulting in smaller values of ,$\epsilon_{ex,3,1}$,$\epsilon_{ex,3,2}$. On another hand, the hot stream outlet temperatures of the third FEHE are different as shown in Fig. 12. In Case Studies 3, and 4 and 5, the cold stream is bypassed across FEHE3, so we have small ϵ_1 's. In Case Study 1 and 2 (without bypass and bypass only at the second FEHE) we have larger ϵ_1 . We see that larger energy maintained within the process (Q3) reflect in small values of $\epsilon_{ex,3,1}$, $\epsilon_{ex,3,2}$ and large value of ϵ_1 in Case Study 1 and 2 (also large value of ϵ_o), see table 6.13.

The heat flow represents the movement of heat from place to place; the energy maintained within the process can be obtained from the sum of heat duty of

Table 6.13 Effectiveness of each of heat exchangers in five case studies and heat flow in two paths

case	ε_1 (FEHE3)	ε_2 (FEHE2)	ε_3 (FEHE1)	$\varepsilon_{ex,2}$	$\varepsilon_{ex,3,1}$	$\varepsilon_{ex,3,2}$	ε_o ($Cp_{,H}=Cp_{,C}$)	ε_o (general eq.)	Q1+Q2 (kJ/h)	Q 3 (kJ/h)
1	0.5115	0.3118	0.546	0.0466	0.11	0.1623	0.6752	0.8158	31,554,965.85	43,923,458.88
2	0.5253	0.2849	0.5462	0.0411	0.1128	0.1644	0.6771	0.8158	31,557,715.36	43,698,093.18
3	0.4981	0.3018	0.5444	0.0383	0.1187	0.1700	0.5620	0.7998	31,867,330.87	43,398,215.64
4	0.4976	0.2918	0.5440	0.0369	0.1237	0.1751	0.6636	0.7954	32,071,527.66	43,080,776.82
5	0.5000	0.2798	0.5437	0.0352	0.1255	0.1765	0.6623	0.7917	32,106,476.65	42,934,702.50

Table 6.14 The quantities of heat in Path 1+2, Path 3 and ε_o are in order

property	Quatity : large ⟶ small				
	(Case Study)				
Q1+Q2	5	4	3	2	1
Q3	1	2	3	4	5
ε_o(Chen and Yu's)	2	1	4	5	3
ε_o(Our Equations)	1 ≈ 2		3	4	5

FEHE1, FEHE1 and FEHE3. When most of heat is brought back in process (Q3), small amount of heat is dissipated to the environment (Q1+Q2). This translates into a reduction in utility cost and improves the thermodynamic efficiency of the process. The quantities of heat in Path 1+2, Path 3 and ϵ_o are in order as shown in Table 6.14.

It can be seen that the Chen and Yu's overall effectiveness (derived by assuming m$C_{P,H}$ = m$C_{P,C}$) cannot reveal the correct quantity of energy maintained within the process (Q3) of each case studies due to the difference between capacity flow rates of hot and cold stream inlet of heat exchangers. Our overall effectiveness equations which include explicit capacity flow rates in equation gives more accurate values of energy maintained within the process (Q3).

We also show the dynamic responses of production rate of Benzene out of the reactor and distilate of product column to set-point change of total toluene feed ±5 kmol/h and load change of toluene feed temperature ±20 ^{o}C in both control structures. See appendix C.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusion

Energy conservation has always been important in process design. Use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost. Thus, it was common practice to install feed-effluent exchangers around reactors and distillation columns as Hydrodealkylation of toluene (HDA) process (alternative 6). Positive feedback can occur and makes the plants more difficult to control (Luyben, 1999). There are conflicts between steady-state economics and dynamic controllability. Recent study has suggested three different "heat pathways" of HDA process (Luyben, 1999). The first pathway is from inside the process and flows out to the environment through cooler. The second pathway carries heat from utilities into the process and flows out to the environment through three reboilers. The third pathway is internal to the process. Here heat flows back and forth between different unit operations.

The ideas of Luyben's heat pathways were taken into account in order to get insight where energy source, energy sink and paths of energy were. These ideas helped us to design several levels of energy maintained within the process (third pathway, Q3) for HDA process (alt.6) in five case studies. The other two Case Studies were simulated for HDA process (alt.1) and HDA process (without energy integration). Then the performances of the those designed processes were evaluated dynamically for two different control structures: with and without ratio control. Two disturbances were tested as set-point change of total toluene feed and load disturbances of toluene feed temperature. Set-point change of total toluene feed is adjusted for production rate, and load disturbances of toluene feed temperature represent fluctuations in fresh feed streams caused by environmental effect. The overall effectiveness was introduced to relate with energy maintained within the process (Q3) and derived in general equations.

The following conclusions can be made from the simulation of present investigation:

1. Overall effectiveness is rederived in general form, which realistically represents the thermal efficiency of a process.
2. Overall effectiveness relates with the amount of Q3 and the control performance. More energy maintained within the process more is the overall effectiveness.
3. Without energy integration in the separation section, the disturbance does not propagate to this section through heat-integrated heat exchangers, i.e., reboiler of distillation columns and the FEHE behaves like the buffer tank to attenuate the disturbances.
4. In this study, the case with less energy maintained within the process (Q3), i.e., more amount of heat is required from utility, has better control performance because the process containing big furnace (large heat to the furnace) can handle more disturbances load, i.e., available desired outlet temperature.
5. The lowest ratio of IAE/Q3 is referred to indicate optimum energy maintained within the process (Q3) in this work.
6. When ratio control (CS2) is used to keep hydrogen/toluene constant, give the same results of the effect of levels of energy maintained within the process on control performance and also give the smoother operations in control loop relating to those reactants, e.g. temperature control loop of recycle column.

7.2 Recommendations

Find the measurements that can be used to indicate the optimum heat flow maintained within the process (Q in path3).

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APPENDICES

APPENDIX A

Table A.1 Data of HDA process (alt. 6) for simulation

Name	FFtol	FFH2	v1out	v2out	Rtol	Rgas	hHE1in	cHE1out	hHE2in
temperature (^oC)	30.00	30.00	30.00	30.11	183.86	76.15	174.43	145.30	434.90
pressure (kPa)	4378.17	4378.17	4171.33	4171.33	4171.33	4171.33	3178.48	3950.70	3275.01
Molar flow (kgmole/h)	131.09	222.72	222.72	131.09	38.32	1596.30	2037.96	1988.43	2037.96
Comp Mole Frac (Hydrogen)	0.0000	0.9700	0.9700	0.0000	0.0000	0.4005	0.3571	0.4302	0.3571
Comp Mole Frac (Methane)	0.0000	0.0300	0.0300	0.0000	0.0000	0.5879	0.5289	0.4753	0.5289
Comp Mole Frac (Benzene)	0.0000	0.0000	0.0000	0.0000	0.0003	0.0104	0.0869	0.0084	0.0869
Comp Mole Frac (Toluene)	1.0000	0.0000	0.0000	1.0000	0.9987	0.0012	0.0253	0.0861	0.0253
Comp Mole Frac (BiPhenyl)	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0018	0.0000	0.0018
Name	hHE2out	hHE3in	hHE3out	Rin	quench	coolout	grecycle	dischg	v5out
temperature (^oC)	352.00	620.84	450.00	621.11	45.38	45.00	45.00	76.15	45.95
pressure (kPa)	3233.64	3350.85	3309.48	3468.06	3350.85	3115.05	3115.05	4171.33	1038.00
Molar flow (kgmole/h)	2037.96	2037.96	2037.96	1988.43	49.50	2037.96	1596.30	1596.30	172.18
Comp Mole Frac (Hydrogen)	0.3571	0.3571	0.3571	0.4302	0.0044	0.3571	0.4001	0.4001	0.0044
Comp Mole Frac (Methane)	0.5289	0.5289	0.5289	0.4753	0.0427	0.5289	0.5882	0.5882	0.0427
Comp Mole Frac (Benzene)	0.0869	0.0869	0.0869	0.0084	0.7140	0.0869	0.0104	0.0104	0.7132
Comp Mole Frac (Toluene)	0.0253	0.0253	0.0253	0.0861	0.2221	0.0253	0.0012	0.0012	0.2229
Comp Mole Frac (BiPhenyl)	0.0018	0.0018	0.0018	0.0000	0.0168	0.0018	0.0000	0.0000	0.0167

Table A.1 Data of HDA process (alt. 6) for simulation (cont.)

Name	boil1	d1	toR1	v7out	boil2	d2	v9out	boil3	ref
temperature (^oC)	215.00	51.07	189.93	115.56	193.00	105.47	144.35	350.70	182.18
pressure (kPa)	1041.11	1034.00	1297.95	214.10	223.46	206.84	543.30	549.90	540.00
Molar flow (kgmole/h)	183.83	8.47	183.83	163.71	386.56	122.54	41.17	47.26	10.04
Comp Mole Frac (Hydrogen)	0.0000	0.0895	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0000	0.8681	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Benzene)	0.7487	0.0420	0.7483	0.7483	0.0002	0.9997	0.0002	0.0000	0.0003
Comp Mole Frac (Toluene)	0.2337	0.0004	0.2341	0.2341	0.9299	0.0003	0.9299	0.0012	0.9987
Comp Mole Frac (BiPhenyl)	0.0176	0.0000	0.0176	0.0176	0.0699	0.0000	0.0699	0.9988	0.0010

Name	b3	condout	d3	reflux	toCR	toR3
temperature (^oC)	349.44	180.80	183.84	183.84	144.27	349.44
pressure (kPa)	798.21	526.21	4378.17	4378.17	902.67	798.21
Molar flow (kgmole/h)	2.84	48.37	38.33	10.04	386.56	47.26
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Benzene)	0.0000	0.0003	0.0003	0.0003	0.0002	0.0000
Comp Mole Frac (Toluene)	0.0012	0.9987	0.9987	0.9987	0.9299	0.0012
Comp Mole Frac (BiPhenyl)	0.9988	0.0010	0.0010	0.0010	0.0699	0.9988

Name	qfur	qcooler	qc1	qc2	wkcomp
Heat flow (kJ/h)	21,613,744.05	6,989,807.11	1,413,073.93	18,119,250.77	1,680,449.24
Name	wkp1	wkp2	wkp3	wkp4	wkp5
Heat flow (kJ/h)	14,388.94	14,453.27	48,991.82	32,651.57	3,454.77

Table A.2 Data of HDA process (alt. 1) for simulation

Name	FFtol	FFH2	v1out	v2out	Rtol	Rgas	Rin	quench	hHEin	coolout
temperature (^oC)	30.00	30.00	30.00	30.11	140.27	70.33	621.11	45.46	621.06	45.00
pressure (kPa)	4378.17	4378.17	4171.33	4171.33	4171.33	4171.33	3468.06	3350.85	3350.85	3287.42
Molar flow (kgmole/h)	131.09	222.72	222.72	131.09	38.30	1596.30	1988.40	49.49	2037.72	2037.72
Comp Mole Frac (Hydrogen)	0.0000	0.9700	0.9700	0.0000	0.0000	0.4012	0.4308	0.0047	0.3580	0.3580
Comp Mole Frac (Methane)	0.0000	0.0300	0.0300	0.0000	0.0000	0.5875	0.4750	0.0449	0.5284	0.5284
Comp Mole Frac (Benzene)	0.0000	0.0000	0.0000	0.0000	0.0006	0.0101	0.0081	0.7124	0.0866	0.0866
Comp Mole Frac (Toluene)	1.0000	0.0000	0.0000	1.0000	0.9993	0.0012	0.0861	0.2215	0.0252	0.0252
Comp Mole Frac (BiPhenyl)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0165	0.0018	0.0018

Name	grecycle	dischg	v5out	d1	v7out	d2	v9out	b3	d3
temperature (^oC)	70.33	70.33	45.97	51.04	116.68	105.55	143.44	292.68	137.64
pressure (kPa)	4171.33	4171.33	1048.00	1034.21	220.63	206.84	220.63	213.74	206.84
Molar flow (kgmole/h)	1596.30	1815.57	172.93	8.95	163.98	122.84	41.14	2.85	38.30
Comp Mole Frac (Hydrogen)	0.4012	0.4012	0.0047	0.0902	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.5875	0.5875	0.0449	0.8674	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Benzene)	0.0101	0.0101	0.7124	0.0420	0.7490	0.9997	0.0006	0.0000	0.0006
Comp Mole Frac (Toluene)	0.0012	0.0012	0.2215	0.0003	0.2336	0.0003	0.9302	0.0003	0.9993
Comp Mole Frac (BiPhenyl)	0.0000	0.0000	0.0165	0.0000	0.0174	0.0000	0.0692	0.9997	0.0000

Name	qfur	qcooler	qc1	qc2	qc3	qr1	qr2	qr3	wkp1	wkp2	wkp3	wkcomp
Heat flow (kJ/h)	3,307,481.92	9,820,691.14	654,454.83	14,520,425.79	1,548,728.69	4,540,128.45	12,393,568.38	1,708,502.91	14,397.27	955.28	26,106.46	1,547,238.49

Table A.3 Data of HDA process (NO FEHE) for simulation

Name	FFtol	FFH2	v1out	v2out	Rtol	Rgas	Rin	quench	hHEin	coolout
temperature (^{o}C)	30.00	30.00	30.00	30.11	140.27	70.33	621.11	45.46	621.06	45.00
pressure (kPa)	4378.17	4378.17	4171.33	4171.33	4171.33	4171.33	3468.06	3350.85	3350.85	3287.42
Molar flow (kgmole/h)	131.09	222.72	222.72	131.09	38.30	1596.30	1988.40	49.49	2037.72	2037.72
Comp Mole Frac (Hydrogen)	0.0000	0.9700	0.9700	0.0000	0.0000	0.4012	0.4308	0.0047	0.3580	0.3580
Comp Mole Frac (Methane)	0.0000	0.0300	0.0300	0.0000	0.0000	0.5875	0.4750	0.0449	0.5284	0.5284
Comp Mole Frac (Benzene)	0.0000	0.0000	0.0000	0.0000	0.0006	0.0101	0.0081	0.7124	0.0866	0.0866
Comp Mole Frac (Toluene)	1.0000	0.0000	0.0000	1.0000	0.9993	0.0012	0.0861	0.2215	0.0252	0.0252
Comp Mole Frac (BiPhenyl)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0165	0.0018	0.0018

Name	grecycle	dischg	v5out	d1	v7out	d2	v9out	b3	d3
temperature (^{o}C)	70.33	70.33	45.97	51.04	116.68	105.55	143.44	292.68	137.64
pressure (kPa)	4171.33	4171.33	1048.00	1034.21	220.63	206.84	220.63	213.74	206.84
Molar flow (kgmole/h)	1596.30	1815.57	172.93	8.95	163.98	122.84	41.14	2.85	38.30
Comp Mole Frac (Hydrogen)	0.4012	0.4012	0.0047	0.0902	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.5875	0.5875	0.0449	0.8674	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Benzene)	0.0101	0.0101	0.7124	0.0420	0.7490	0.9997	0.0006	0.0000	0.0006
Comp Mole Frac (Toluene)	0.0012	0.0012	0.2215	0.0003	0.2336	0.0003	0.9302	0.0003	0.9993
Comp Mole Frac (BiPhenyl)	0.0000	0.0000	0.0165	0.0000	0.0174	0.0000	0.0692	0.9997	0.0000

Name	qfur	qcooler	qc1	qc2	qc3	qr1	qr2	qr3	wkp1	wkp2	wkp3	wkcomp
Heat flow (kJ/h)	68,041,393.96	74,554,603.18	655,853.35	14,521,133.34	1,548,740.69	4,541,767.16	12,394,279.74	1,708,515.76	14,397.27	955.28	26,106.46	1,547,238.50

Equipment data and specifications

Table A.4 Column specifications

	Stabilizer column	Product column	Recycle column
Number of theoretical trays	6	27	7
Feed tray	3	15	5
Diameter (ft)	3.5	16.97	2
Reboiler volume (ft^3)	250	320	100
Condenser volume (ft^3)	18	366.2	150
Reflux ratio	3.86	4.05	0.32
Specification 1	Benzene fraction in overhead = 0.042	Toluene fraction in distillate = 0.0003	Diphenyl fraction in distillate = 0.00002
Specification 2 .	Methane fraction in bottom =1ppm.	Benzene fraction in bottom = 0.0006	Toluene fraction in bottom = 0.00026

Table A.5 Equipment data

HDA process (alt. 6)

Reactor	Length (ft)	57
	Diameter (ft)	9.53
Furnace	Tube volume	300
Separator	Volume (ft^3)	80
FEHE 1	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	3.64E+05
FEHE 2	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	2.76E+04
FEHE 3	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	6.85E+04

Table A.5 Equipment data (cont.)

R1	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	2.11E+04
R2	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	1.64E+05
R3	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	1.15E+04

HDA process (alt. 1)

Reactor	Length (ft)	57
	Diameter (ft)	9.53
Furnace	Tube volume	300
Separator	Volume (ft^3)	80
FEHE 1	Shell volume (ft^3)	500
	Tube volume (ft^3)	500
	UA (Btu/F-hr)	8.19E+05

HDA process (NO FEHE)

Reactor	Length (ft)	57
	Diameter (ft)	9.53
Furnace	Tube volume	300
Separator	Volume (ft^3)	80

APPENDIX B

PARAMETER TUNING

Tuning Flow, Level, Pressure and Temperature Loops

Flow Controllers

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

In a real plant application, filtering of the flow signal is also recommended because of the noise. So filter is put at controller output signal and a good number to use for a flow loop is τ_F = 0.1 minute.

Level Controllers

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

Pressure Controllers

Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Of course the gain used depends on the span of the pressure transmitter. Some simple step tests can be used to find the value of controller gain that yields satisfactory pressure control.

Typical pressure controller tuning constants for columns and tanks are $K_C = 2$ and $\tau_I = 10$ minutes.

Temperature Controllers

If we have a controller that needs tuning and after we have inserted reasonable lags and deadtimes, we need a quick and simple method for identifying the dynamic parameters that are important for designing a feedback controller. The relay-feedback test is a tool that serves this purpose well. The results of the test are the ultimate gain and the ultimate frequency. This information is usually sufficient to permit us to calculate some reasonable controller tuning constants.

The method consists of merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the height of the relay h. This height is typically 5 to 10% of the controller-output scale. The loop starts to oscilate around the setpoint, with the controller output switching every time the process varisble (PV) signal crosses the setpoint.

The maximum amplitude of the PV signal is used to calculate the ultimate gain K_u from the equation:

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

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

Relay feedback testing can be done in HYSYS. It simply click the Tuning botton on the controller faceplate, select Autotuning and click the Start Autotuning button. The loop will start to oscilate. After several cycles, the tuning is stoppedand some recommended settings for a PID controller are suggested.

Inclusion of Lags

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

In this plant, we include lags at temperature control loops of TCQ, TCR, TC2 and TC3. Some lags are recommended in table below:

Table B.1 Typical measurement lags

		Number	Time constant (minutes)	Type
Temperature	Liquid	2	0.5	First-Order Lag
	Gas	3	1	First-Order Lag

Table B.2 Parameter tuning of HDA process (alt.6) for case study 1

Controller	Process variable	Output	Control action	Set point	K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 auxilary duty (qar1)	Reverse	166.43 °C	3.8070	1.5884	0.3530
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00 kPa	2	10	-
FCB1	column1 boilup flowrate	column1 boilup valve (V18)	Reverse	183.83 kgmole/h	0.5	0.3	-
LC11	column1 tank level	column2 feed valve (V7)	Direct	50.00 %	2	-	-
LC12	column1 reflux drum level	column1 condenser duty (qc1)	Reverse	50.00 %	2	-	-
TC2	column2 stage 12 temperature	column2 auxilary duty (qar2)	Reverse	121.11 °C	3	2.5936	0.5764
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84 kPa	2	10	-
FCB2	column2 boilup flowrate	column2 boilup valve (V10)	Reverse	386.56 kgmole/h	0.5	0.3	-
LC21	column2 tank level	column3 feed valve (V9)	Direct	50.00 %	2	-	-
LC22	column2 reflux drum level	column2 distillate flow valve (V8)	Direct	50.00 %	2	-	-
TC3	column3 average temperature	exchanger R3 bypass valve(vbp4)	Direct	331.11 °C	3.1100	45.7670	10.1704
PC3	column3 tank pressure	exchanger CR bypass valve(vbp7)	Reverse	526.21 kPa	2	10	-
FCB3	column3 boilup flowrate	column3 boilup valve (V19)	Reverse	47.26 kgmole/h	0.5	0.3	-
LC31	column3 bottom tank level	column3 bottom valve (V12)	Direct	50.00 %	2	-	-
LC32	column3 top tank level	column3 top valve (V3)	Direct	50.00 %	2	-	-
FCR	column3 reflux flowrate	column3 reflux valve (V11)	Reverse	10.04 kgmole/h	0.5	0.3	-
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41 kgmole/h	0.5	0.3	-

Table B.2 Parameter tuning of HDA process (alt.6) for case study 1 (cont.)

Controller	Process variable	Output	Control action	Set point	K_C	τ_I (min)	τ_d (min)
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33 kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59 -	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00 %	2	-	-
TCQ	quenched temperature	quenched valve (V13)	Direct	621.11 ^{o}C	0.2311	1.6844	0.3743
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	621.11 ^{o}C	1.6631	0.9281	0.2062
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00 ^{o}C	1.6767	0.3197	0.0711
TCE2H	FEHE2 hot stream outlet temperature	valve bypass across FEHE2(vbp2)	Reverse	352.00 ^{o}C	1	2	-
TCE3H	FEHE3 hot stream outlet temperature	valve bypass across FEHE3(vbp3)	Reverse	450.00 ^{o}C	1	2	-

Table B.3 Parameter tuning of HDA process (alt.6) for case study 2

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 auxilary duty (qar1)	Reverse	166.43	°C	4.6951	1.3351	0.2967
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	2	10	-
FCB1	column1 boilup flowrate	column1 boilup valve (V18)	Reverse	183.83	kgmole/h	0.5	0.3	-
LC11	column1 tank level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 reflux drum level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 auxilary duty (qar2)	Reverse	121.11	°C	5.6000	1.9072	0.4238
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	2	10	-
FCB2	column2 boilup flowrate	column2 boilup valve (V10)	Reverse	386.56	kgmole/h	0.5	0.3	-
LC21	column2 tank level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 reflux drum level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	exchanger R3 bypass valve(vbp4)	Direct	331.11	°C	11.3851	27.2240	6.0498
PC3	column3 tank pressure	exchanger CR bypass valve(vbp7)	Reverse	526.21	kPa	2	10	-
FCB3	column3 boilup flowrate	column3 boilup valve (V19)	Reverse	47.26	kgmole/h	0.5	0.3	-
LC31	column3 bottom tank level	column3 bottom valve (V12)	Direct	50.00	%	2	-	-
LC32	column3 top tank level	column3 top valve (V3)	Direct	50.00	%	2	-	-
FCR	column3 reflux flowrate	column3 reflux valve (V11)	Reverse	10.04	kgmole/h	0.5	0.3	-
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	kgmole/h	0.5	0.3	-

Table B.3 Parameter tuning of HDA process (alt.6) for case study 2 (cont.)

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V13)	Direct	621.11	^{o}C	0.1293	0.2142	0.0476
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	621.11	^{o}C	0.0835	0.2165	0.0481
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	^{o}C	1.6288	0.3301	0.0733
TCE2H	FEHE2 hot stream outlet temperature	valve bypass across FEHE2(vbp2)	Reverse	353.19	^{o}C	1	2	-
TCE3H	FEHE3 hot stream outlet temperature	valve bypass across FEHE3(vbp3)	Reverse	449.91	^{o}C	1	2	-

Table B.4 Parameter tuning of HDA process (alt.6) for case study 3

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 auxilary duty (qar1)	Reverse	166.43	^oC	4.0282	1.5244	0.3387
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	2	10	-
FCB1	column1 boilup flowrate	column1 boilup valve (V18)	Reverse	183.83	kgmole/h	0.5	0.3	-
LC11	column1 tank level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 reflux drum level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 auxilary duty (qar2)	Reverse	121.11	^oC	5.8000	1.5135	0.3363
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	2	10	-
FCB2	column2 boilup flowrate	column2 boilup valve (V10)	Reverse	386.56	kgmole/h	0.5	0.3	-
LC21	column2 tank level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 reflux drum level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	exchanger R3 bypass valve(vbp4)	Direct	331.11	^oC	10.8537	30.4211	6.7602
PC3	column3 tank pressure	exchanger CR bypass valve(vbp7)	Reverse	526.21	kPa	2	10	-
FCB3	column3 boilup flowrate	column3 boilup valve (V19)	Reverse	47.26	kgmole/h	0.5	0.3	-
LC31	column3 bottom tank level	column3 bottom valve (V12)	Direct	50.00	%	2	-	-
LC32	column3 top tank level	column3 top valve (V3)	Direct	50.00	%	2	-	-
FCR	column3 reflux flowrate	column3 reflux valve (V11)	Reverse	10.04	kgmole/h	0.5	0.3	-
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	kgmole/h	0.5	0.3	-

Table B.4 Parameter tuning of HDA process (alt.6) for case study 3 (cont.)

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V13)	Direct	621.11	°C	1.2881	1.3074	0.2905
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	621.11	°C	0.4213	1.2158	0.2701
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	°C	1.5622	0.3497	7.7716
TCE2H	FEHE2 hot stream outlet temperature	valve bypass across FEHE2(vbp2)	Reverse	358.54	°C	1	2	-
TCE3H	FEHE3 hot stream outlet temperature	valve bypass across FEHE3(vbp3)	Reverse	455.69	°C	1	2	-

Table B.5 Parameter tuning of HDA process (alt.6) for case study 4

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 auxilary duty (qar1)	Reverse	166.43	°C	4.8777	1.2850	0.2856
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	2	10	-
FCB1	column1 boilup flowrate	column1 boilup valve (V18)	Reverse	183.83	kgmole/h	0.5	0.3	-
LC11	column1 tank level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 reflux drum level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 auxilary duty (qar2)	Reverse	121.11	°C	5	1.9260	0.4280
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	2	10	-
FCB2	column2 boilup flowrate	column2 boilup valve (V10)	Reverse	386.56	kgmole/h	0.5	0.3	-
LC21	column2 tank level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 reflux drum level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	exchanger R3 bypass valve(vbp4)	Direct	331.11	°C	10.4441	21.9813	4.8847
PC3	column3 tank pressure	exchanger CR bypass valve(vbp7)	Reverse	526.21	kPa	2	10	-
FCB3	column3 boilup flowrate	column3 boilup valve (V19)	Reverse	47.26	kgmole/h	0.5	0.3	-
LC31	column3 bottom tank level	column3 bottom valve (V12)	Direct	50.00	%	2	-	-
LC32	column3 top tank level	column3 top valve (V3)	Direct	50.00	%	2	-	-
FCR	column3 reflux flowrate	column3 reflux valve (V11)	Reverse	10.04	kgmole/h	0.5	0.3	-
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	kgmole/h	0.5	0.3	-

Table B.5 Parameter tuning of HDA process (alt.6) for case study 4 (cont.)

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V13)	Direct	621.11	^oC	1.0180	1.2638	0.2808
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	621.11	^oC	0.4196	1.2163	0.2703
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	^oC	1.6214	0.3221	0.0716
TCE2H	FEHE2 hot stream outlet temperature	valve bypass across FEHE2(vbp2)	Reverse	358.54	^oC	1	2	-
TCE3H	FEHE3 hot stream outlet temperature	valve bypass across FEHE3(vbp3)	Reverse	455.69	^oC	1	2	-

Table B.6 Parameter tuning of HDA process (alt.6) for case study 5

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 auxilary duty (qar1)	Reverse	166.43	°C	5.8023	1.0874	0.2416
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	2	10	-
FCB1	column1 boilup flowrate	column1 boilup valve (V18)	Reverse	183.83	kgmole/h	0.5	0.3	-
LC11	column1 tank level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 reflux drum level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 auxilary duty (qar2)	Reverse	121.11	°C	10	1.5987	0.3553
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	2	10	-
FCB2	column2 boilup flowrate	column2 boilup valve (V10)	Reverse	386.56	kgmole/h	0.5	0.3	-
LC21	column2 tank level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 reflux drum level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	exchanger R3 bypass valve(vbp4)	Direct	331.11	°C	11.4631	39.6076	8.8017
PC3	column3 tank pressure	exchanger CR bypass valve(vbp7)	Reverse	526.21	kPa	2	10	-
FCB3	column3 boilup flowrate	column3 boilup valve (V19)	Reverse	47.26	kgmole/h	0.5	0.3	-
LC31	column3 bottom tank level	column3 bottom valve (V12)	Direct	50.00	%	2	-	-
LC32	column3 top tank level	column3 top valve (V3)	Direct	50.00	%	2	-	-
FCR	column3 reflux flowrate	column3 reflux valve (V11)	Reverse	10.04	kgmole/h	0.5	0.3	-
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	kgmole/h	0.5	0.3	-

Table B.6 Parameter tuning of HDA process (alt.6) for case study 5 (cont.)

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V13)	Direct	621.11	°C	0.4168	1.2170	0.2704
TCR	reactor inlet temperature	furnace duty (qfur)	Reverse	621.11	°C	1.5626	0.9325	0.2072
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	°C	1.6380	0.3296	0.0733
TCE2H	FEHE2 hot stream outlet temperature	valve bypass across FEHE2(vbp2)	Reverse	359.40	°C	1	2	-
TCE3H	FEHE3 hot stream outlet temperature	valve bypass across FEHE3(vbp3)	Reverse	455.47	°C	1	2	-

Table B.7 Parameter tuning of HDA process (alt.1) for case study 6

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 reboiler duty (qr1)	Reverse	154.02	^oC	2	12	0.1210
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	1	10	-
LC11	column1 reboiler level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 condenser level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 reboiler duty (qr2)	Reverse	121.11	^oC	3.5171	3.7325	0.8294
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	1	10	-
LC21	column2 reboiler level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 condenser level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	column3 bottom flow valve(V10)	Direct	260.00	^oC	1.4360	19.4755	4.3279
PC3	column3 condenser pressure	column3 condenser duty (qc3)	Direct	206.84	kPa	1	10	-
LC31	column3 reboiler level	column3 reboiler duty (qr3)	Direct	50.00	%	2	-	-
LC32	column3 condenser level	column3 top valve (V3)	Direct	50.00	%	2	-	-
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V11)	Direct	621.11	^oC	1.2180	1.0499	0.2333
TCR	reacter inlet temperature	furnace duty (qfur)	Reverse	621.11	^oC	0.1776	1.2707	0.2823
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	^oC	0.4779	0.1987	4.4156
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	^oC	0.5	0.3	-

Table B.8 Parameter tuning of HDA process (NO FEHE) for case study 7

Controller	Process variable	Output	Control action	Set point		K_C	τ_I (min)	τ_d (min)
TC1	column1 top stage temperature	column1 reboiler duty (qr1)	Reverse	154.06	°C	2	12	0.1210
PC1	column1 condenser pressure	column1distilate flow valve (V6)	Direct	1034.00	kPa	1	10	-
LC11	column1 reboiler level	column2 feed valve (V7)	Direct	50.00	%	2	-	-
LC12	column1 condenser level	column1 condenser duty (qc1)	Reverse	50.00	%	2	-	-
TC2	column2 stage 12 temperature	column2 reboiler duty (qr2)	Reverse	121.11	°C	3.5636	3.6228	0.8050
PC2	column2 condenser pressure	column2 condenser duty (qc2)	Direct	206.84	kPa	1	10	-
LC21	column2 reboiler level	column3 feed valve (V9)	Direct	50.00	%	2	-	-
LC22	column2 condenser level	column2 distillate flow valve (V8)	Direct	50.00	%	2	-	-
TC3	column3 average temperature	column3 bottom flow valve(V10)	Direct	260.00	°C	0.6679	21.2567	4.7237
PC3	column3 condenser pressure	column3 condenser duty (qc3)	Direct	206.84	kPa	1	10	-
LC31	column3 reboiler level	column3 reboiler duty (qr3)	Direct	50.00	%	2	-	-
LC32	column3 condenser level	column3 top valve (V3)	Direct	50.00	%	2	-	-
PCG	recycle gas pressure	fresh feed hydrogen valve (V1)	Reverse	4171.33	kPa	2	10	-
CCG	recycle gas methane mole fraction	purge valve (V4)	Direct	0.59	-	0.2	15	-
LCS	separator tank level	column1 feed valve (V5)	Direct	50.00	%	2	-	-
TCQ	quenched temperature	quenched valve (V11)	Direct	621.11	°C	0.9983	1.0866	0.2414
TCR	reacter inlet temperature	furnace duty (qfur)	Reverse	621.11	°C	8.1520	1.7656	0.3923
TCS	cooler outlet temperature	cooler duty (qcooler)	Direct	45.00	°C	0.3520	0.2038	4.5300
FCtol	total toluene flow rate	fresh feed toluene valve (V2)	Reverse	169.41	°C	0.5	0.3	-

APPENDIX C

DYNAMIC RESPONSES

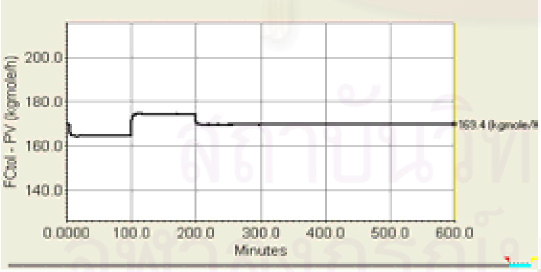
Two control structures, CS1 and CS2, are considered for evaluating the interaction of energy integration and control performance. In CS1, pressure of recycle gas stream is controlled by manipulating fresh feed hydrogen because pressure of recycle gas stream relates to the amount of recycled hydrogen to the process as shown in Fig. C.5-C.7. In CS2, the proportion of hydrogen/toluene is controlled by measuring total toluene feed flow rate to calculate set-point of fresh feed hydrogen flow rate. This loop also controls indirectly the pressure of recycle gas stream as shown in Fig. C.8-C.10.

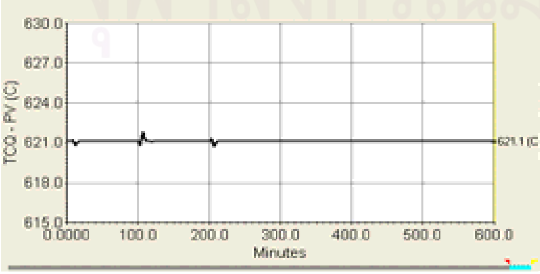
The graph responses and table of IAEs of six different levels of heat in path 3 designed by bypassing at different FEHEs (i.e., FEHE 2,3) in HDA (alt.6), HDA (alt.1) and HDA (NO FEHE) are shown in figures and tables below.

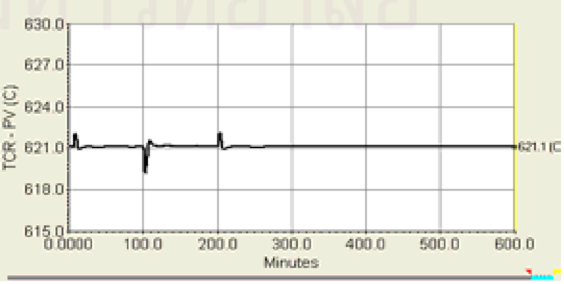
C.1 Test set-point change of Total toluene feed ±5 kmol/h

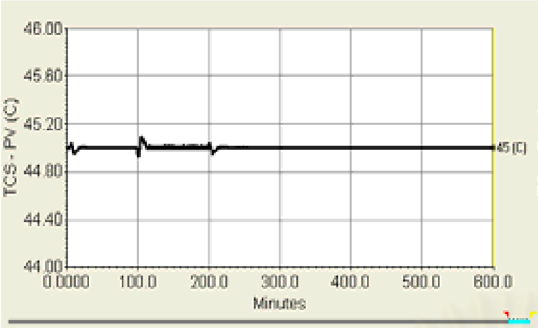
C.1.1 Control structure 1

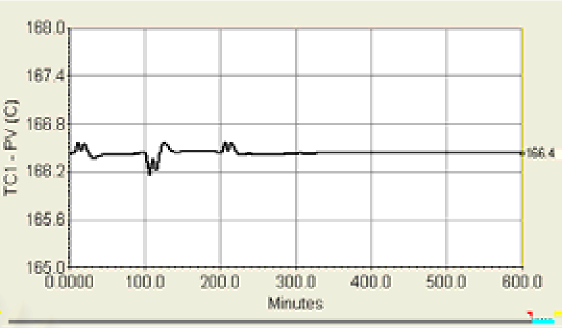
<u>Case Study1</u>

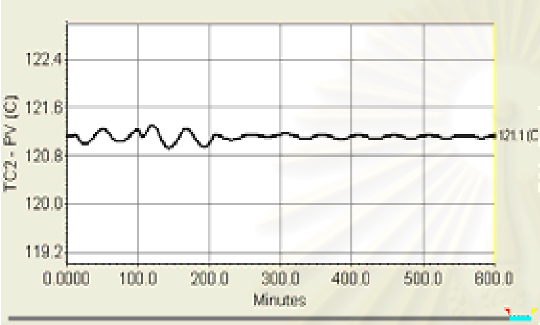


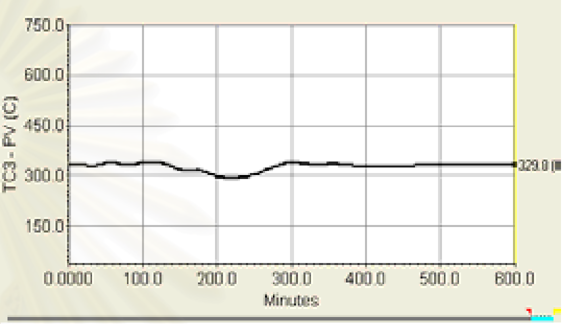


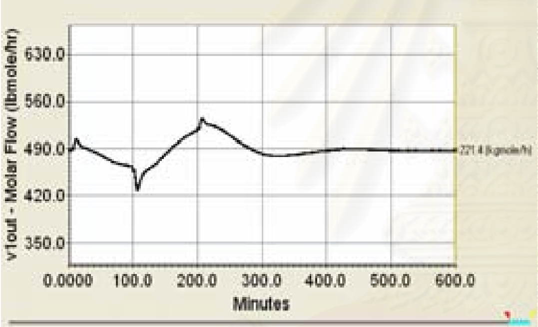


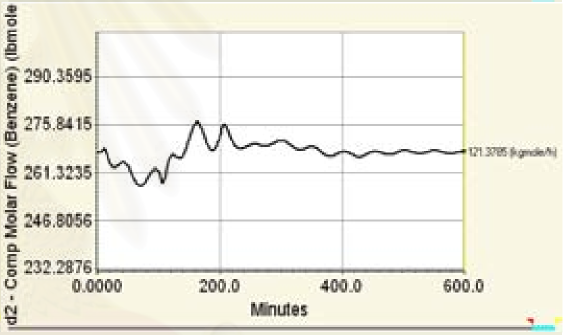

TC5 - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

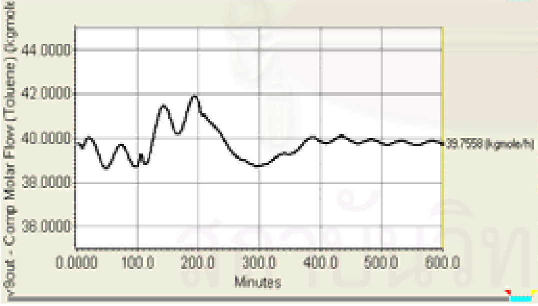

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4

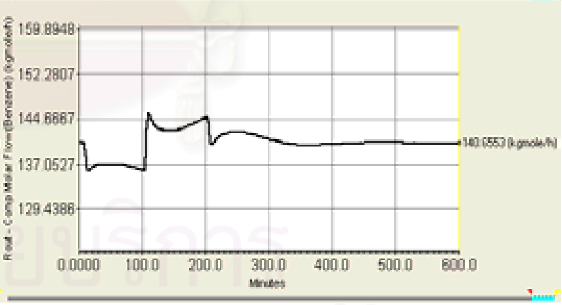

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
329.0

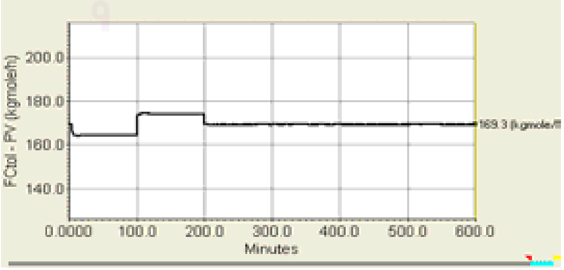

v1out - Molar Flow (lbmole/hr)
630.0
560.0
490.0
420.0
350.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
221.4 (kgmole/h)

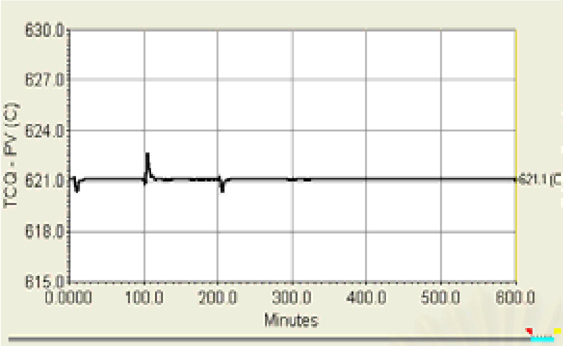

d2 - Comp Molar Flow (Benzene) (lbmole
290.3595
275.8415
261.3235
246.8056
232.2876
0.0000
200.0
400.0
600.0
Minutes
121.3785 (kgmole/h)

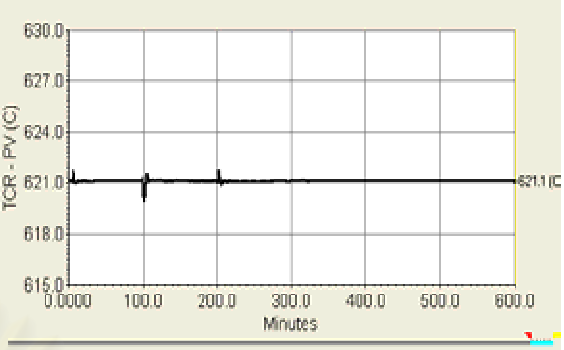

v3out - Comp Molar Flow (Toluene) (kgmole
44.0000
42.0000
40.0000
38.0000
36.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
39.7558 (kgmole/h)

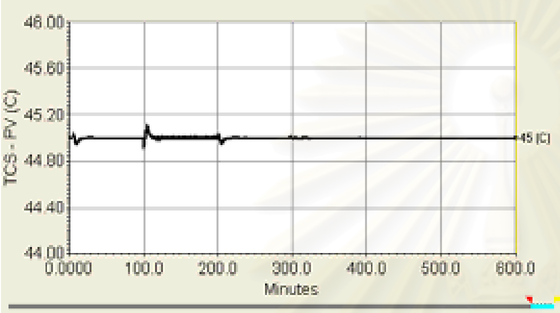

Rout - Comp Molar Flow (Benzene) (kgmole/h)
159.8948
152.2807
144.6667
137.0527
129.4386
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
140.6553 (kgmole/h)

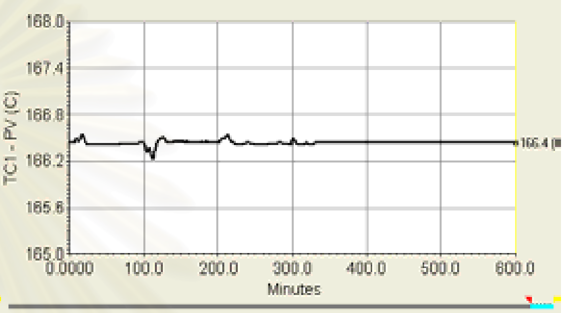
Case Study2

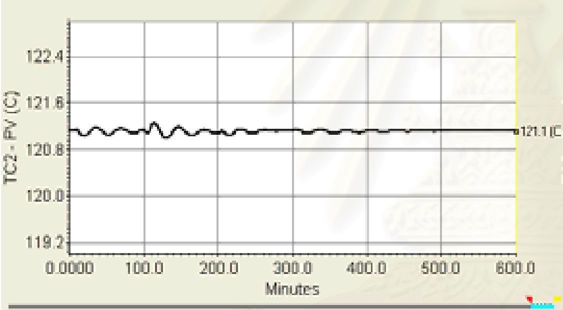

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.3 (kgmole/h

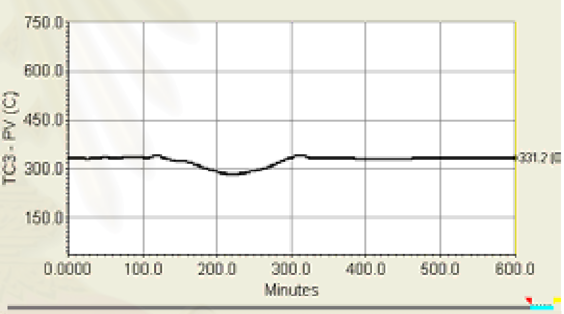

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

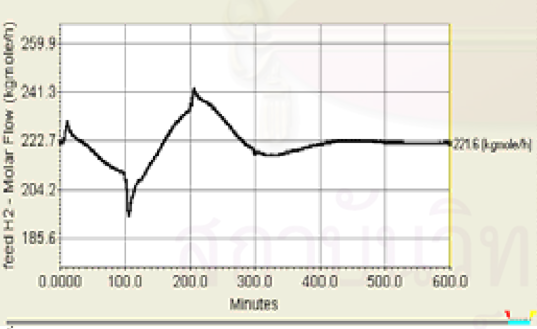

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

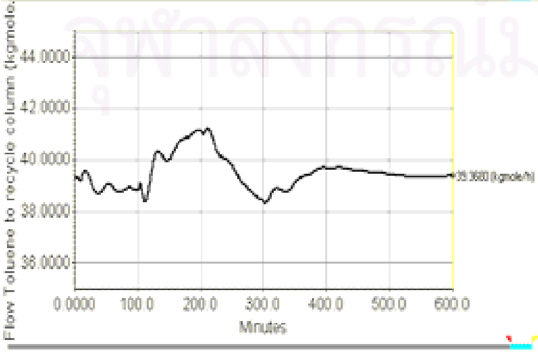

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
166.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

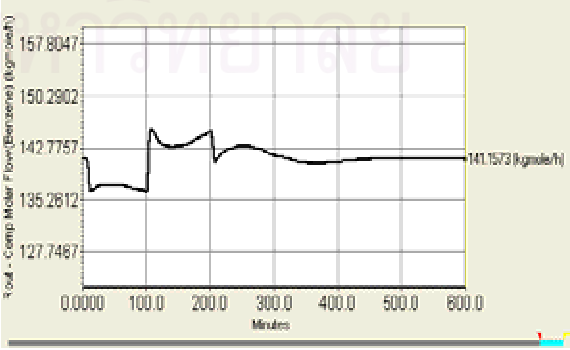

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
121.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
331.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

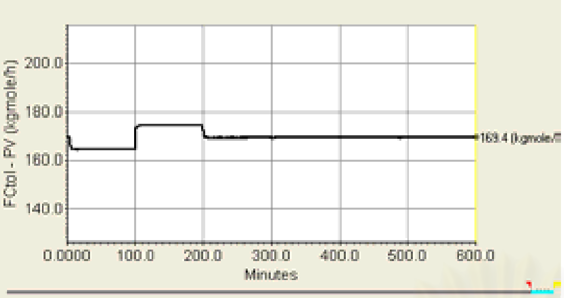

feed H2 - Molar Flow (kgmole/h)
259.9
241.3
222.7
204.2
185.6
221.6 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

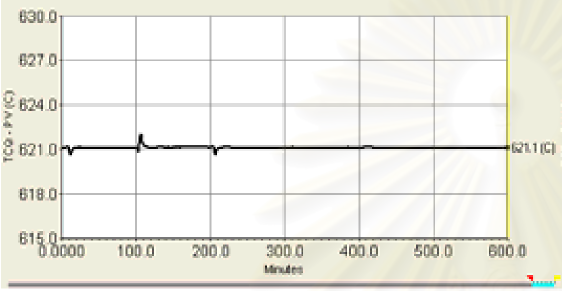

d2 - Comp Molar Flow (Benzene) (kgmole
132.5634
126.2508
119.9383
113.6257
107.3132
121.5996 (kgmole/h
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

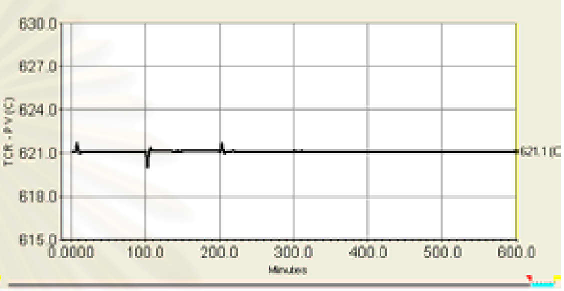

Flow Toluene to recycle column (kgmole
44.0000
42.0000
40.0000
38.0000
36.0000
39.3680 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

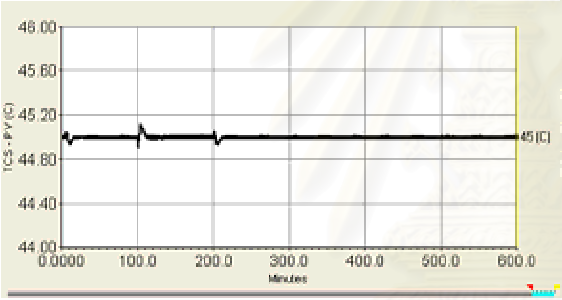

Fout - Comp Molar Flow(Benzene) (kgmole/h)
157.8047
150.2902
142.7757
135.2812
127.7467
141.1573 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

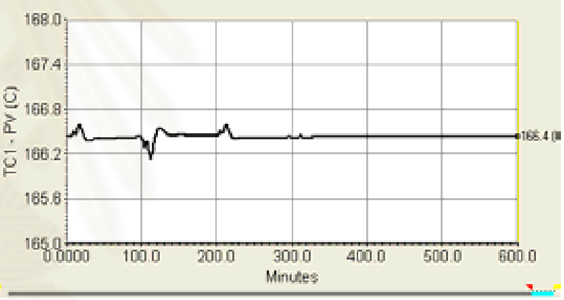
Case Study3

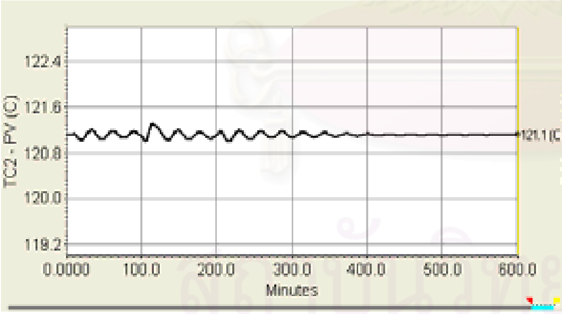

FCtbl - PV (kgmole/h)
200.0
180.0
160.0
140.0
169.4 (kgmole/
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

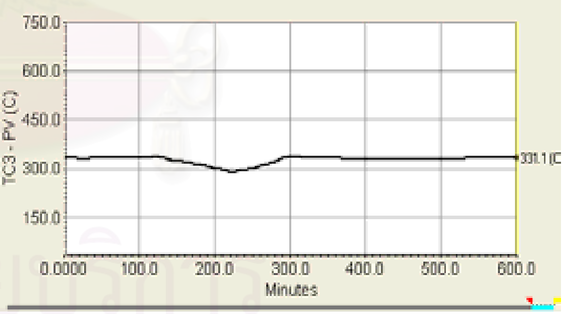

TC0 - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

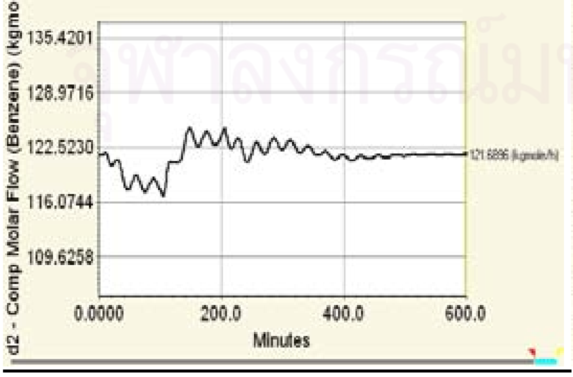

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

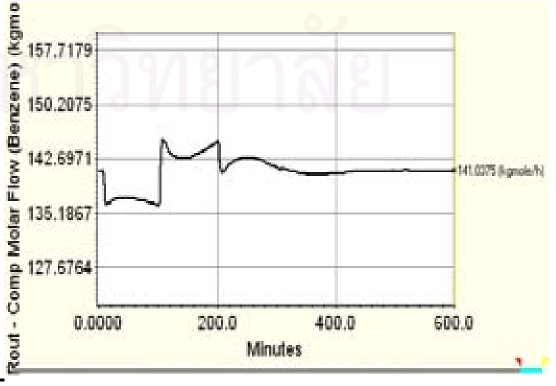

TC5 - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
166.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

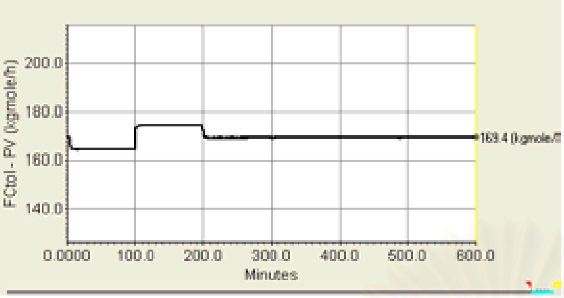

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
121.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

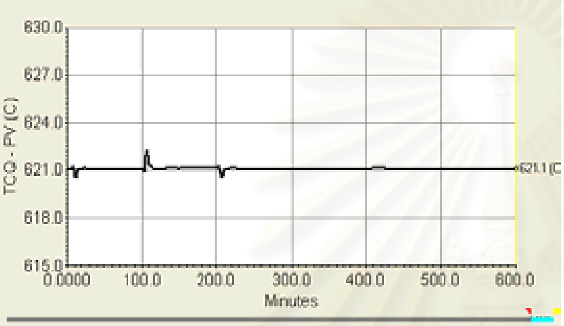

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
331.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

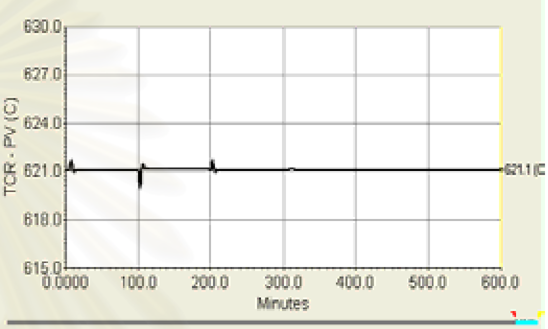

d2 - Comp Molar Flow (Benzene) (kgmole
135.4201
128.9716
122.5230
116.0744
109.6258
121.6896 (kgmole/h)
0.0000
200.0
400.0
600.0
Minutes

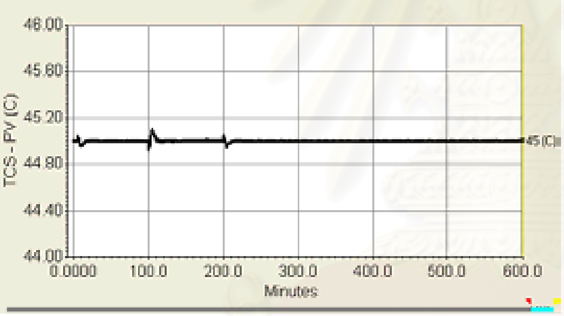

Rout - Comp Molar Flow (Benzene) (kgmo
157.7179
150.2075
142.6971
135.1867
127.6764
141.0375 (kgmole/h)
0.0000
200.0
400.0
600.0
Minutes

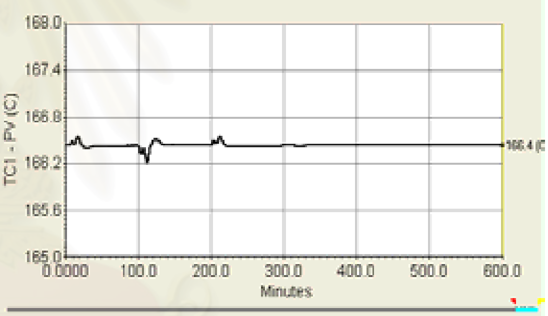
Case Study4

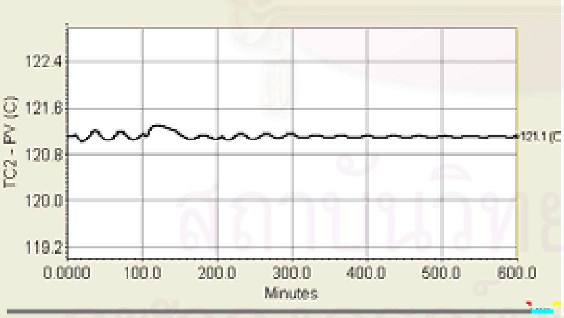

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
169.4 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

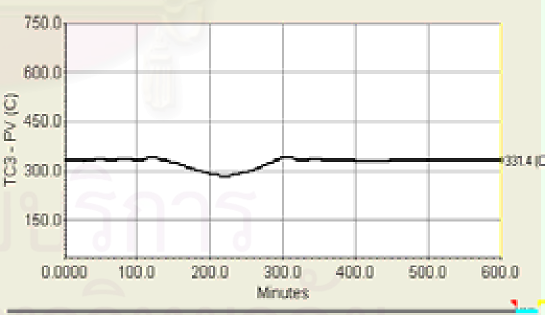

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

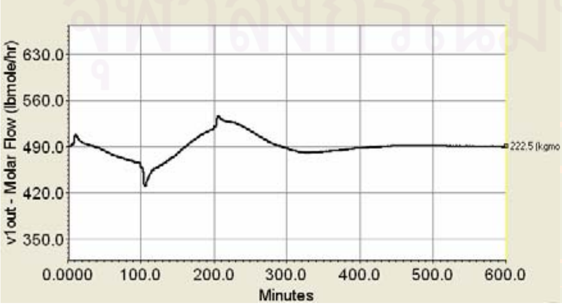

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

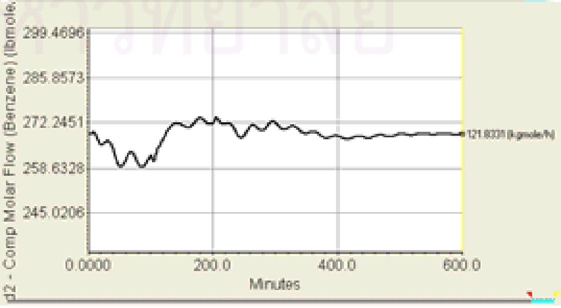

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

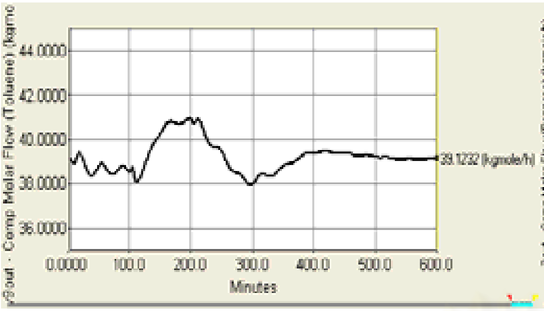

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
166.4 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

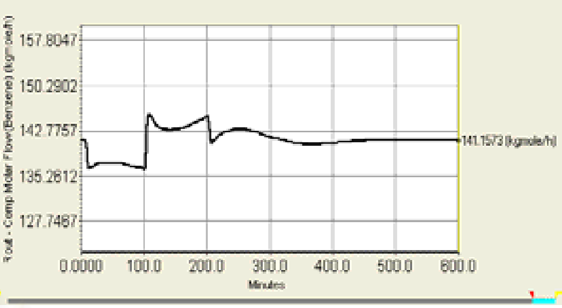

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
121.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
331.4 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

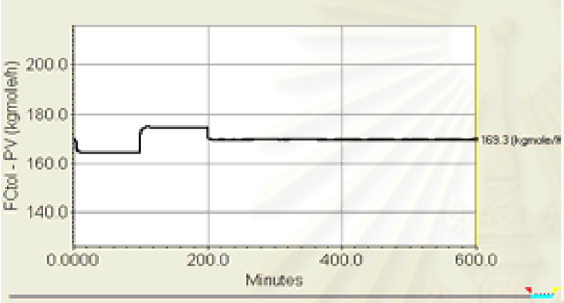

v1out - Molar Flow (lbmole/hr)
630.0
560.0
490.0
420.0
350.0
222.5 (kgmo
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

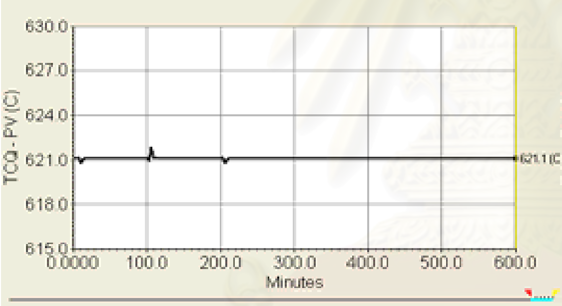

l2 - Comp Molar Flow (Benzene) (lbmole
299.4696
285.8573
272.2451
258.6328
245.0206
121.8331 (kgmole/h)
0.0000
200.0
400.0
600.0
Minutes

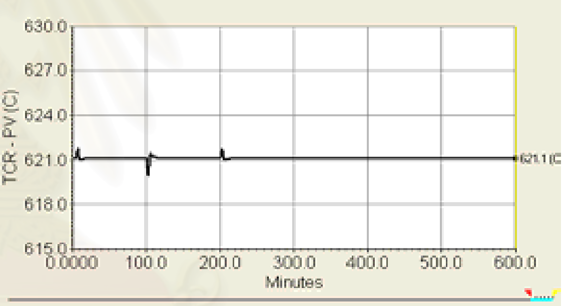

Comp Molar Flow (Toluene) (kgmo
44.0000
42.0000
40.0000
38.0000
36.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
39.1232 (kgmole/h)

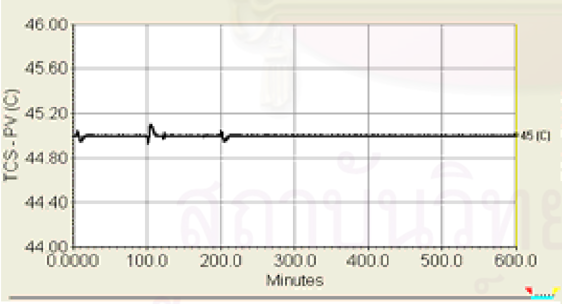

Comp Molar Flow(Benzene) (kgmole/h)
157.8047
150.2902
142.7757
135.2612
127.7467
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.1573 (kgmole/h)

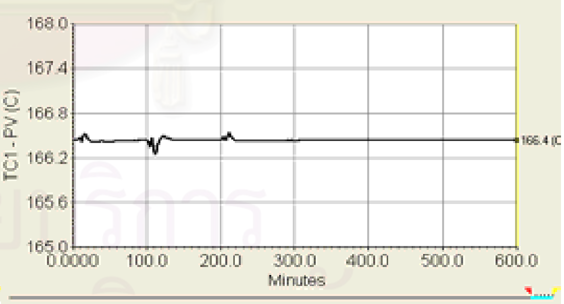
Case Study5

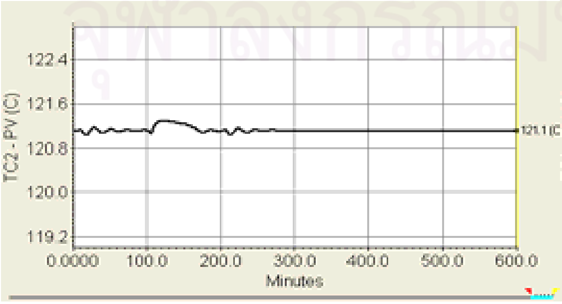

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
200.0
400.0
600.0
Minutes
169.3 (kgmole/h

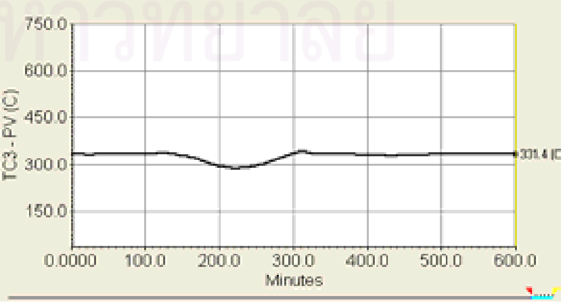

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

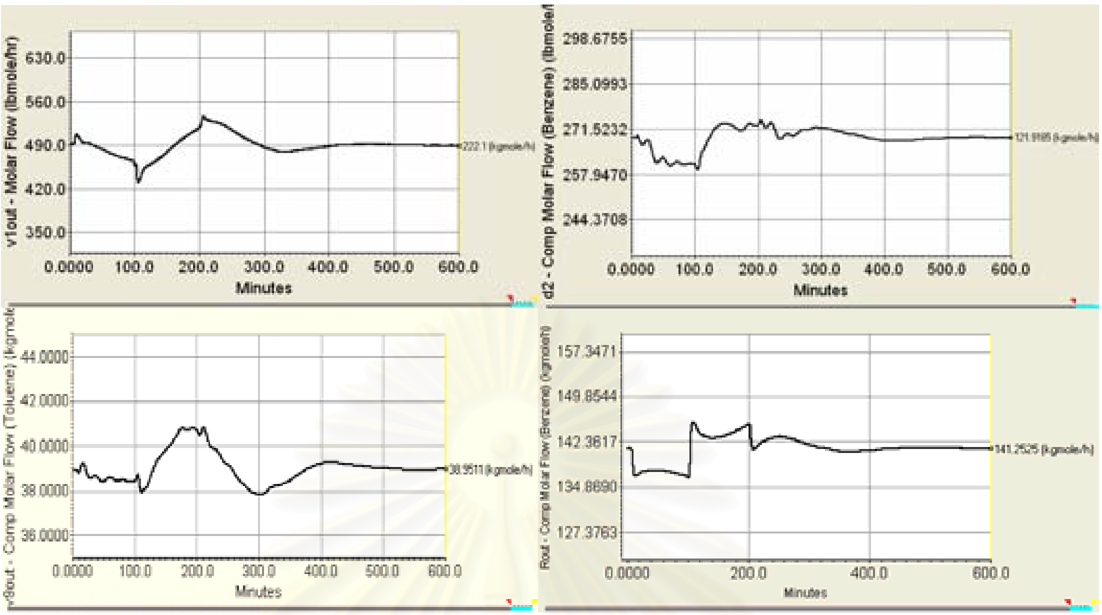

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C


TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

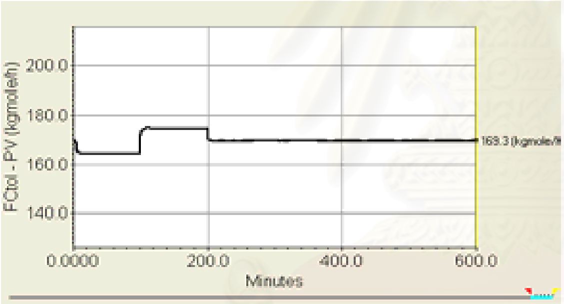

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (C

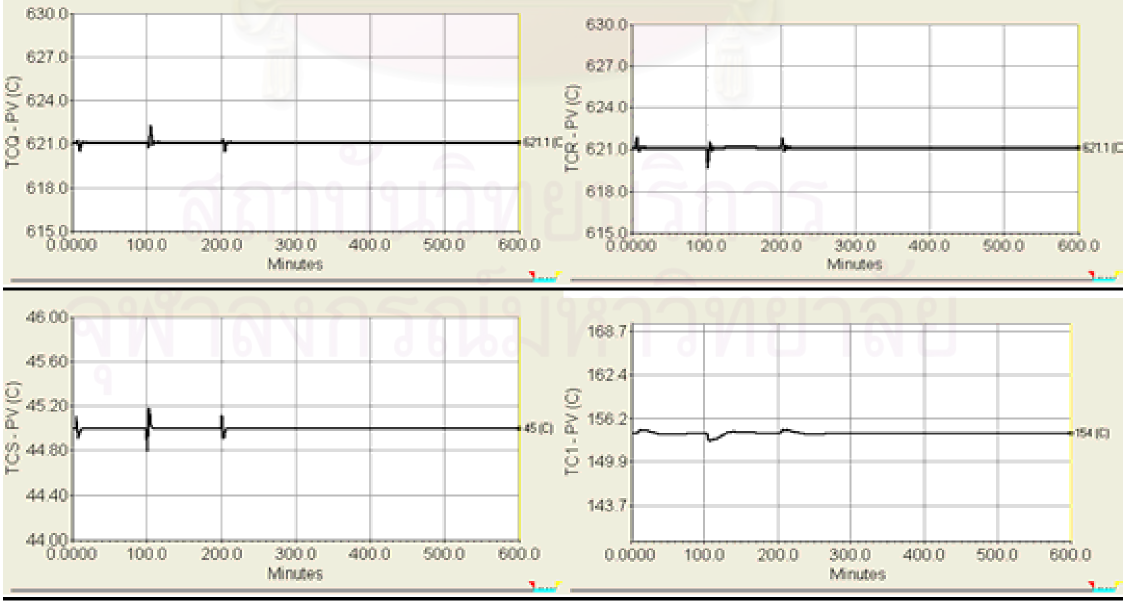

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

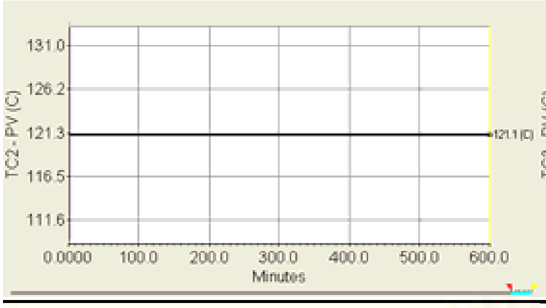

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.4 (C

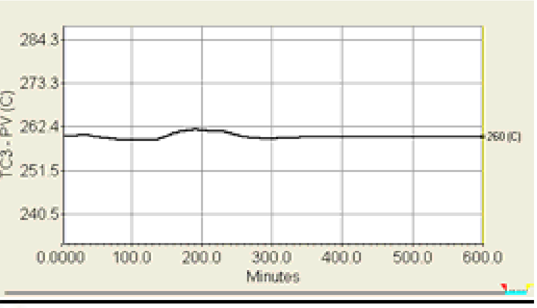

v1out - Molar Flow (lbmole/hr)
630.0
560.0
490.0
420.0
350.0
222.1 (kgmole/h)
d2 - Comp Molar Flow (Benzene) (lbmole/
298.6755
285.0993
271.5232
257.9470
244.3708
121.9185 (kgmole/h)
v8out - Comp Molar Flow (Toluene) (kgmole
44.0000
42.0000
40.0000
38.0000
36.0000
38.9511 (kgmole/h)
Rout - Comp Molar Flow (Benzene) (kgmole/h)
157.3471
149.8544
142.3617
134.8690
127.3763
141.2525 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

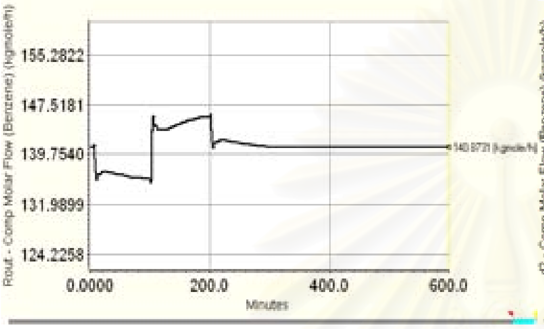
Case Study6

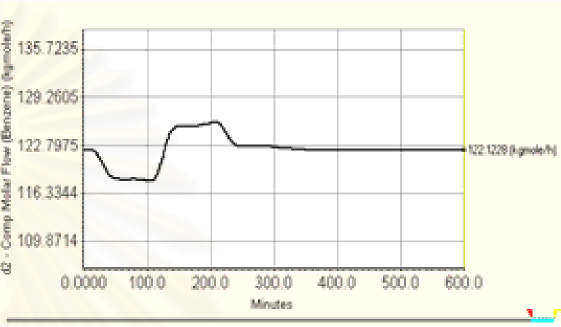

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
169.3 (kgmole/h
0.0000
200.0
400.0
600.0
Minutes


TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
TC1 - PV (C)
168.7
162.4
156.2
149.9
143.7
154 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

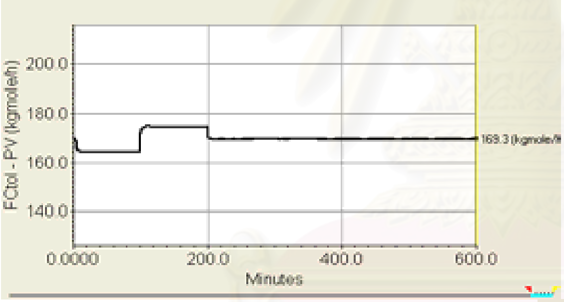

TC2 - PV (C)
131.0
126.2
121.3
116.5
111.6
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C)

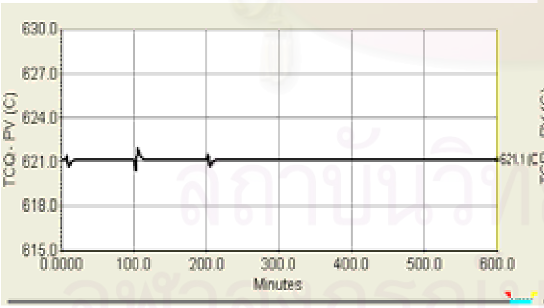

TC3 - PV (C)
284.3
273.3
262.4
251.5
240.5
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
260 (C)

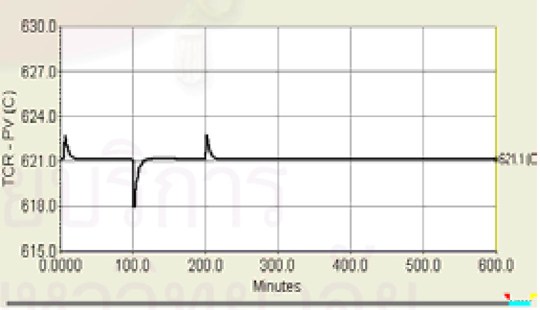

Rout - Comp Molar Flow (Benzene) (kgmole/h)
155.2822
147.5181
139.7540
131.9899
124.2258
0.0000
200.0
400.0
600.0
Minutes
140.9731 (kgmole/h)

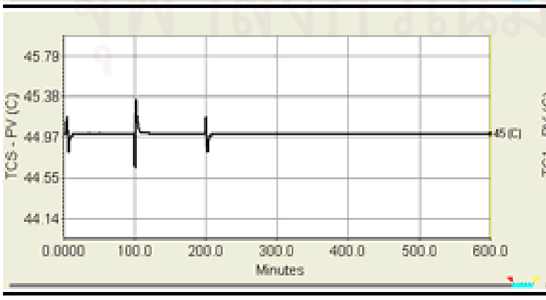

d2 - Comp Molar Flow (Benzene) (kgmole/h)
135.7235
129.2605
122.7975
116.3344
109.8714
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
122.1228 (kgmole/h)

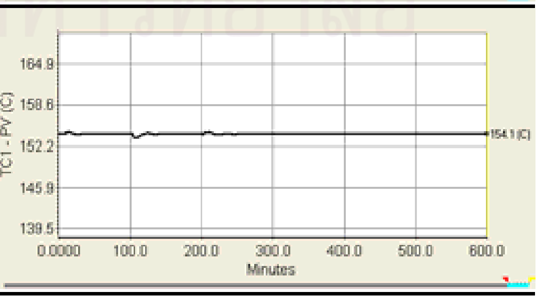
Case Study7


FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
200.0
400.0
600.0
Minutes
169.3 (kgmole/h)


TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)


TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)


TCS - PV (C)
45.79
45.38
44.97
44.55
44.14
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
164.9
158.6
152.2
145.9
139.5
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154.1 (C)

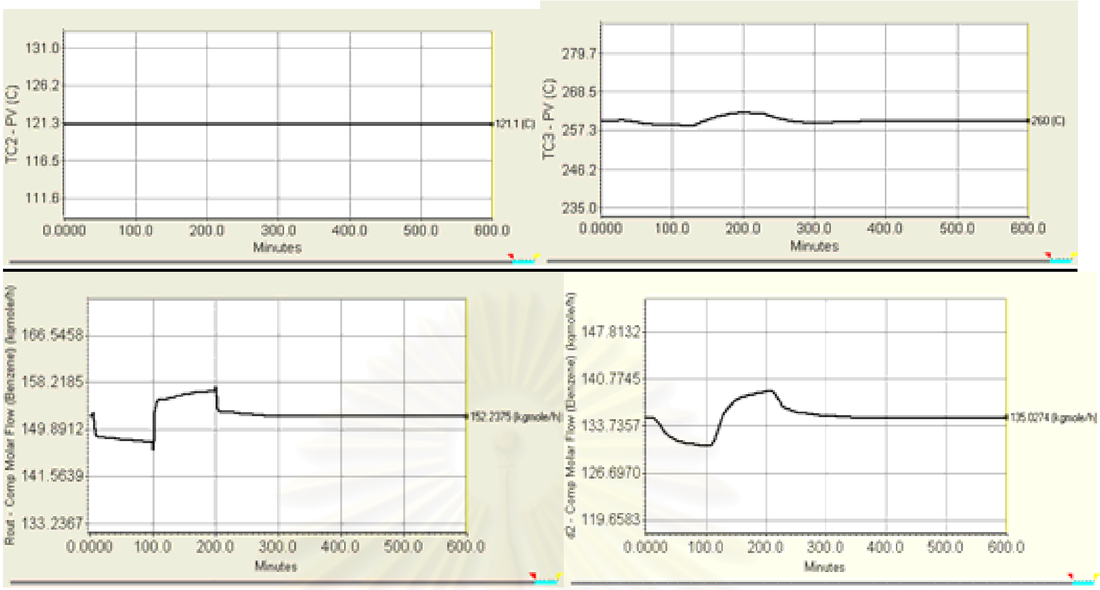
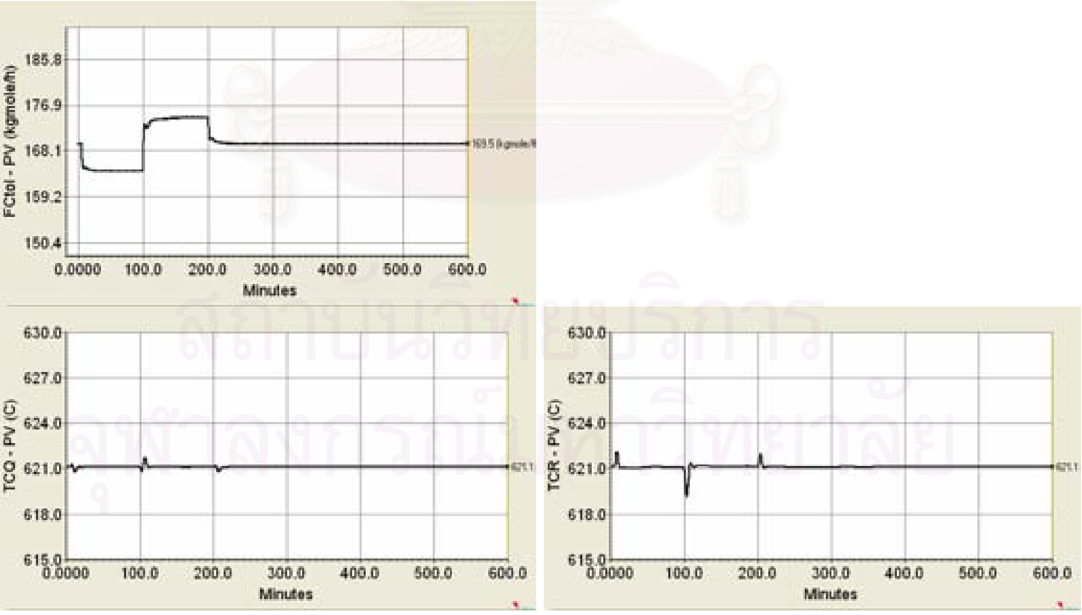
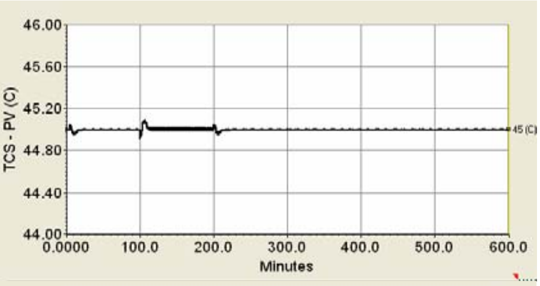


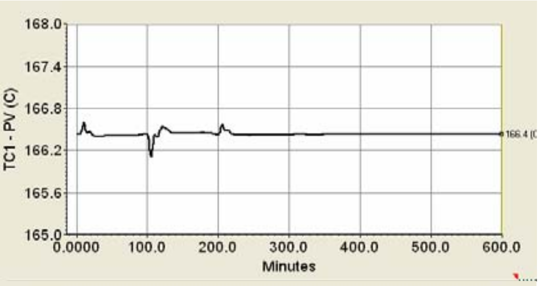
Figure C.1: Dynamic responses of CS1 of seven case studies to set-point change of total toluene feed ±5 kmol/h.

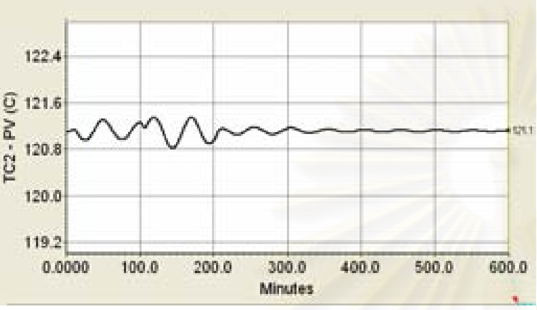
C.1.2 Control structure 2

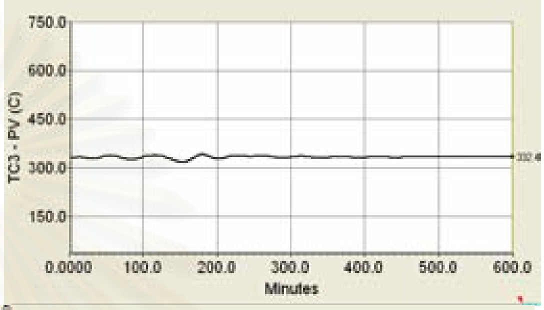
Case Study1

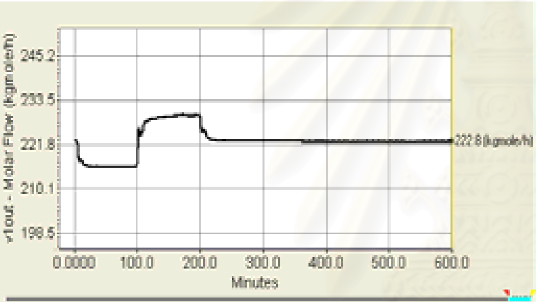


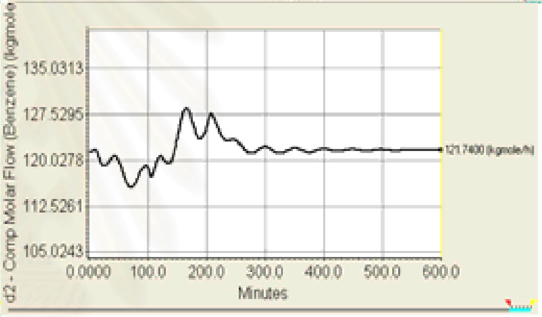

46.00
45.60
45.20
44.80
44.40
44.00
TCS - PV (C)
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

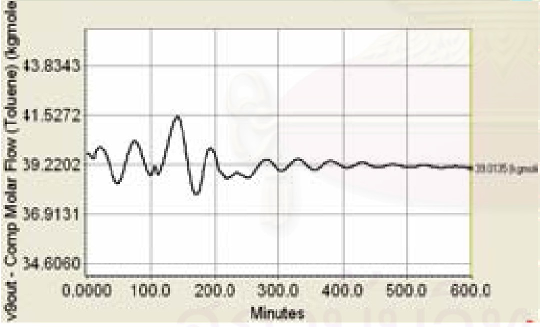

168.0
167.4
166.8
166.2
165.6
165.0
TC1 - PV (C)
166.4 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

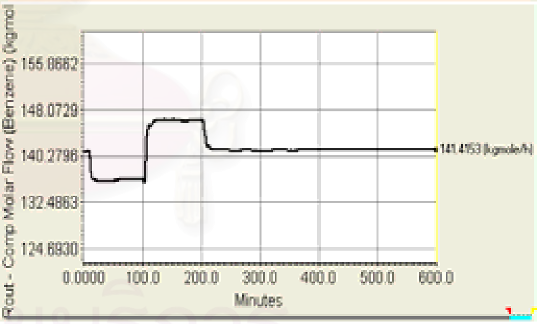

122.4
121.6
120.8
120.0
119.2
TC2 - PV (C)
121.1
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


750.0
600.0
450.0
300.0
150.0
TC3 - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

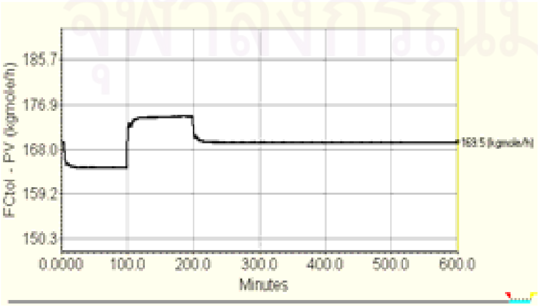

245.2
233.5
221.8
210.1
198.5
v1out - Molar Flow (kgmole/h)
222.8 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

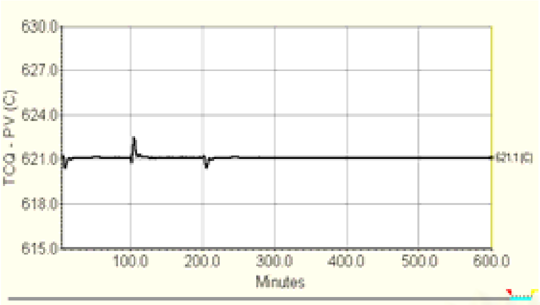

135.0313
127.5295
120.0278
112.5261
105.0243
d2 - Comp Molar Flow (Benzene) (kgmole
121.7400 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

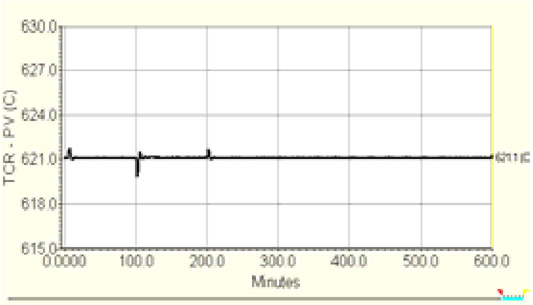

43.8343
41.5272
39.2202
36.9131
34.6060
v8out - Comp Molar Flow (Toluene) (kgmole
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

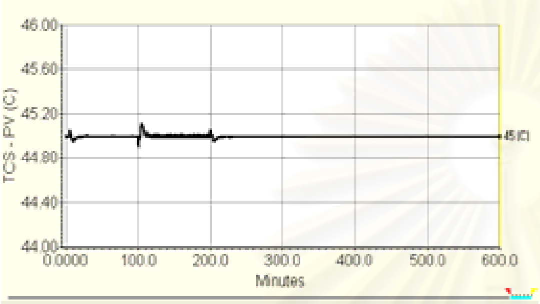

155.8662
148.0729
140.2796
132.4863
124.6930
Rout - Comp Molar Flow (Benzene) (kgmol
141.4153 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

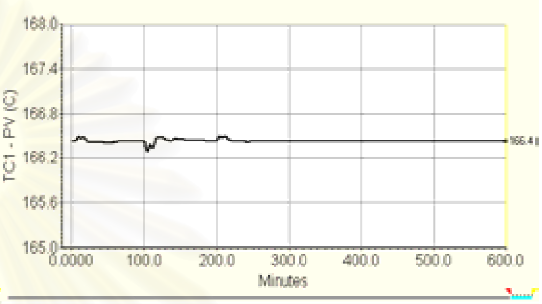
Case Study2

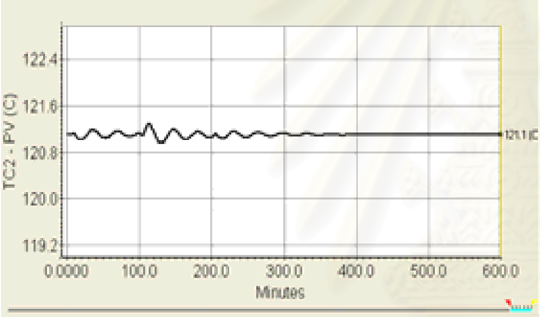

185.7
176.9
168.0
159.2
150.3
FCtol - PV (kgmole/h)
169.5 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

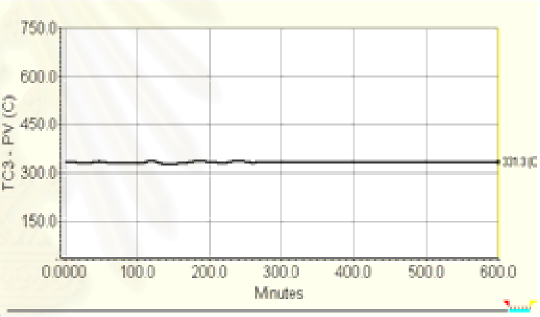

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)

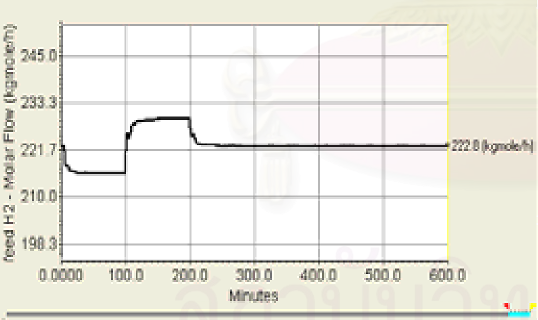

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

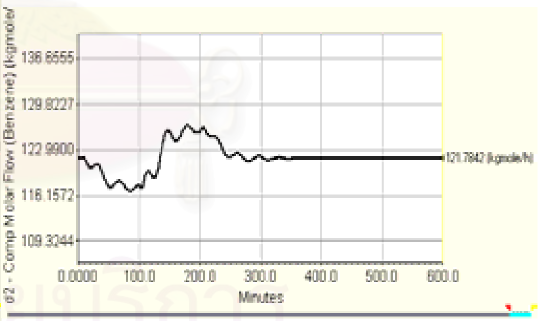

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

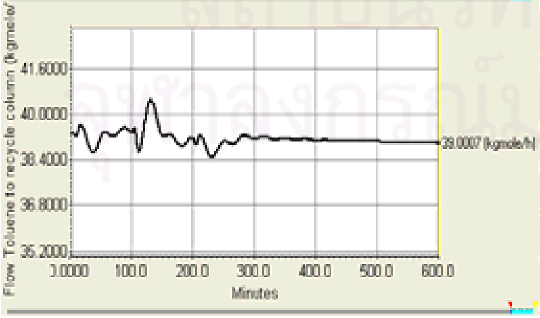

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (

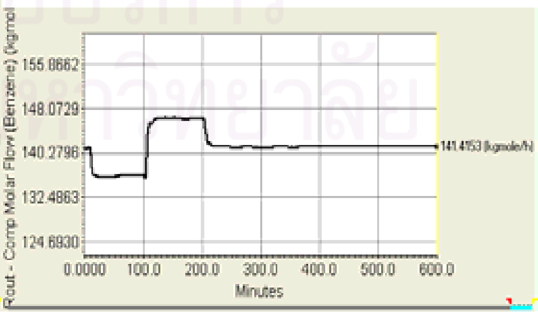

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.3 (C

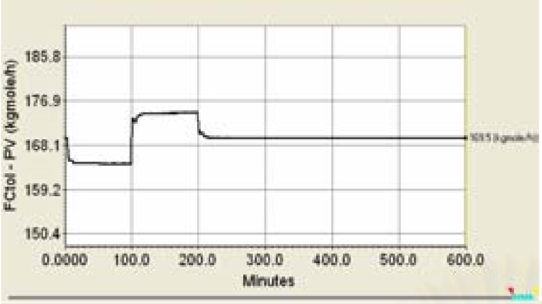

feed H2 - Molar Flow (kgmole/h)
245.0
233.3
221.7
210.0
198.3
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
222.8 (kgmole/h)

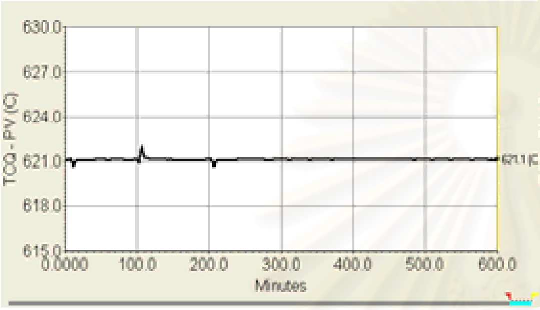

d2 - Comp Molar Flow (Benzene) (kgmole/
136.6555
129.8227
122.9900
116.1572
109.3244
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.7842 (kgmole/h)

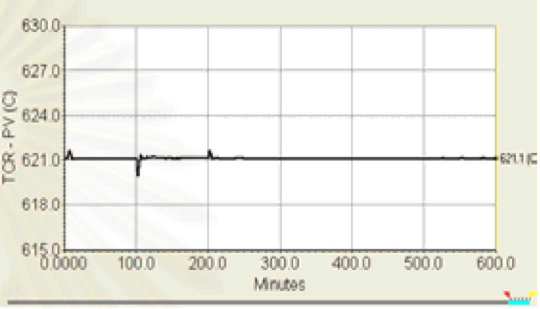

Flow Toluene to recycle column (kgmole/
41.6000
40.0000
38.4000
36.8000
35.2000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
39.0007 (kgmole/h)

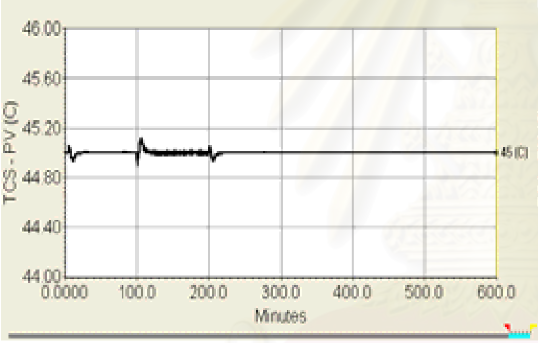

Rout - Comp Molar Flow (Benzene) (kgmol
155.8662
148.0729
140.2796
132.4863
124.6930
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.4153 (kgmole/h)

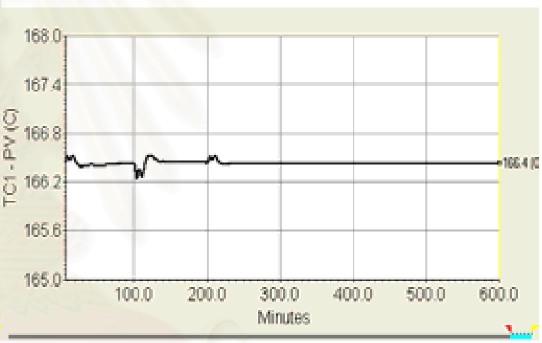
Case Study3

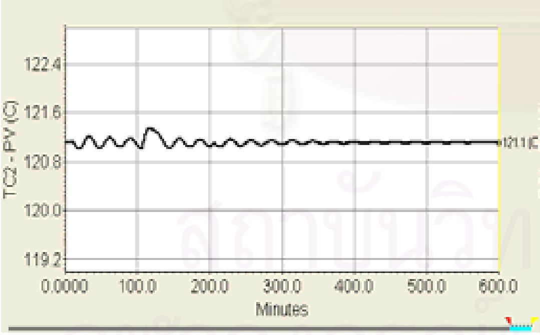

FCtol - PV (kgmole/h)
185.8
176.9
168.1
159.2
150.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

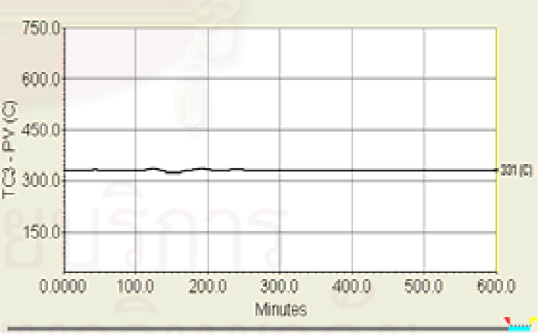

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

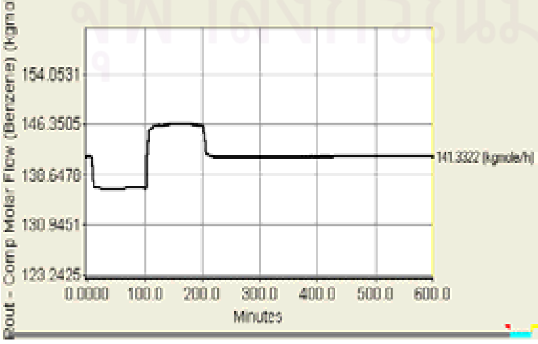

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

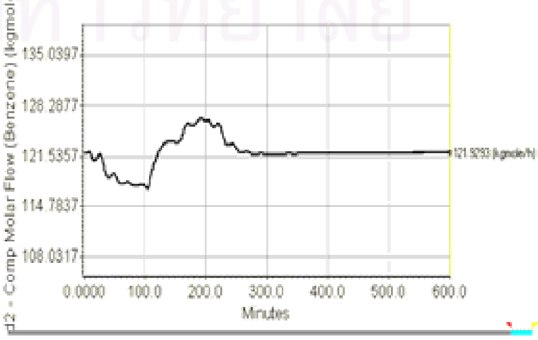

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
166.4 (C)
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

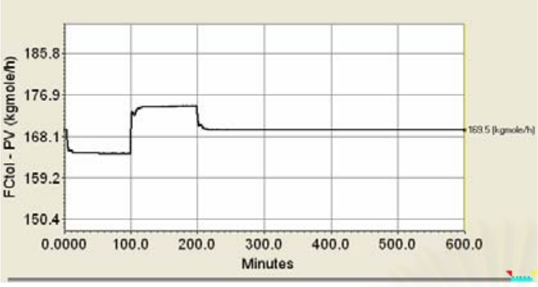

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
121.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

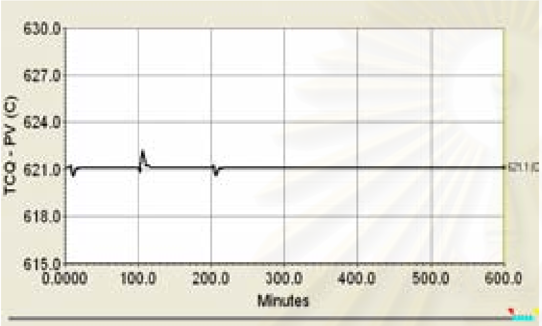

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
331 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

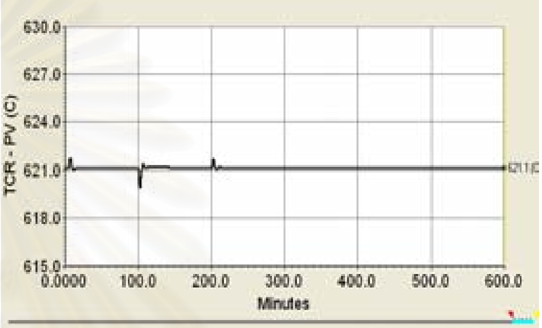

Qout - Comp Molar Flow (Benzene) (kgmol
154.0531
146.3505
138.6478
130.9451
123.2425
141.3322 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

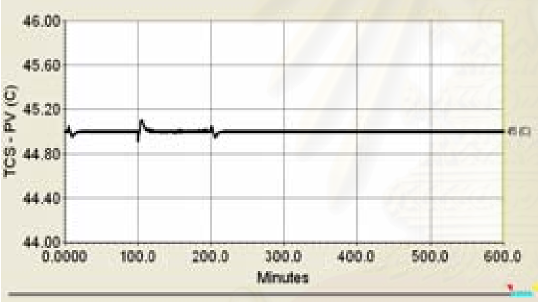

d2 - Comp Molar Flow (Benzene) (kgmol
135.0397
128.2877
121.5357
114.7837
108.0317
121.5293 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

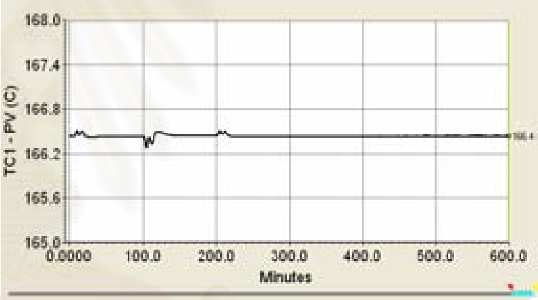
Case Study4

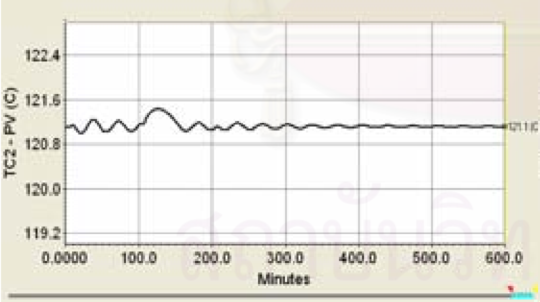

FCtol - PV (kgmole/h)
185.8
176.9
168.1
159.2
150.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h)

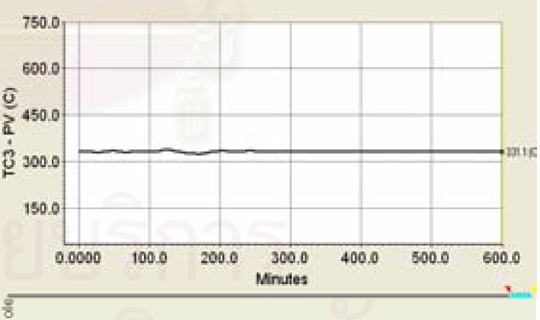

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

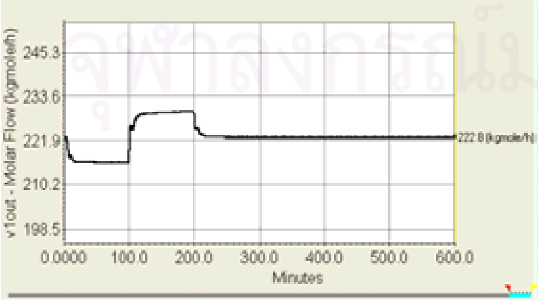

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

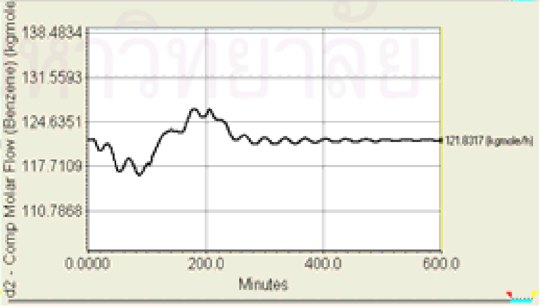

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

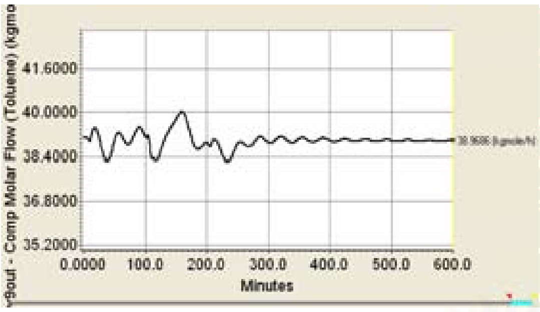

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4

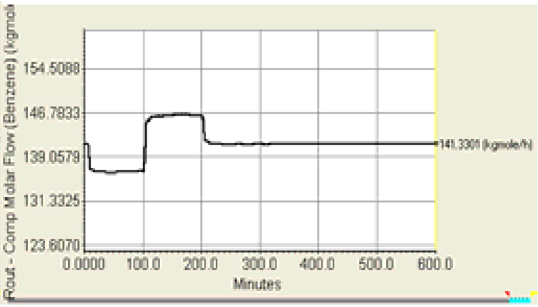

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1 (C

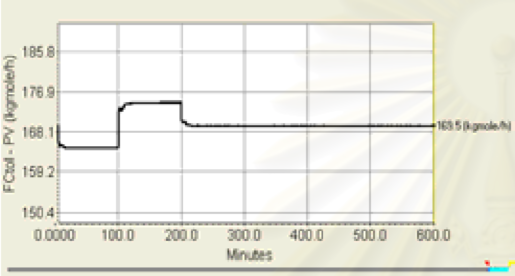

v1out - Molar Flow (kgmole/h)
245.3
233.6
221.9
210.2
198.5
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
222.8 (kgmole/h)

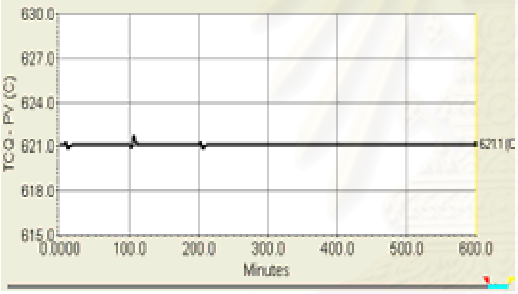

d2 - Comp Molar Flow (Benzene) (kgmole
138.4834
131.5593
124.6351
117.7109
110.7868
0.0000
200.0
400.0
600.0
Minutes
121.8317 (kgmole/h)

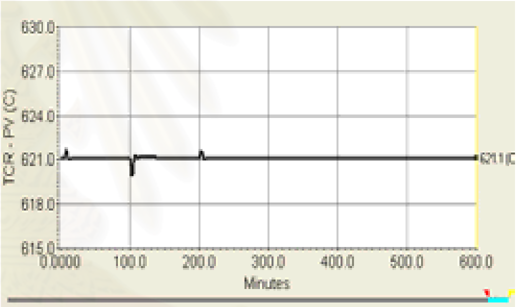

9out - Comp Molar Flow (Toluene) (kgmo
41.6000
40.0000
38.4000
36.8000
35.2000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

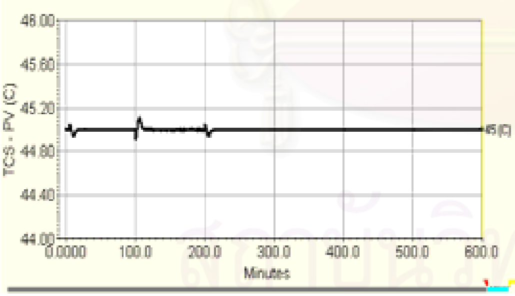

Rout - Comp Molar Flow (Benzene) (kgmol
154.5088
146.7833
139.0579
131.3325
123.6070
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.3301 (kgmole/h)

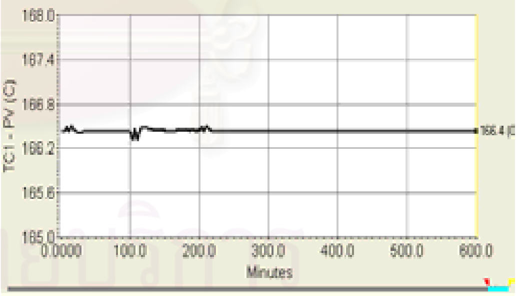
Case Study5

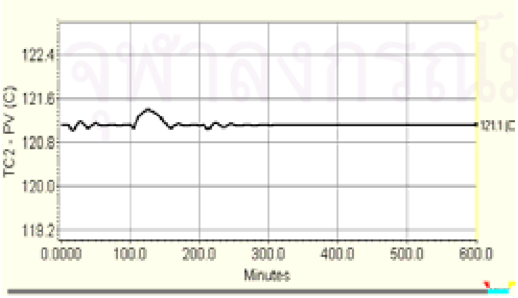

FCtol - PV (kgmole/h)
185.8
176.9
168.1
159.2
150.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

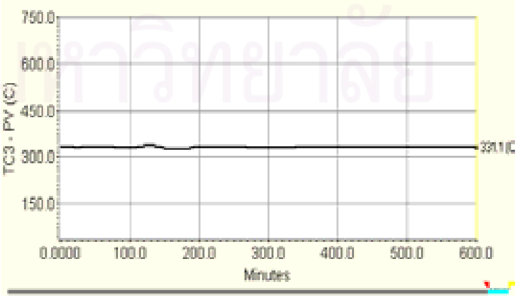

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

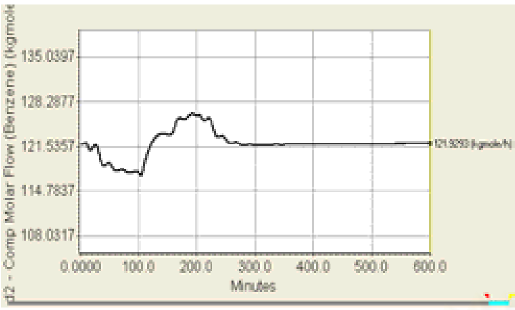

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

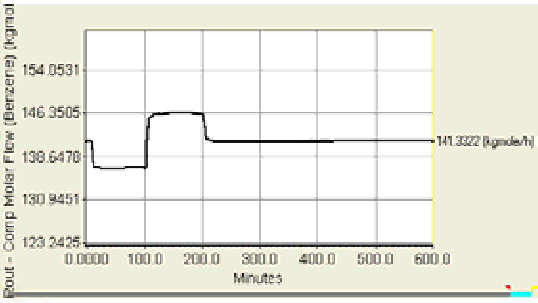

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (C

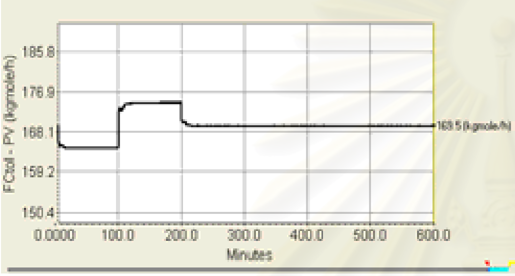

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

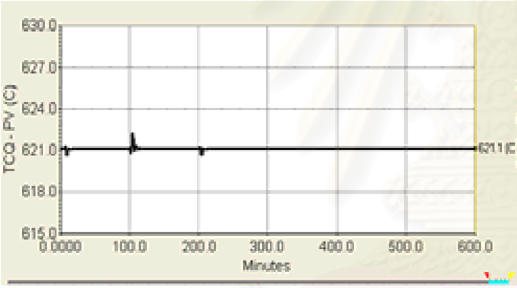

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1 (C

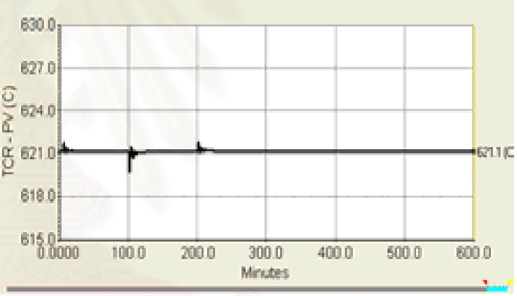

d2 - Comp Molar Flow (Benzene) (kgmole
135.0397
128.2877
121.5357
114.7837
108.0317
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.9293 (kgmole/h)

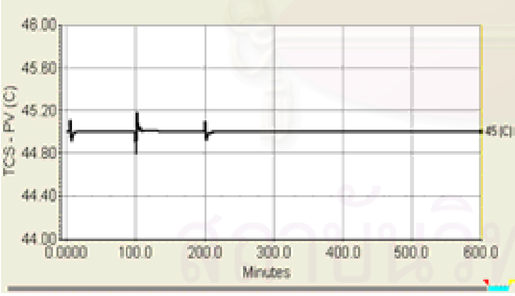

Bout - Comp Molar Flow (Benzene) (kgmol
154.0531
146.3505
138.6478
130.9451
123.2425
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.3322 (kgmole/h)

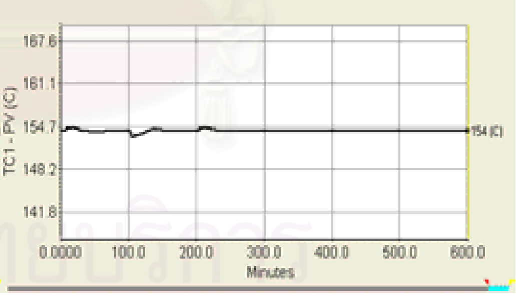
Case Study6

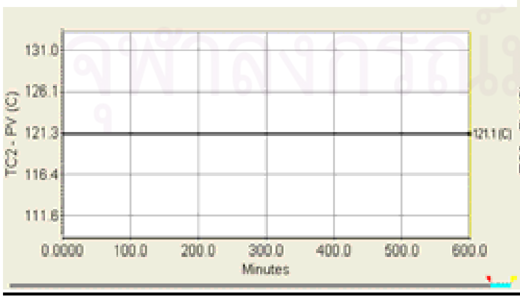

FCbl - PV (kgmole/h)
185.8
176.9
168.1
159.2
150.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h)

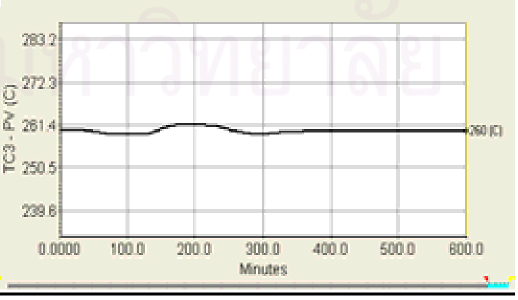

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)

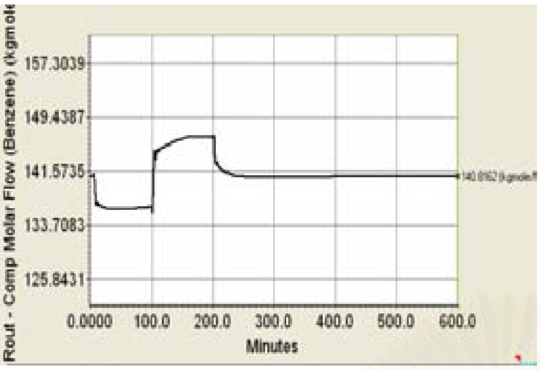

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

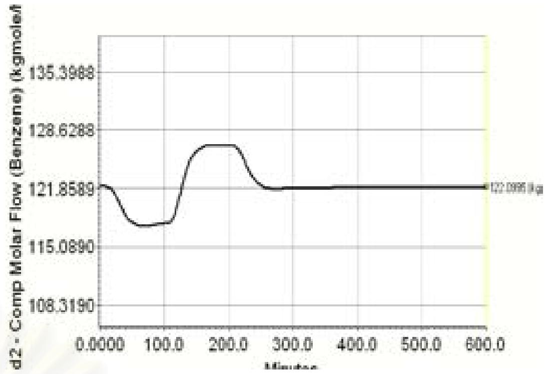

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
167.6
161.1
154.7
148.2
141.8
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154 (C)

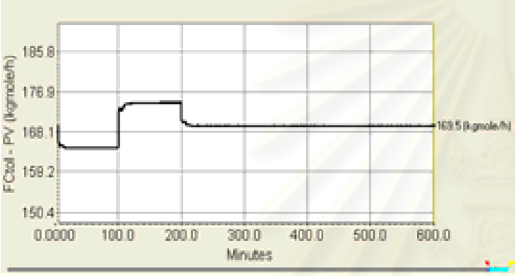

TC2 - PV (C)
131.0
126.1
121.3
116.4
111.6
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C)

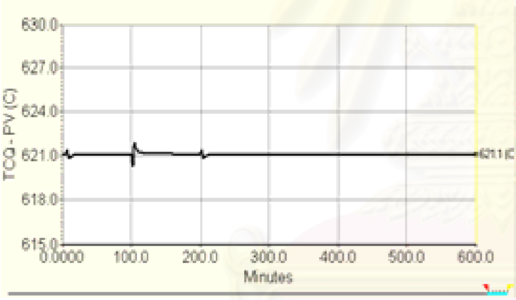

TC3 - PV (C)
283.2
272.3
261.4
250.5
239.6
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
260 (C)

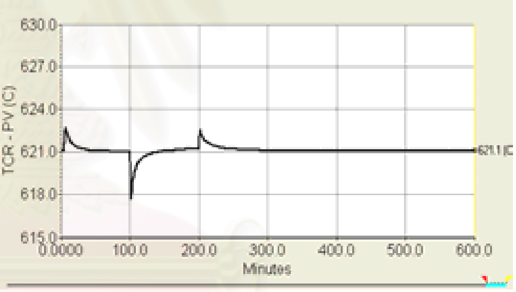

Rout - Comp Molar Flow (Benzene) (kgmole
157.3039
149.4387
141.5735
133.7083
125.8431
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
140.8162 (kgmole/h

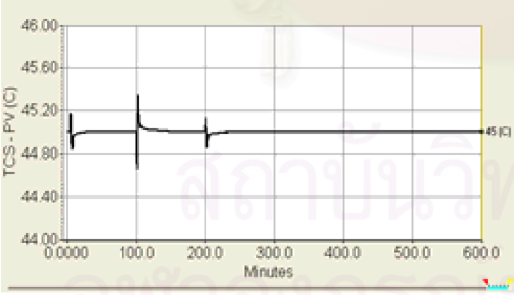

d2 - Comp Molar Flow (Benzene) (kgmole/h
135.3988
128.6288
121.8589
115.0890
108.3190
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
122.0995 (kg

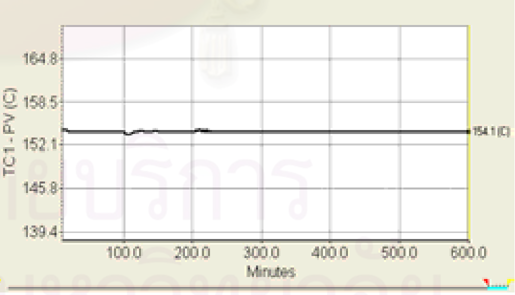
Case Study7

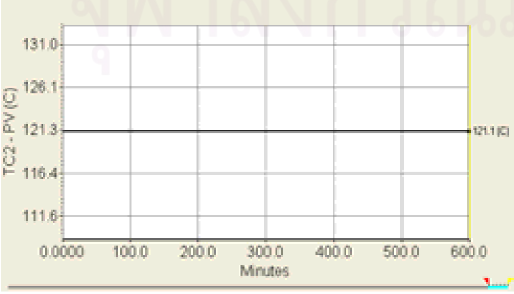

FCtol - PV (kgmole/h)
185.8
176.9
168.1
159.2
150.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h)

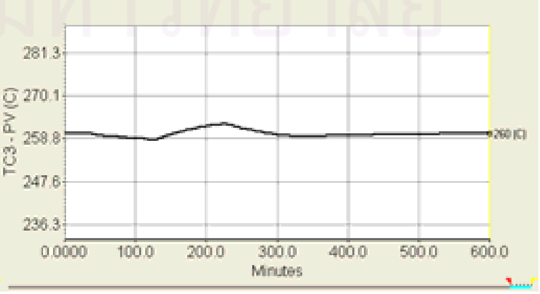

TCO - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C


TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C


TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
164.8
158.5
152.1
145.8
139.4
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154.1 (C)


TC2 - PV (C)
131.0
126.1
121.3
116.4
111.6
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C)


TC3 - PV (C)
281.3
270.1
258.8
247.6
236.3
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
260 (C)

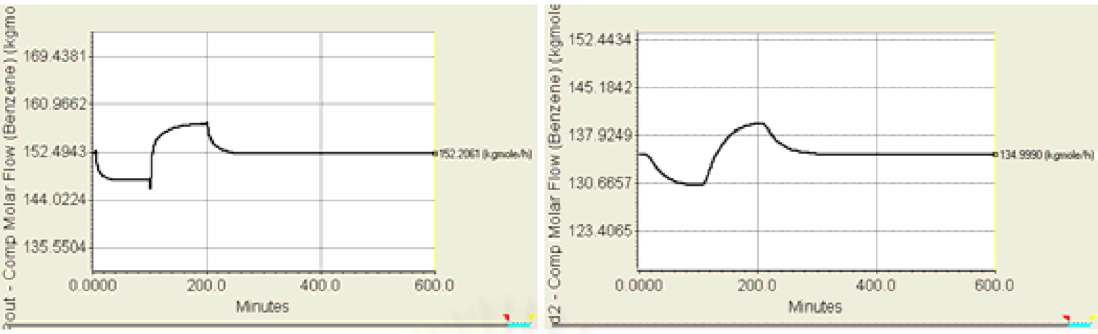
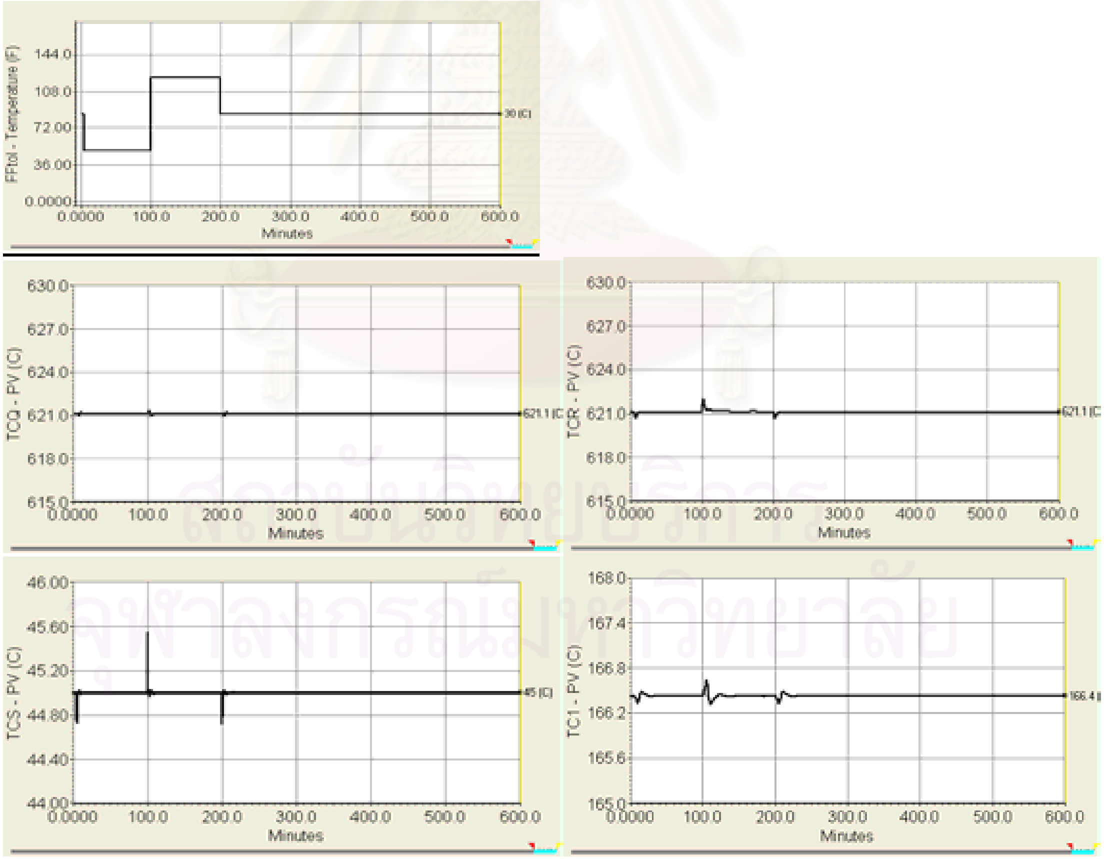


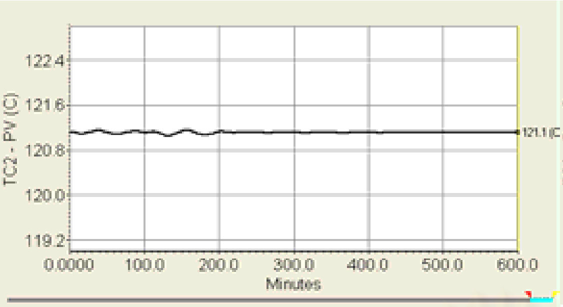
Figure C.2: Dynamic responses of CS2 of seven case studies to set-point change of total toluene feed ±5 kmol/h.

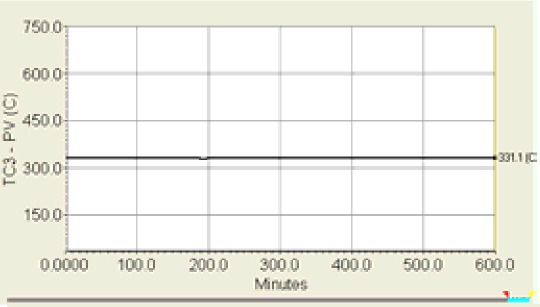
C.2 Test load change of toluene feed temperature ±20 °C

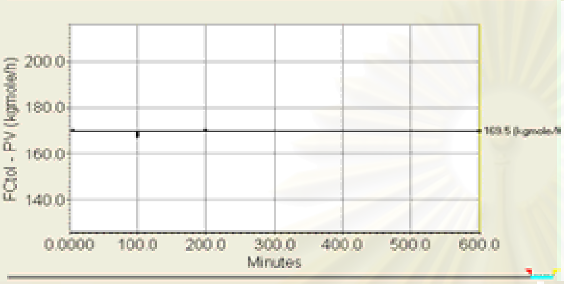
C.1.1 Control structure 1

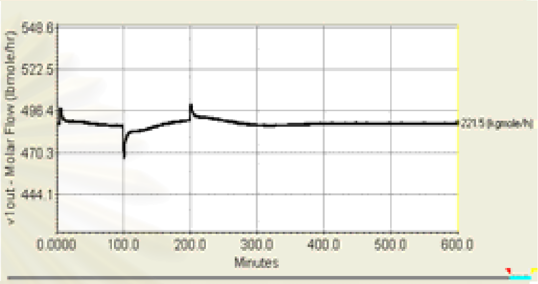
Case Study1

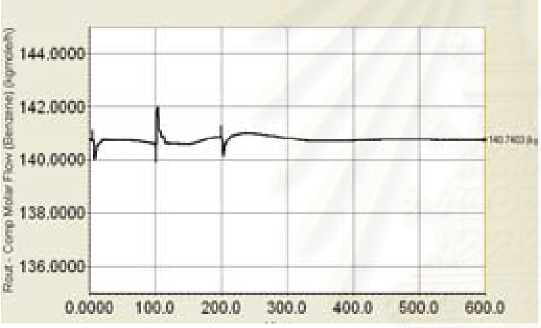


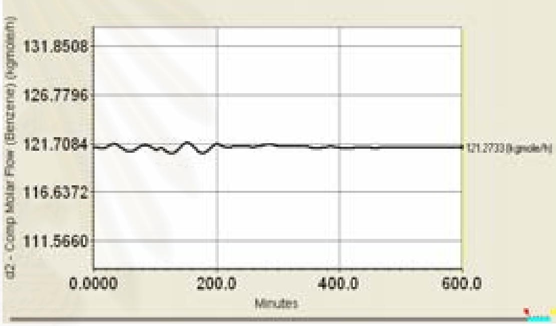

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
121.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
331.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

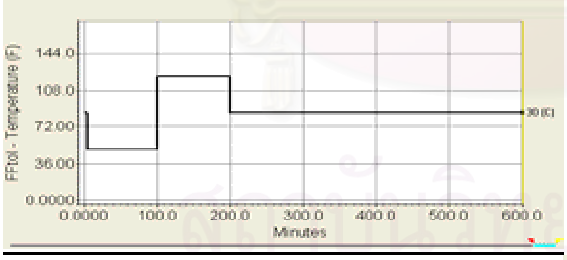

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
169.5 (kgmole/h
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

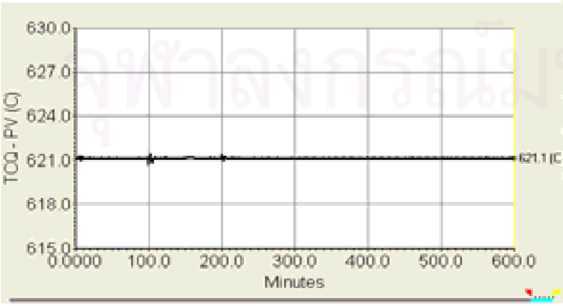

v1out - Molar Flow (lbmole/hr)
548.6
522.5
496.4
470.3
444.1
221.5 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

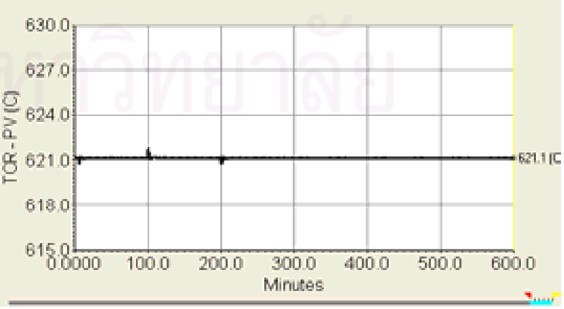

Rout - Comp Molar Flow (Benzene) (kgmole/h)
144.0000
142.0000
140.0000
138.0000
136.0000
140.7403 (kg
0.0000
100.0
200.0
300.0
400.0
500.0
600.0

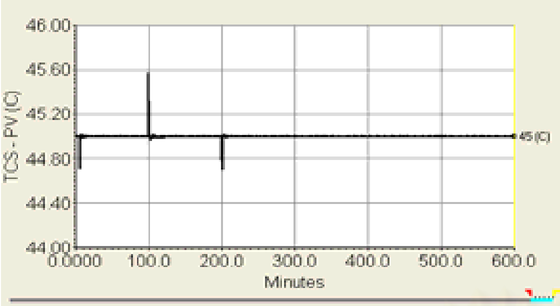

d2 - Comp Molar Flow (Benzene) (kgmole/h)
131.8508
126.7796
121.7084
116.6372
111.5660
121.2733 (kgmole/h)
0.0000
200.0
400.0
600.0
Minutes

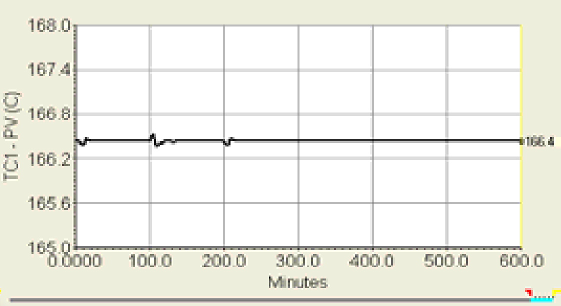
Case Study2

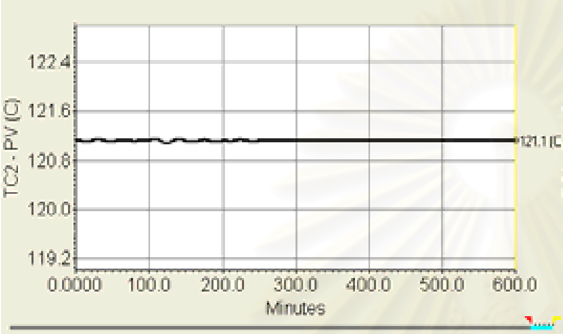

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
30 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

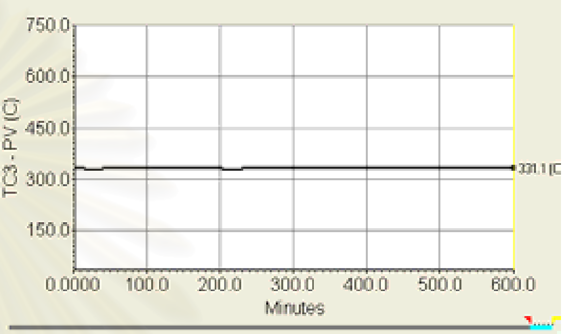

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

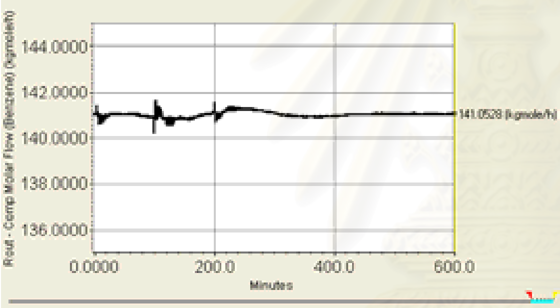

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

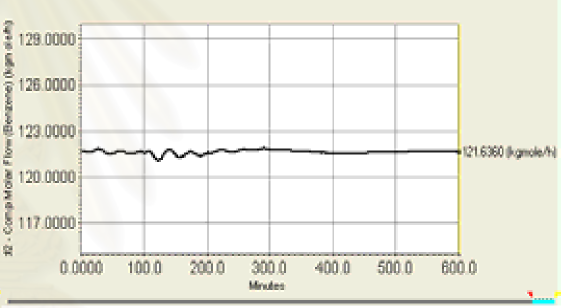

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

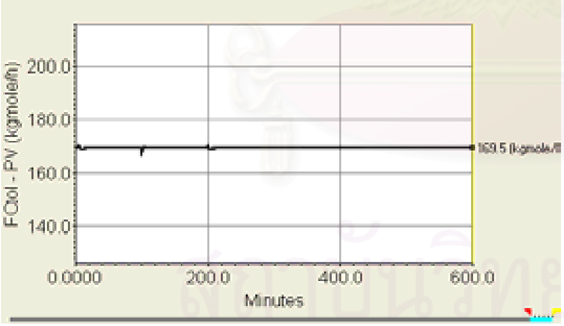

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4


TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

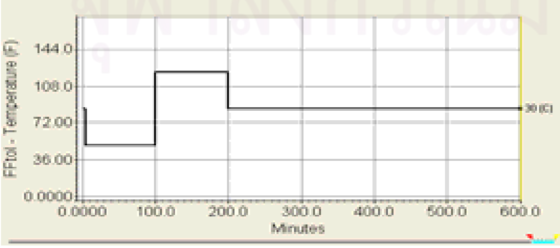

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1 (C

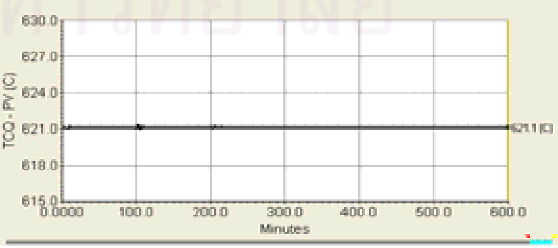

Rout - Comp Molar Flow (Benzene) (kgmole/h)
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
200.0
400.0
600.0
Minutes
141.0528 (kgmole/h)

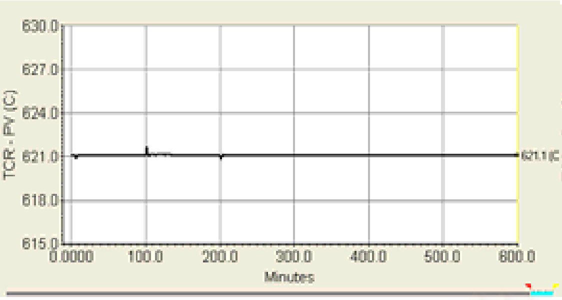

32 - Comp Molar Flow (Benzene) (kgmole/h)
129.0000
126.0000
123.0000
120.0000
117.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.6360 (kgmole/h)

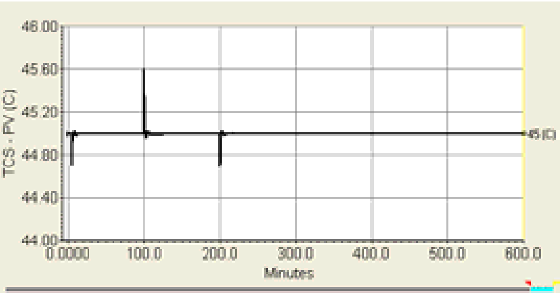

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
200.0
400.0
600.0
Minutes
169.5 (kgmole/h

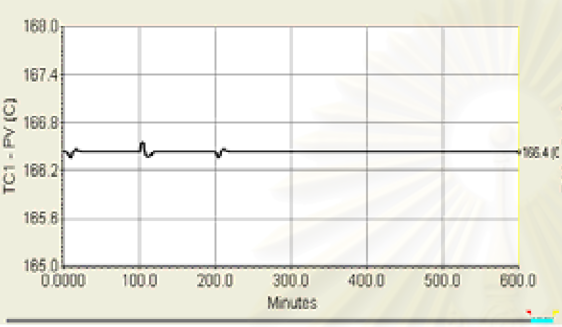
Case Study3

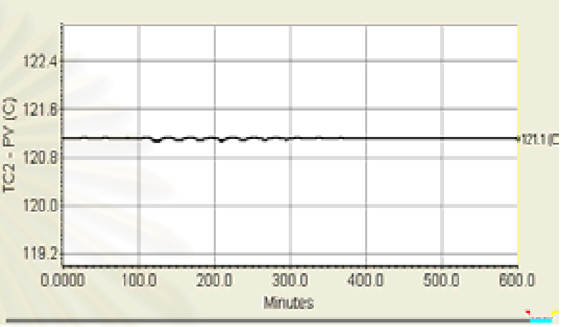

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

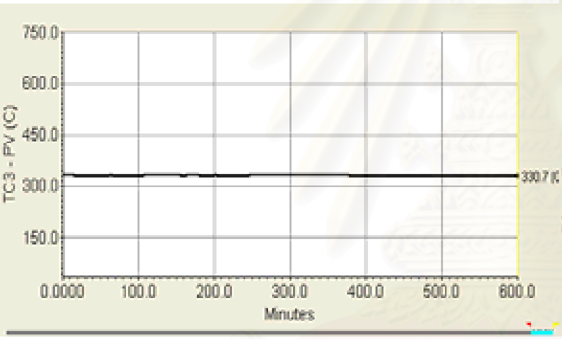

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)

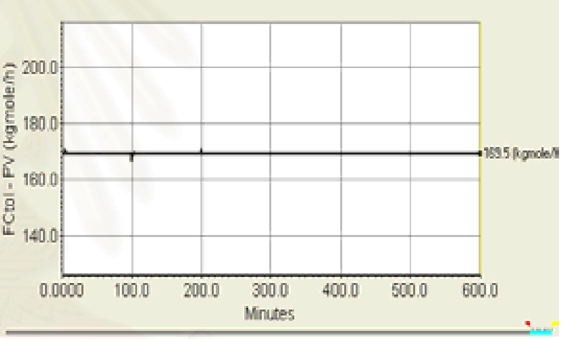

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

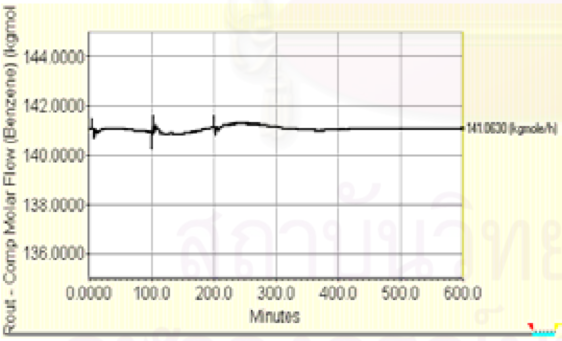

TC5 - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

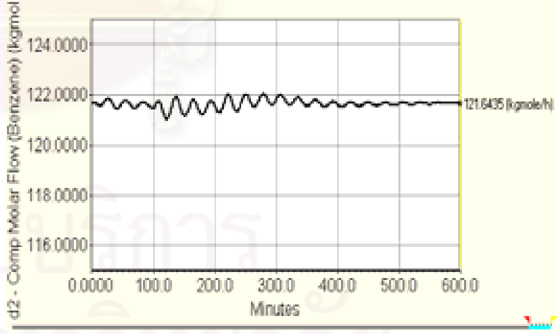

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (C


TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

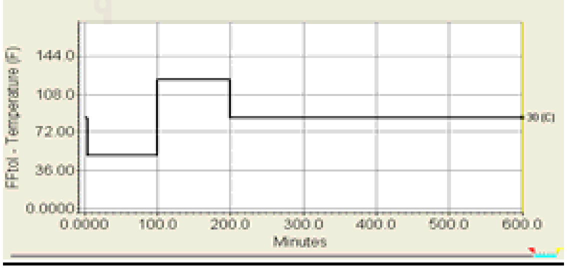

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
330.7 (C

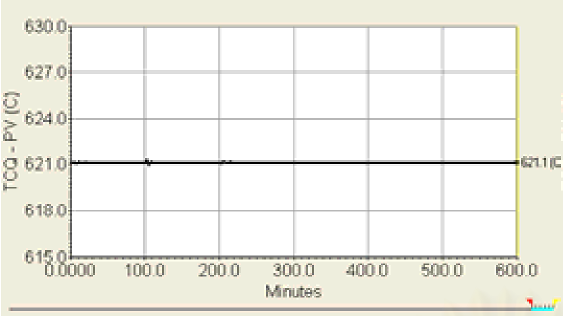

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h

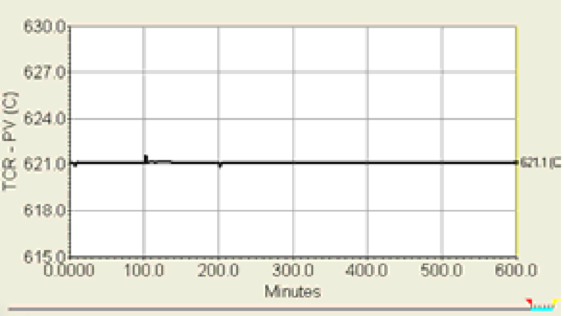

Rout - Comp Molar Flow (Benzene) (kgmol
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.0630 (kgmole/h)

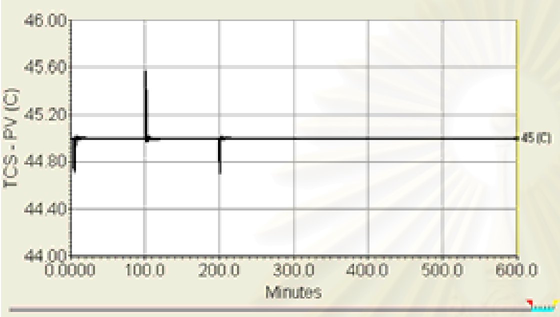

d2 - Comp Molar Flow (Benzene) (kgmole
124.0000
122.0000
120.0000
118.0000
116.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.6435 (kgmole/h)

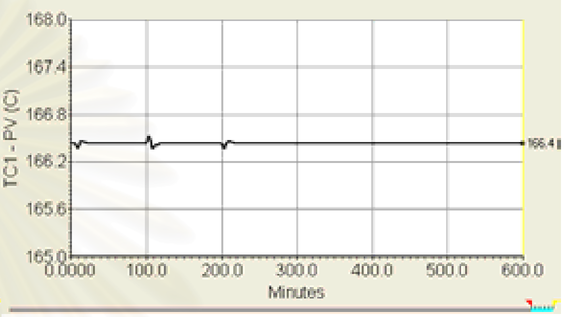
Case Study4

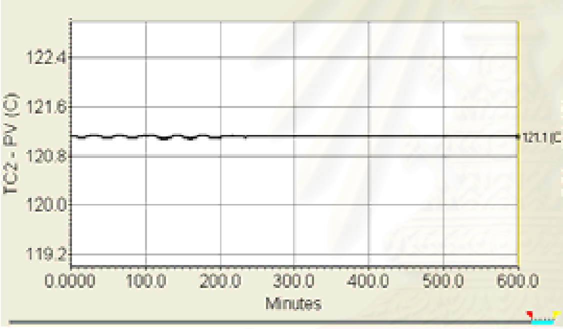

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

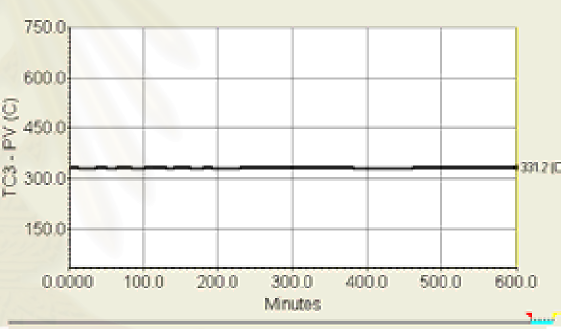

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

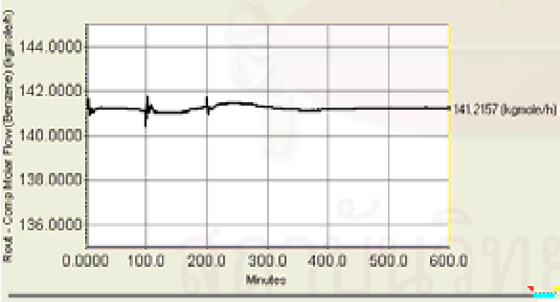

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

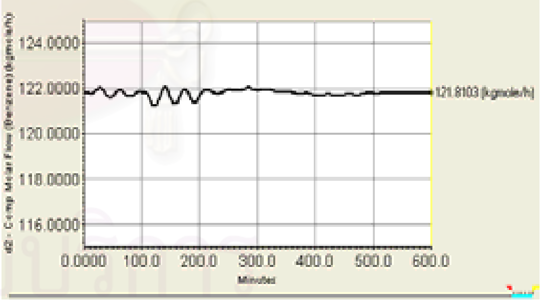

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

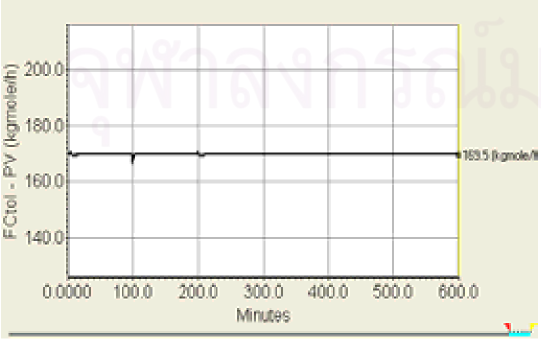

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4


TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

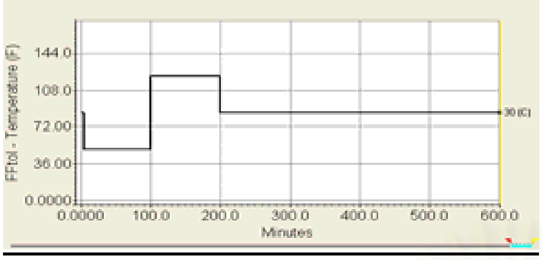

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.2 (C

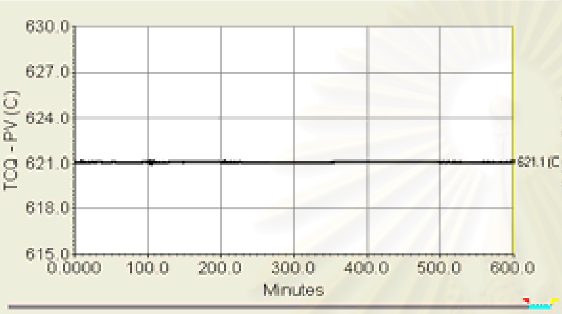

Rout - Comp Molar Flow (Benzene) (kgmole/h)
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.2157 (kgmole/h)

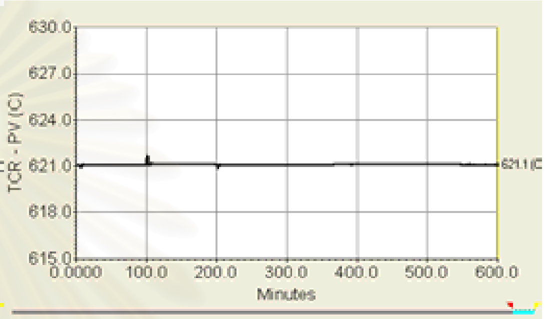

d2 - Comp Molar Flow (Benzene) (kgmole/h)
124.0000
122.0000
120.0000
118.0000
116.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.8103 (kgmole/h)

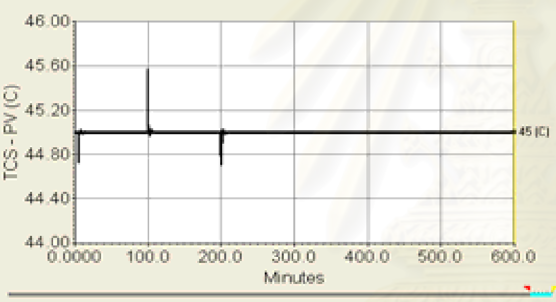

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h

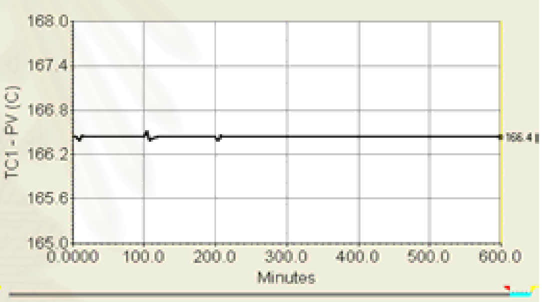
Case Study5

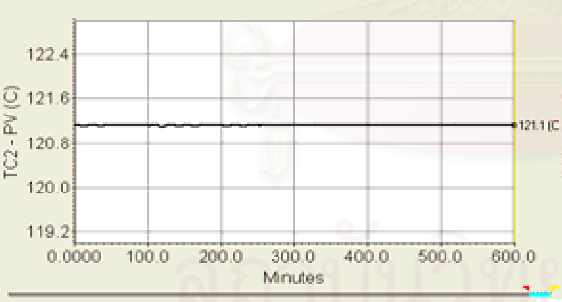

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

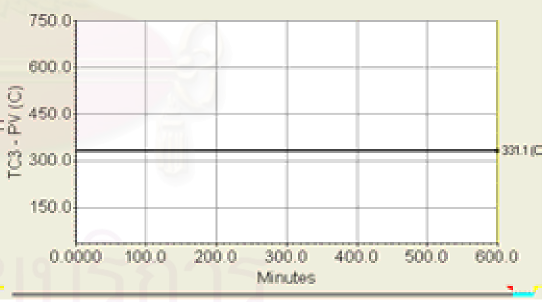

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

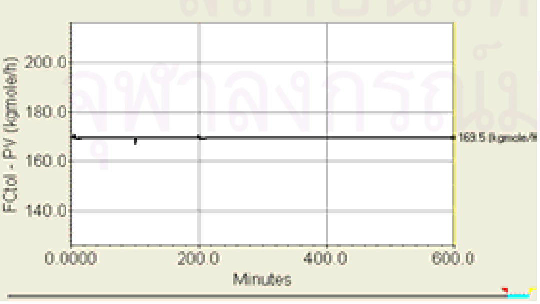

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

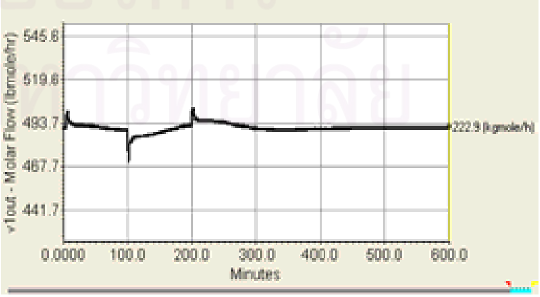

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

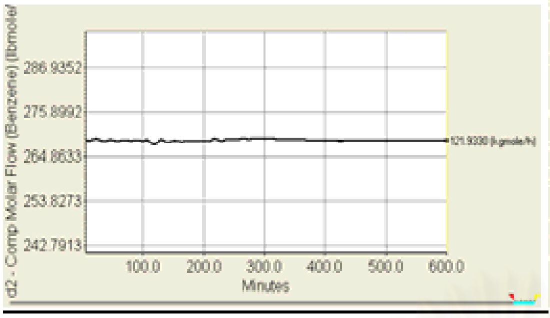

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (

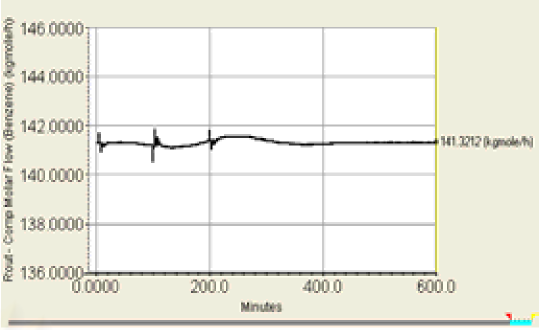

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1 (C

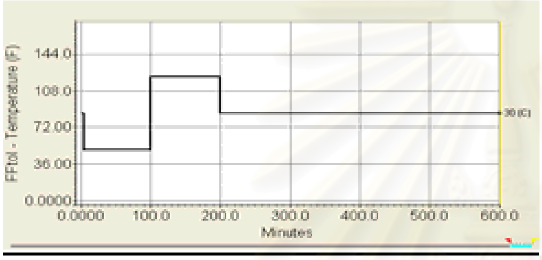

FCtol - PV (kgmole/h)
200.0
180.0
160.0
140.0
0.0000
200.0
400.0
600.0
Minutes
169.5 (kgmole/h

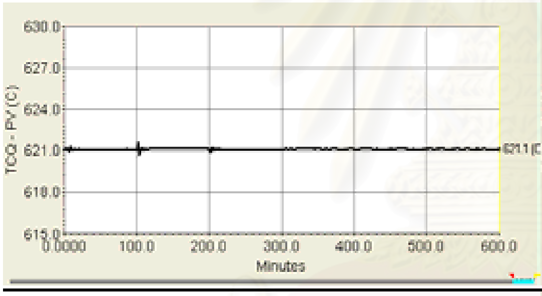

v1out - Molar Flow (lbmole/hr)
545.8
519.8
493.7
467.7
441.7
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
222.9 (kgmole/h)

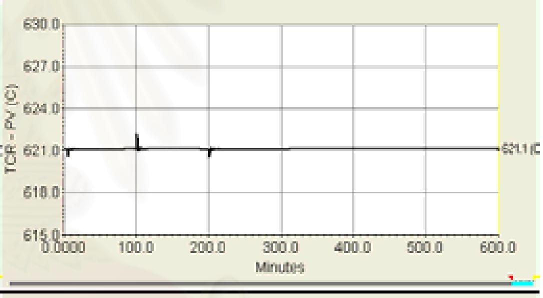

d2 - Comp Molar Flow (Benzene) (lbmole/
286.9352
275.8992
264.8633
253.8273
242.7913
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.9330 (kgmole/h)

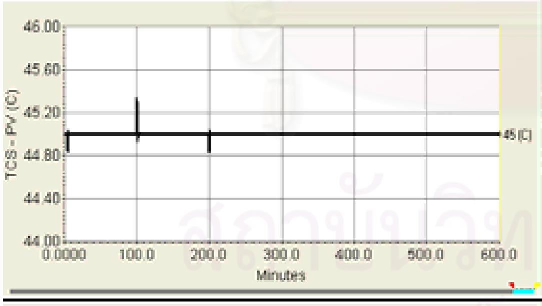

Rout - Comp Molar Flow (Benzene) (kgmole/h)
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
200.0
400.0
600.0
Minutes
141.3212 (kgmole/h)

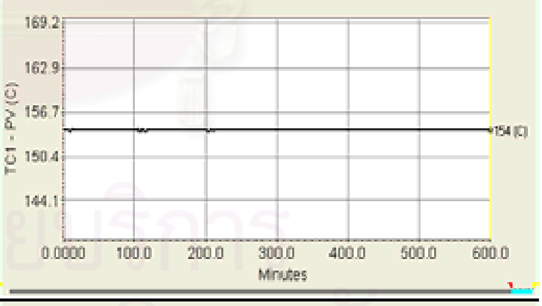
Case Study6

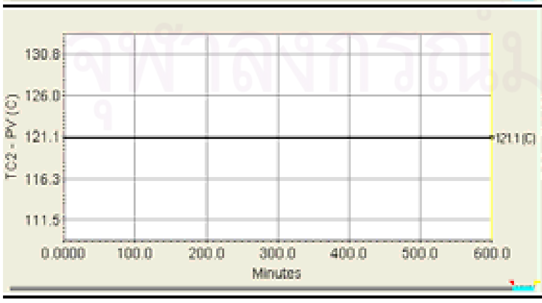

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

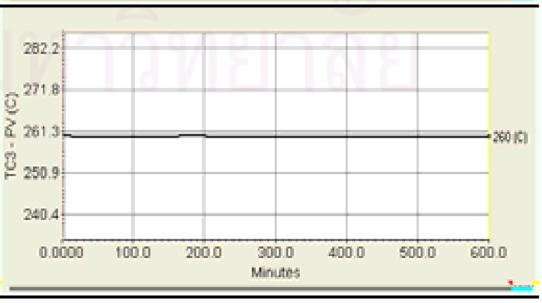

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

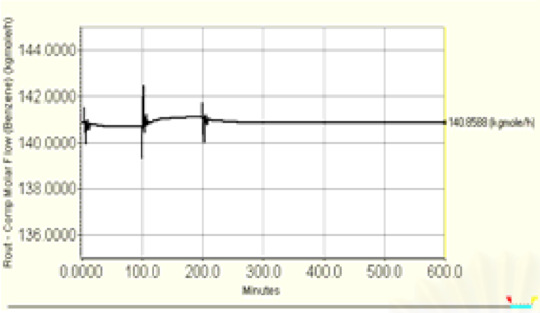

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

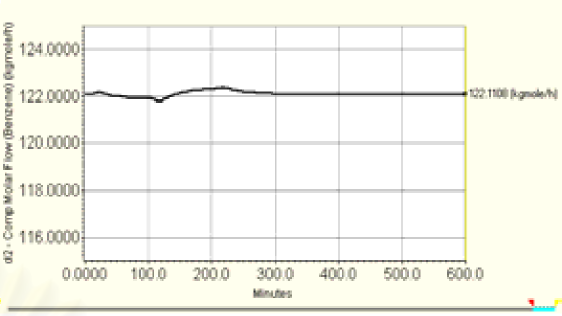

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
169.2
162.9
156.7
150.4
144.1
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154 (C)

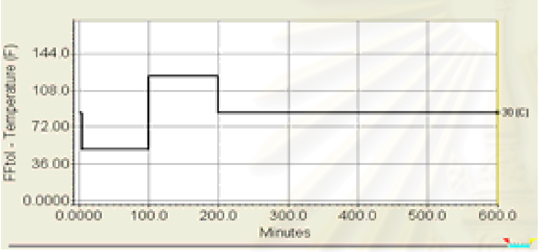

TC2 - PV (C)
130.8
126.0
121.1
116.3
111.5
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C)

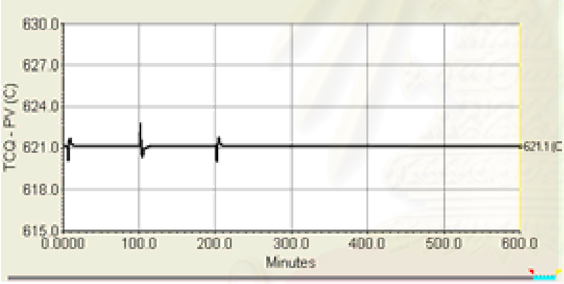

TC3 - PV (C)
282.2
271.8
261.3
250.9
240.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
260 (C)

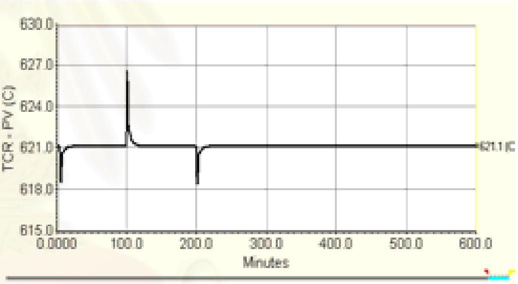

Rout - Comp Molar Flow (Benzene) (kgmole/h)
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
140.8588 (kgmole/h)

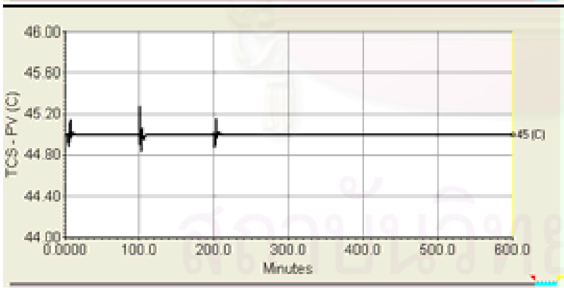

d2 - Comp Molar Flow (Benzene) (kgmole/h)
124.0000
122.0000
120.0000
118.0000
116.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
122.1100 (kgmole/h)

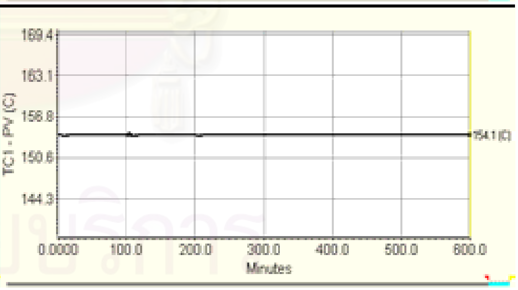
Case Study7

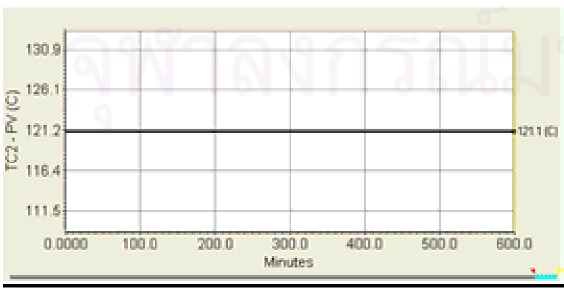

FFtol - Temperature (F)
144.0
108.0
72.00
36.00
0.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

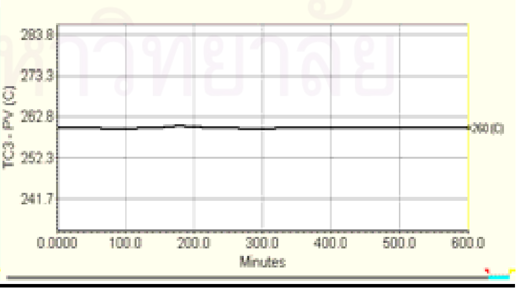

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C


TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C


TC5 - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
169.4
163.1
156.8
150.6
144.3
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154.1 (C)


TC2 - PV (C)
130.9
126.1
121.2
116.4
111.5
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C)


TC3 - PV (C)
283.8
273.3
262.8
252.3
241.7
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
260 (C)

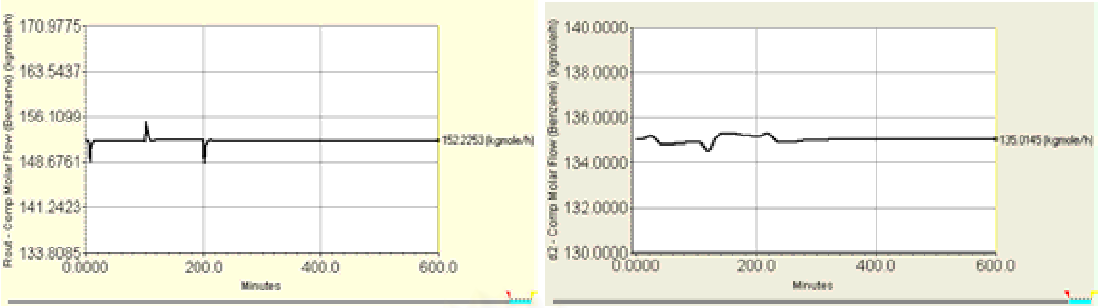
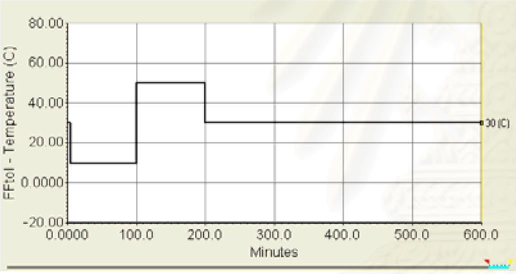
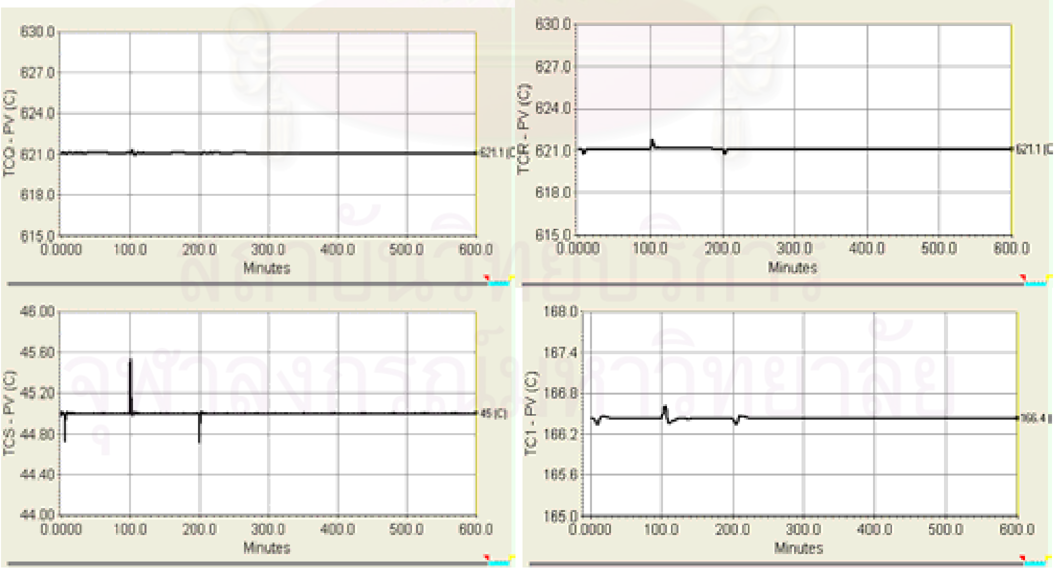


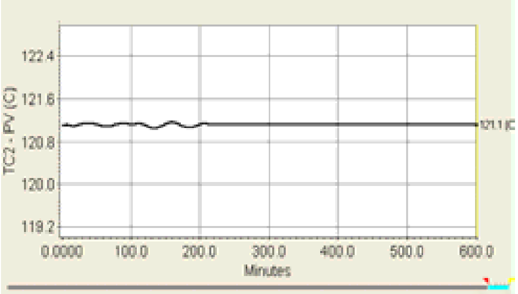
Figure C.3: Dynamic responses of CS1 of seven case studies to load change of toluene feed temperature ±20 °C.

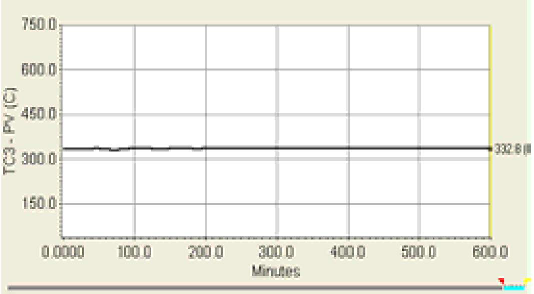
C.1.2 Control structure 2

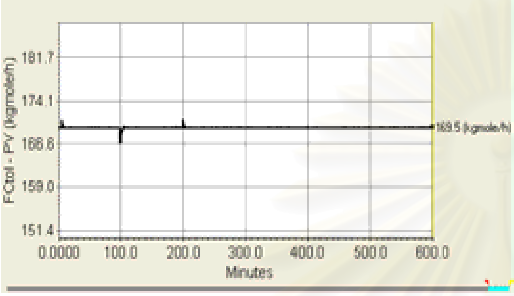
Case Study1

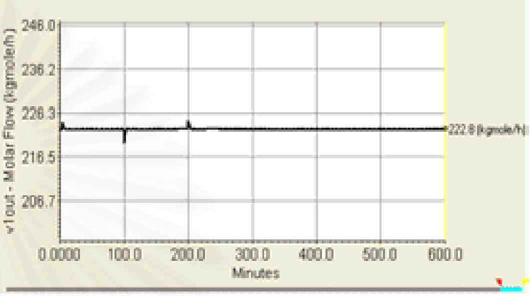


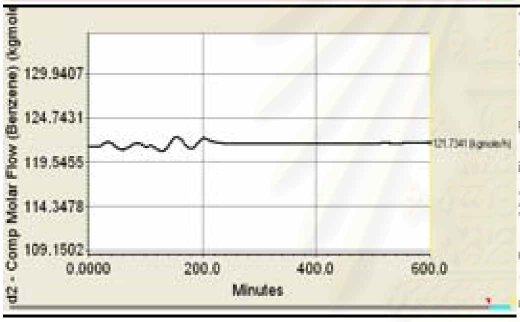


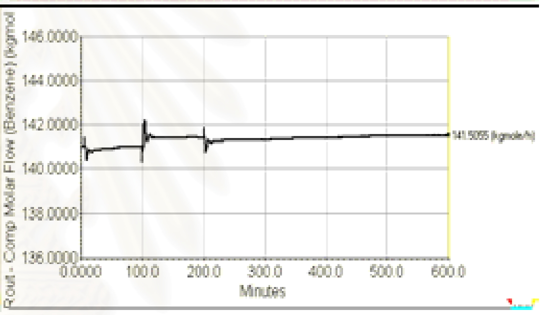

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
332.8 (

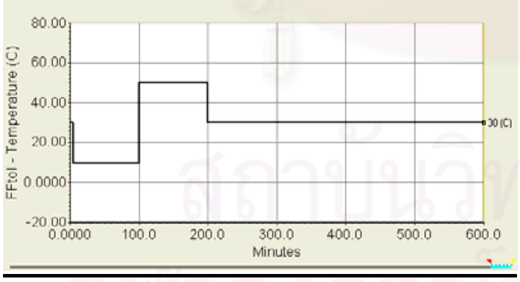

FCtol - PV (kgmole/h)
181.7
174.1
166.6
159.0
151.4
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h)

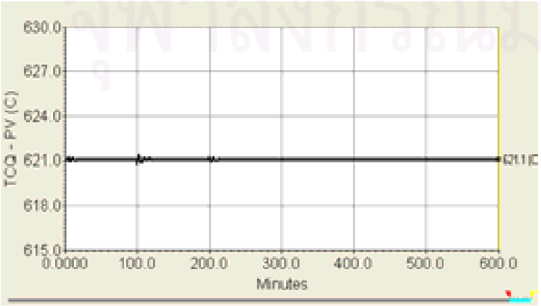

v1out - Molar Flow (kgmole/h)
246.0
236.2
226.3
216.5
206.7
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
222.8 (kgmole/h)

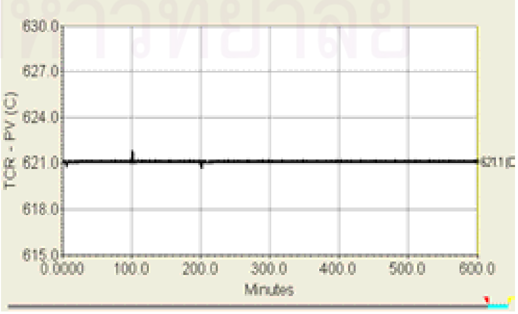

d2 - Comp Molar Flow (Benzene) (kgmol
129.9407
124.7431
119.5455
114.3478
109.1502
0.0000
200.0
400.0
600.0
Minutes
121.7341 (kgmole/h)

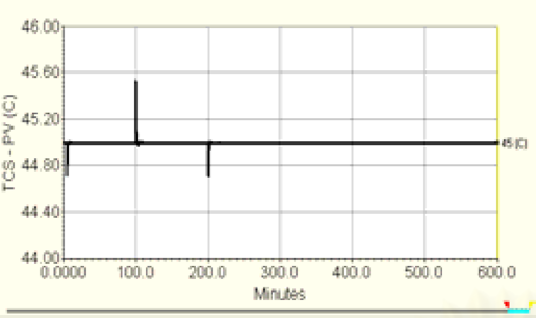

Rout - Comp Molar Flow (Benzene) (kgmol
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
141.5055 (kgmole/h)

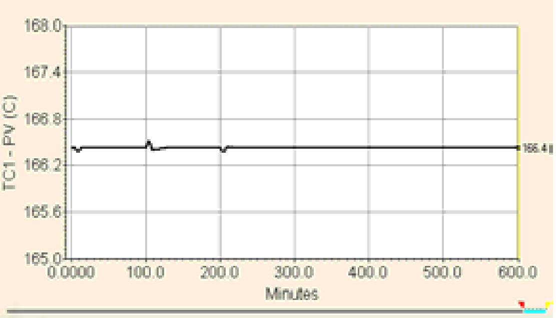
Case Study2

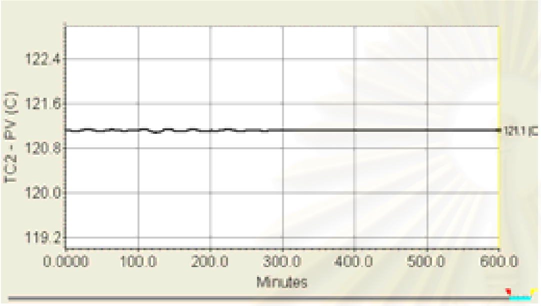

FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

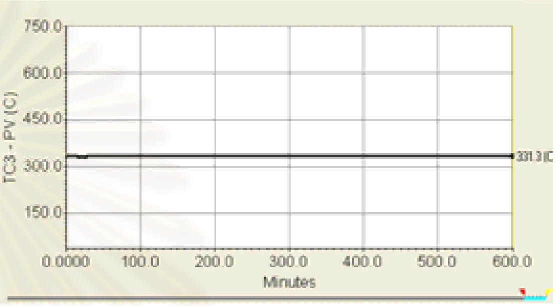

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

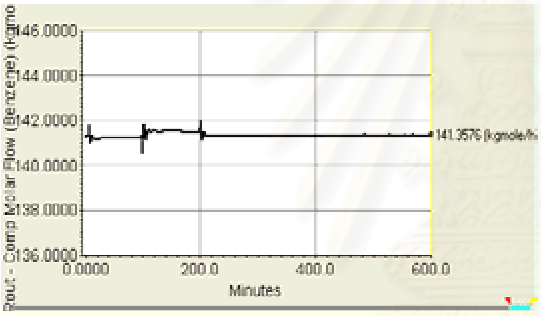

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

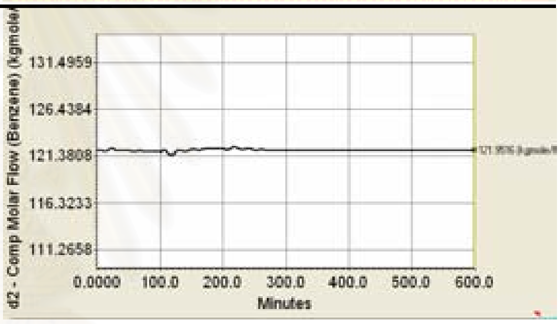

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

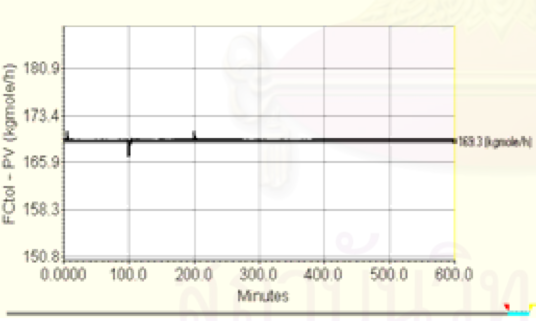

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4


TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

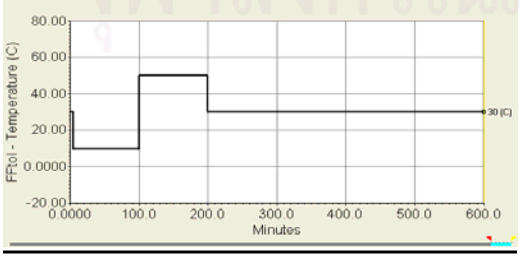

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.3 (C

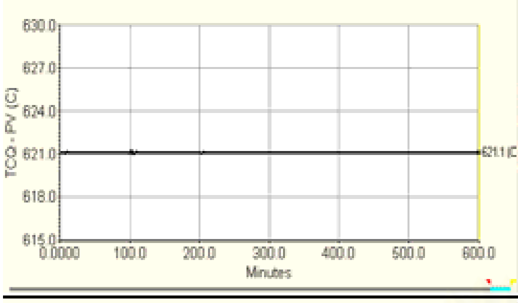

Rout - Comp Molar Flow (Benzene) (kgmo
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
200.0
400.0
600.0
Minutes
141.3576 (kgmole/h

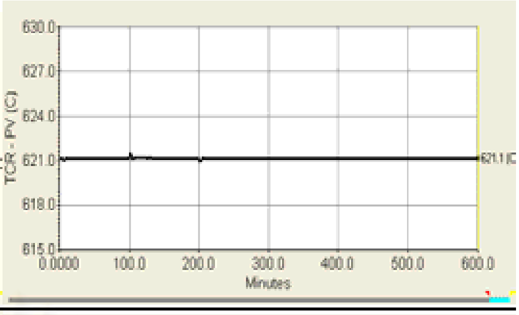

d2 - Comp Molar Flow (Benzene) (kgmole/
131.4959
126.4384
121.3808
116.3233
111.2658
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.3576 (kgmole/h

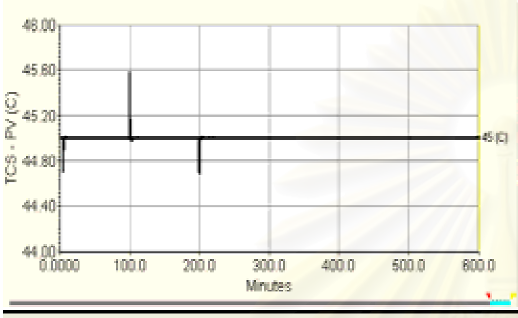

FCtol - PV (kgmole/h)
180.9
173.4
165.9
158.3
150.8
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.3 (kgmole/h)

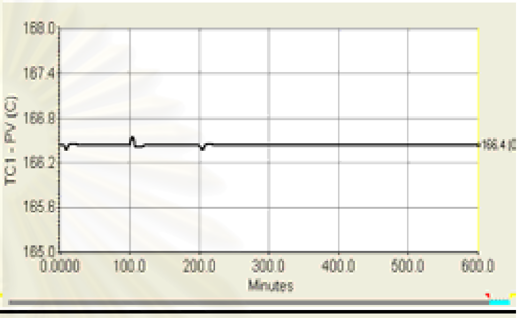
Case Study3

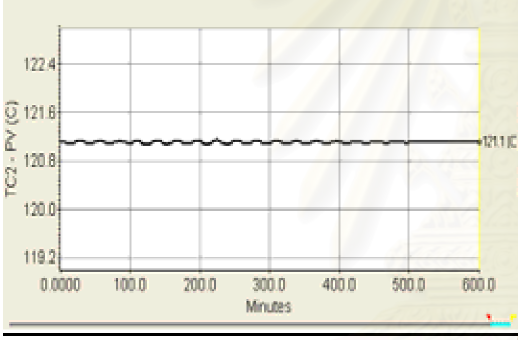

FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

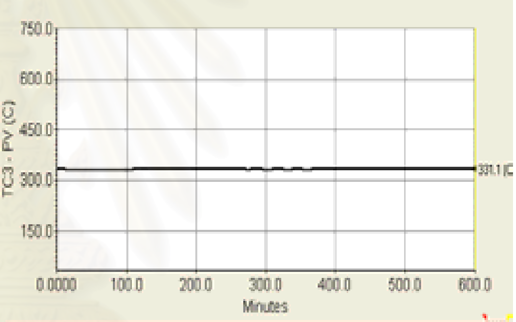

630.0
627.0
624.0
621.0
618.0
615.0
TCO - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

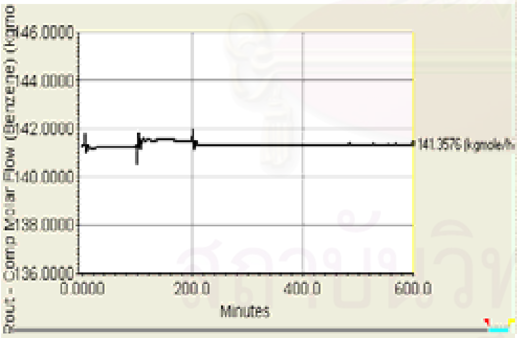

630.0
627.0
624.0
621.0
618.0
615.0
TCR - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

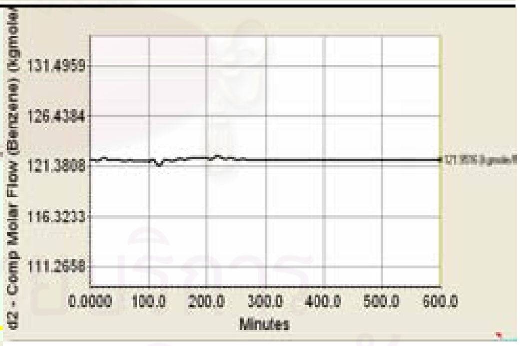

46.00
45.60
45.20
44.80
44.40
44.00
TCS - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

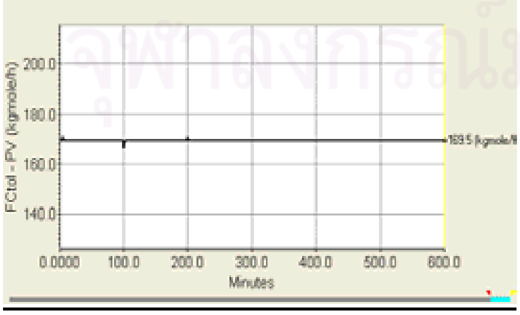

168.0
167.4
166.8
166.2
165.6
165.0
TC1 - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (C


122.4
121.6
120.8
120.0
119.2
TC2 - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

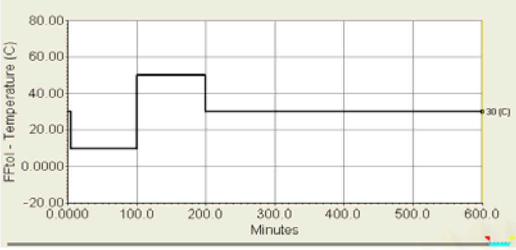

750.0
600.0
450.0
300.0
150.0
TC3 - PV (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1 (C

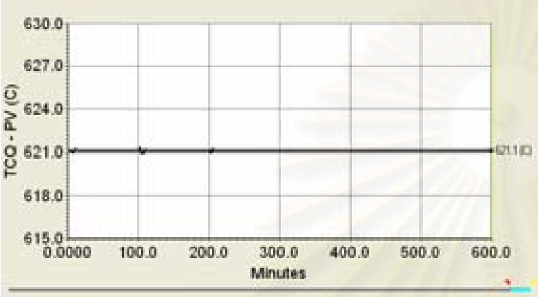

146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
Bout - Comp Molar Flow (Benzene) (kgmo
0.0000
200.0
400.0
600.0
Minutes
141.3576 (kgmole/h

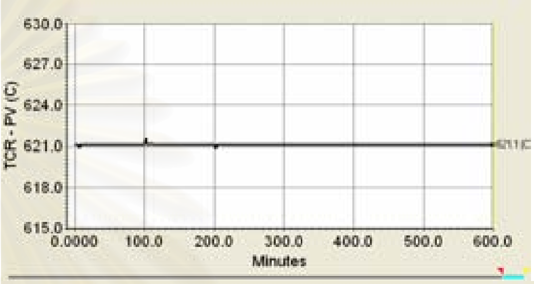

131.4959
126.4384
121.3808
116.3233
111.2658
d2 - Comp Molar Flow (Benzene) (kgmole/
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

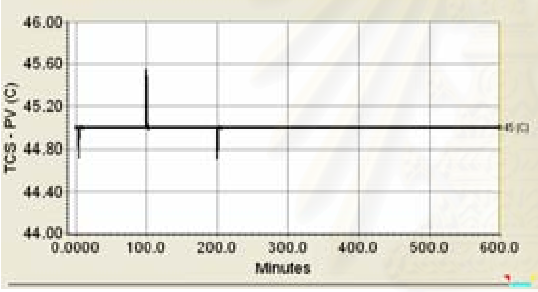

200.0
180.0
160.0
140.0
FCtol - PV (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h

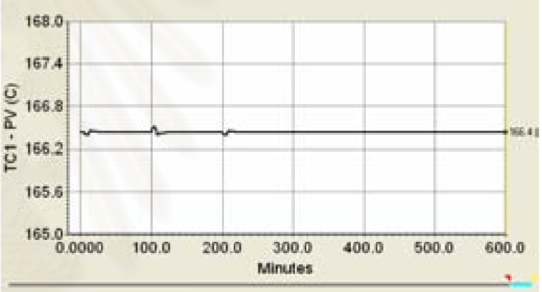
Case Study4

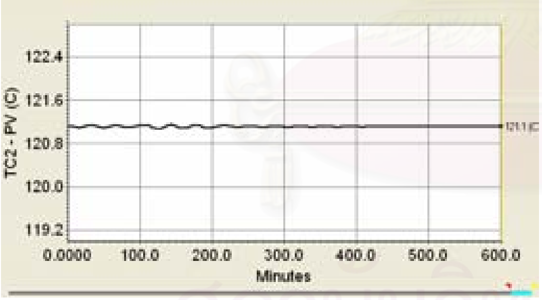

FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

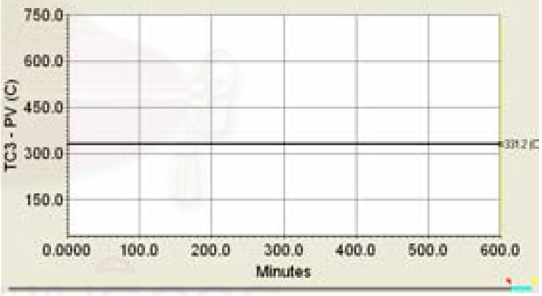

TCO - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C)

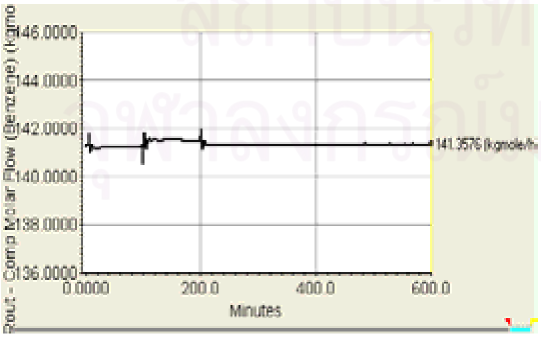

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

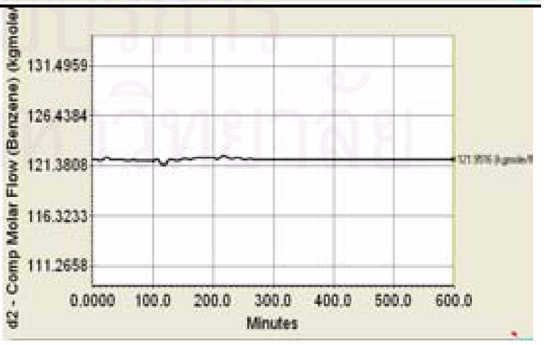

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

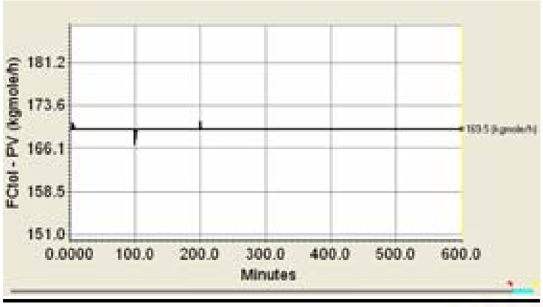

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
166.4 (


TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1 (C

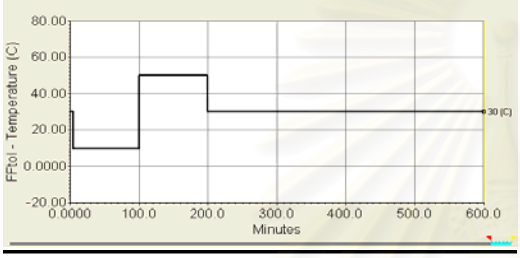

TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.2 (C

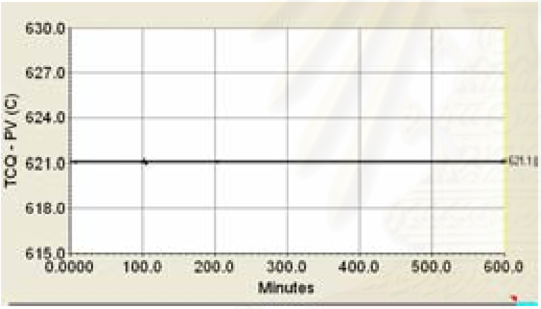

Rout - Comp Molar Flow (Benzene) (kgmo
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
200.0
400.0
600.0
Minutes
141.3576 (kgmole/h

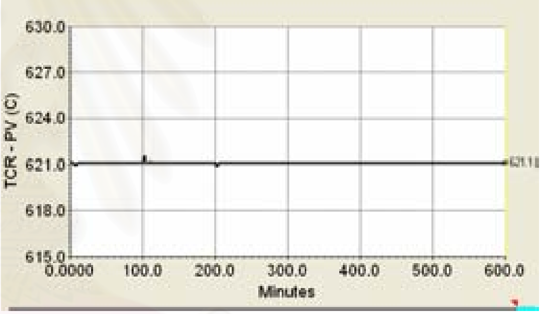

d2 - Comp Molar Flow (Benzene) (kgmole/
131.4959
126.4384
121.3808
116.3233
111.2658
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

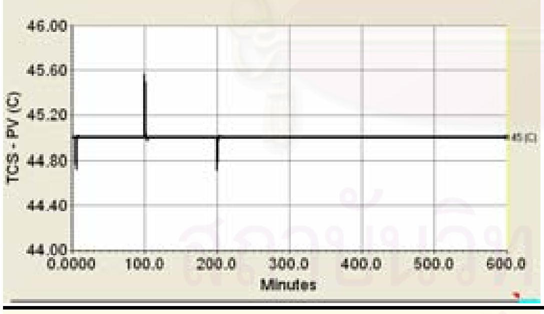

FCtol - PV (kgmole/h)
181.2
173.6
166.1
158.5
151.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h)

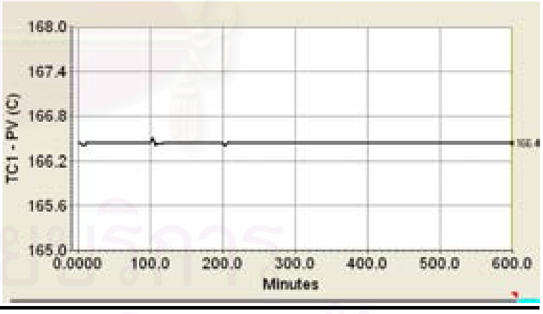
Case Study5

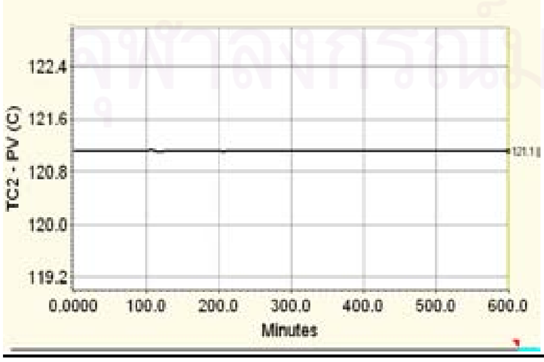

FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

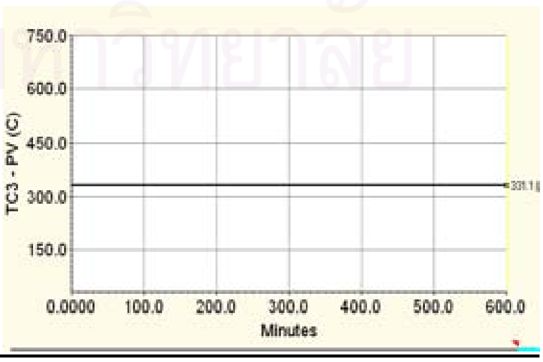

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1

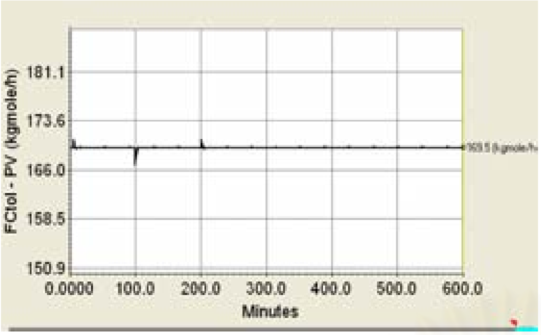

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1

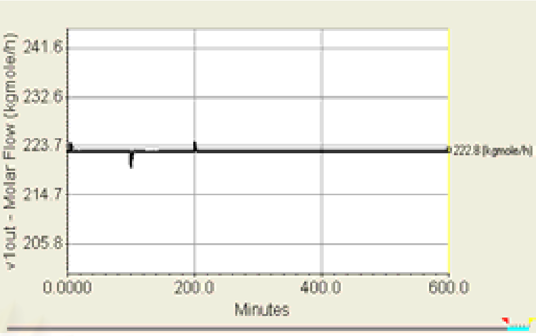

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)

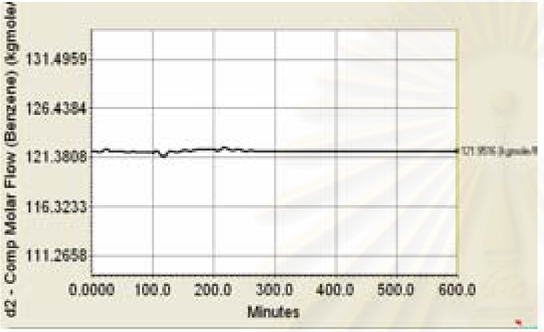

TC1 - PV (C)
168.0
167.4
166.8
166.2
165.6
165.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

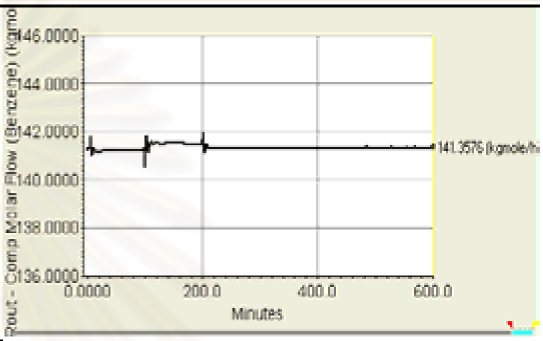

TC2 - PV (C)
122.4
121.6
120.8
120.0
119.2
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
121.1


TC3 - PV (C)
750.0
600.0
450.0
300.0
150.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
331.1

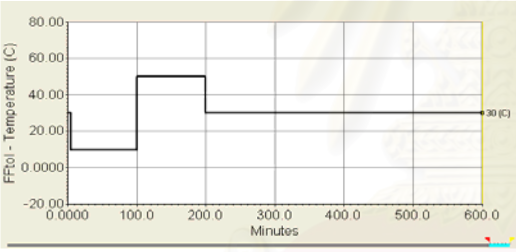

FCtol - PV (kgmole/h)
181.1
173.6
166.0
158.5
150.9
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
169.5 (kgmole/h

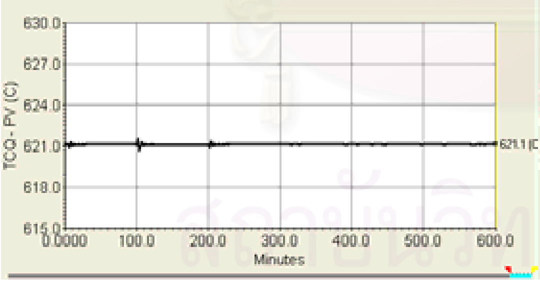

v1out - Molar Flow (kgmole/h)
241.6
232.6
223.7
214.7
205.8
0.0000
200.0
400.0
600.0
Minutes
222.8 (kgmole/h)

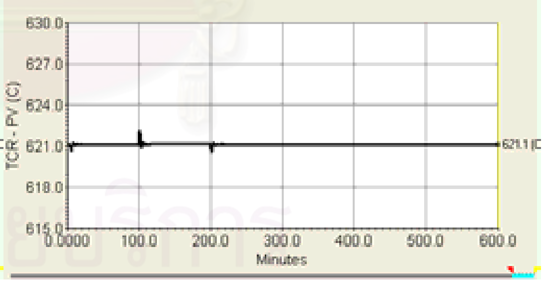

d2 - Comp Molar Flow (Benzene) (kgmole/
131.4959
126.4384
121.3808
116.3233
111.2658
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

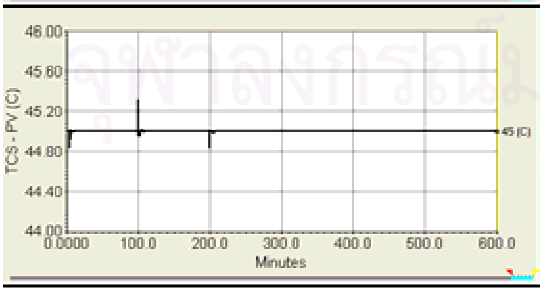

Rout - Comp Molar Flow (Benzene) (kgmo
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
0.0000
200.0
400.0
600.0
Minutes
141.3576 (kgmole/h

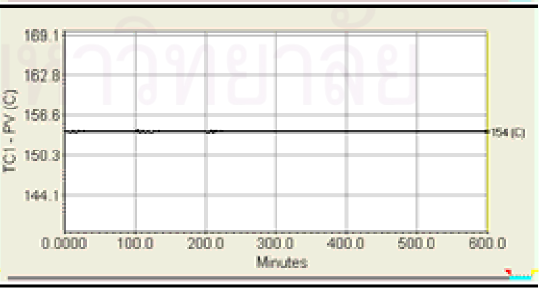
Case Study6

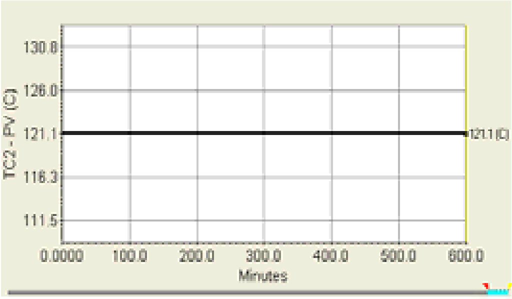

FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
30 (C)

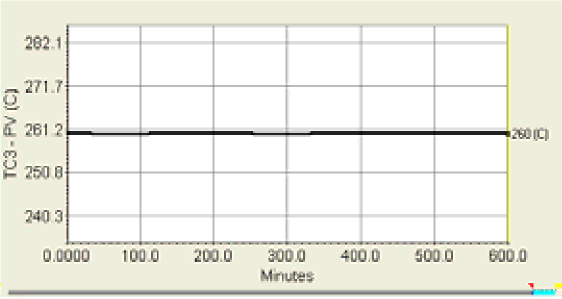

TCQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

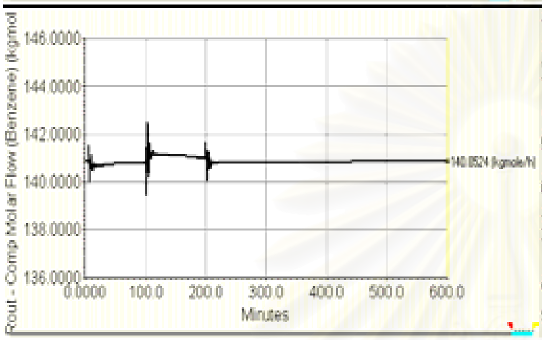

TCR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
621.1 (C

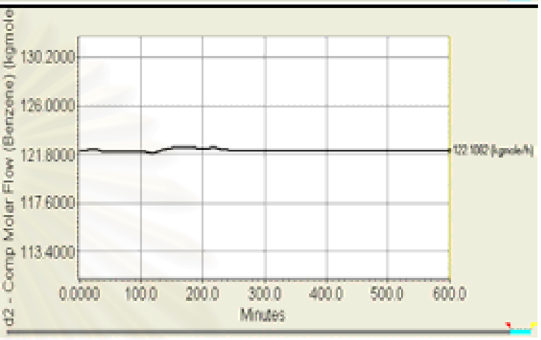

TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
45 (C)


TC1 - PV (C)
169.1
162.8
156.6
150.3
144.1
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes
154 (C)

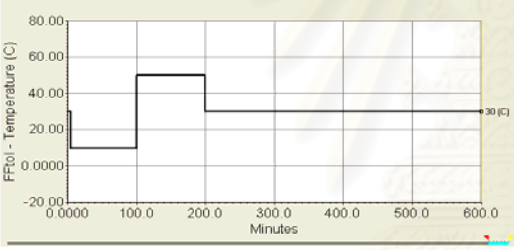

TC2 - PV (C)
130.8
126.0
121.1
116.3
111.5
121.1 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

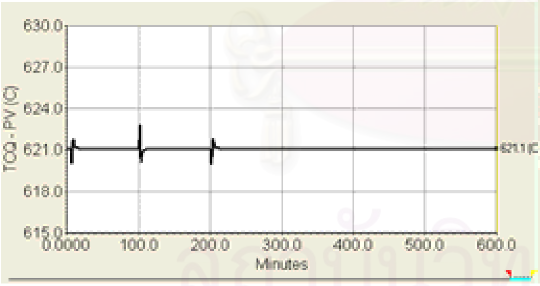

TC3 - PV (C)
282.1
271.7
261.2
250.8
240.3
260 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

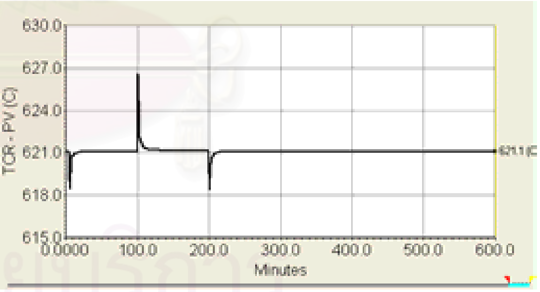

Rout - Comp Molar Flow (Benzene) (kgmol
146.0000
144.0000
142.0000
140.0000
138.0000
136.0000
140.8524 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

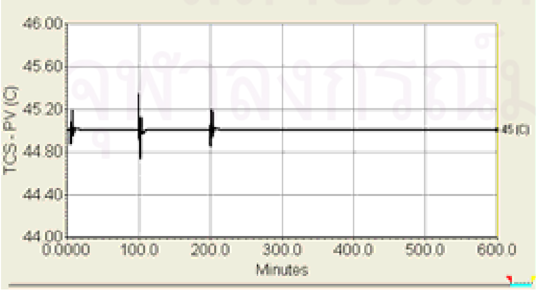

d2 - Comp Molar Flow (Benzene) (kgmole
130.2000
126.0000
121.8000
117.6000
113.4000
122.1082 (kgmole/h)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

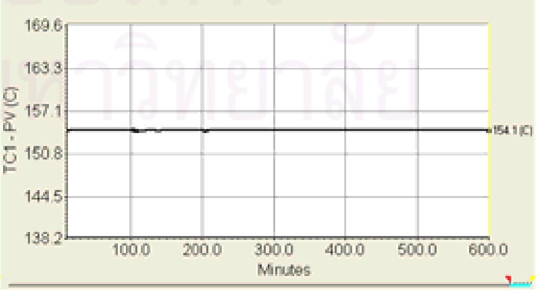
Case Study7


FFtol - Temperature (C)
80.00
60.00
40.00
20.00
0.0000
-20.00
30 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TOQ - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TOR - PV (C)
630.0
627.0
624.0
621.0
618.0
615.0
621.1 (C
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TCS - PV (C)
46.00
45.60
45.20
44.80
44.40
44.00
45 (C)
0.0000
100.0
200.0
300.0
400.0
500.0
600.0
Minutes


TC1 - PV (C)
169.6
163.3
157.1
150.8
144.5
138.2
154.1 (C)
100.0
200.0
300.0
400.0
500.0
600.0
Minutes

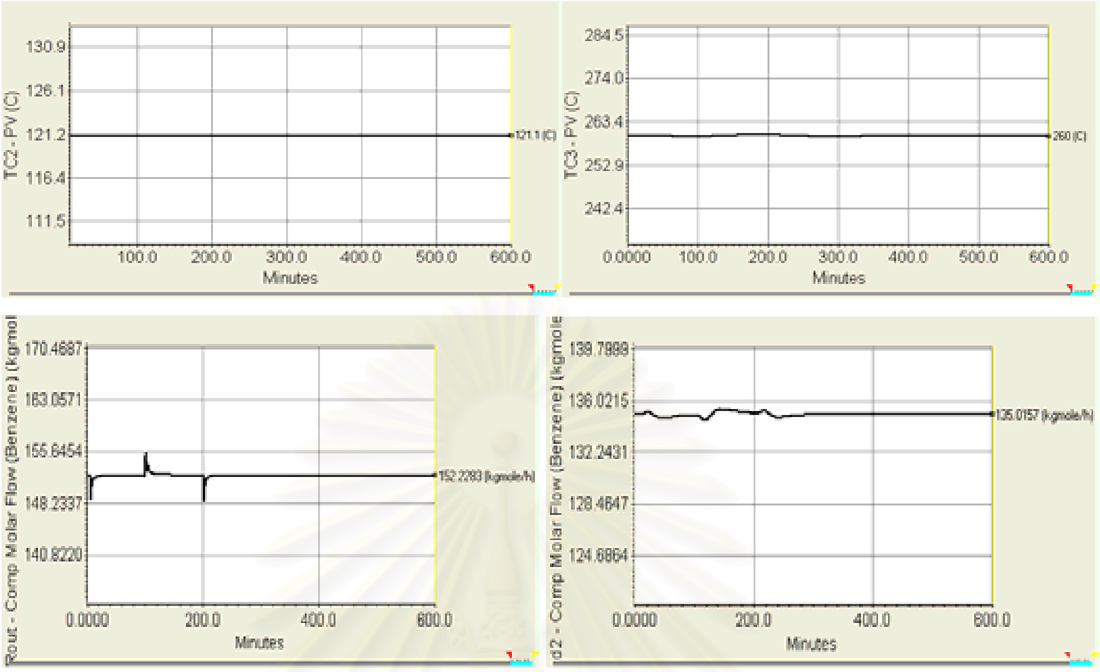


Figure C.4: Dynamic responses of CS2 of seven case studies to load change of toluene feed temperature ±20 °C.

Table C.1 Integral absolute error (IAE) from set-point change and load disturbance of product quality control loops (CS1)

IAE **test SP change of Total toluene feed ±5 kmol/h**

case	TCQ	TCR	TCS	TC1	TC2	TC3	FCtol	**sum**
1	8.18	26.137	3.752	11.663	24.978	4,525.60	40.192	4,640.50
2	19.145	20.192	3.662	8.096	11.684	5,389.200	41.488	5,493.47
3	11.199	11.856	3.7965	10.981	18.493	4,286.50	41.917	4,384.74
4	13.968	12.476	3.526	7.133	17.934	4,983.000	40.735	5,078.77
5	6.934	12.217	3.591	5.100	12.342	4,692.300	42.690	4,775.17
6	8.2462	9.7834	1.3347	45.337	1.5674	246.67	21.482	334.42
7	10.498	41.143	2.6588	16.328	1.3249	352.52	22.723	447.20

IAE **test load change of toluene feed temperature ±20 °C**

case	TCQ	TCR	TCS	TC1	TC2	TC3	FCtol	**sum**
1	1.941	9.41	3.448	3.577	5.479	272.26	28.017	324.13
2	4.505	13.450	3.497	1.843	2.007	240.930	29.052	295.28
3	1.8492	3.712	3.6136	2.3523	4.5602	260.72	27.723	304.53
4	2.298	3.946	3.451	1.752	2.995	205.670	28.597	248.71
5	1.613	3.850	3.465	1.315	1.078	206.070	29.120	246.51
6	3.533	5.047	0.556	6.548	0.135	23.63	6.902	46.35
7	11.555	35.386	1.252	3.792	0.659	43.35	12.130	108.13

Table C.2 Integral absolute error IAE from set-point change and load disturbance of product quality control loops (CS2)

IAE **test SP change of Total toluene feed ±5 kmol/h**

case	TCQ	TCR	TCS	TC1	TC2	TC3	FCtol	**sum**
1	7.786	26.289	3.960	8.244	33.418	1,534.10	82.448	1,696.250
2	18.579	20.182	3.810	5.556	13.571	521.260	75.133	658.090
3	10.757	11.705	3.9842	8.079	17.581	737.530	67.142	856.780
4	13.105	12.067	3.676	5.229	25.903	719.840	71.342	851.160
5	6.253	11.567	3.703	3.927	13.390	600.150	69.393	708.380
6	8.441	15.341	1.787	41.656	1.143	251.480	124.170	444.020
7	11.165	74.750	3.603	15.857	1.197	378.660	125.940	611.170

IAE **test load change of toluene feed temperature ±20 °C**

case	TCQ	TCR	TCS	TC1	TC2	TC3	FCtol	**sum**
1	1.96	9.512	3.363	3.297	5.758	1,002.10	39.526	1,065.52
2	4.717	14.159	3.445	1.567	2.659	206.840	37.455	270.840
3	1.873	3.5413	3.522	1.910	5.648	221.060	32.217	269.770
4	2.271	3.867	3.372	1.402	4.158	177.600	34.211	226.88
5	1.377	3.670	3.405	1.082	1.111	186.320	33.604	230.570
6	4.026	6.155	0.682	6.155	0.173	22.034	15.786	55.010
7	11.264	38.503	1.805	4.540	0.695	54.080	24.574	135.460

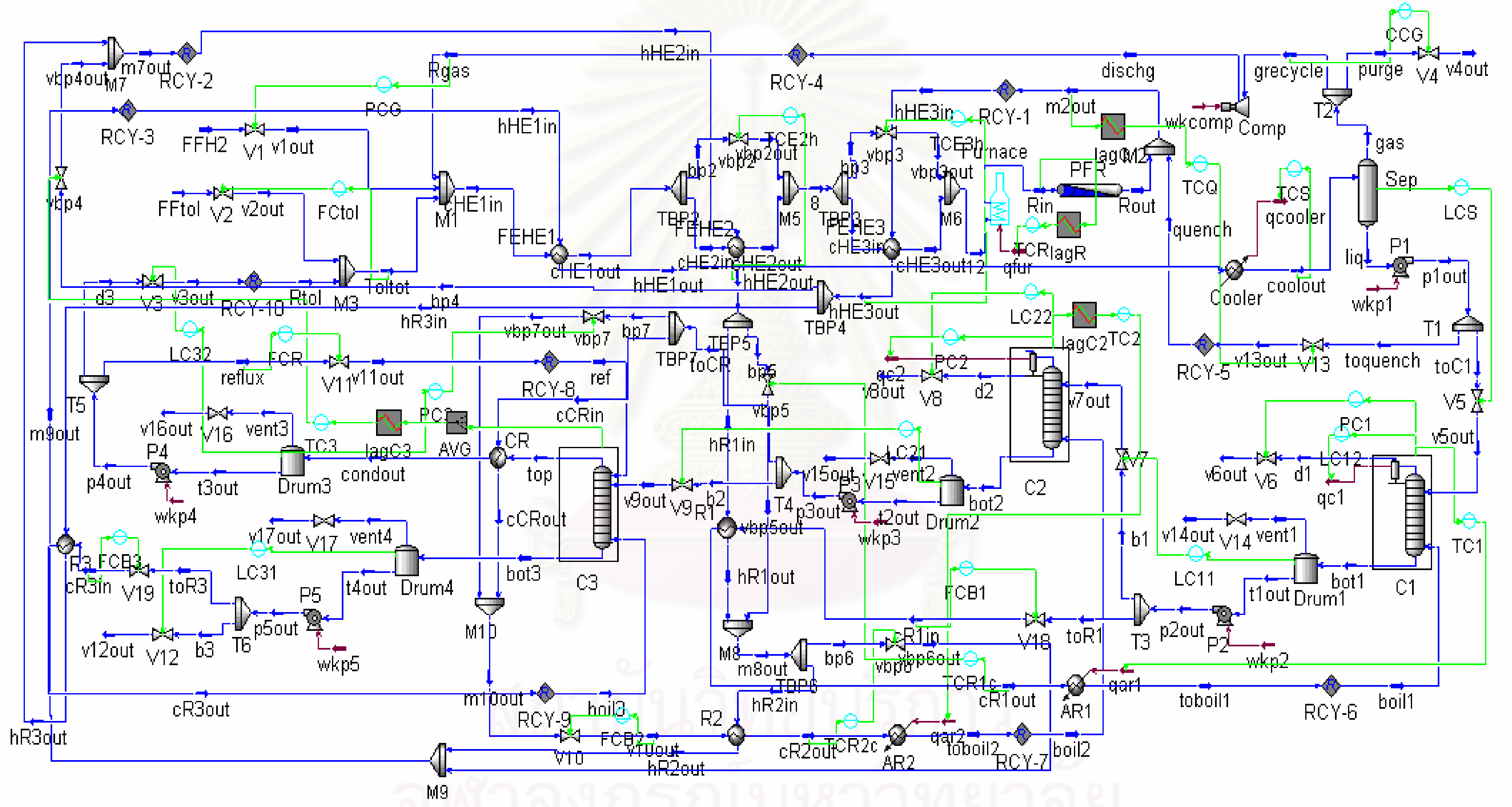


Figure C.5: The hysys flowsheet of HDA process (alt.6) with control scheme (CS1).

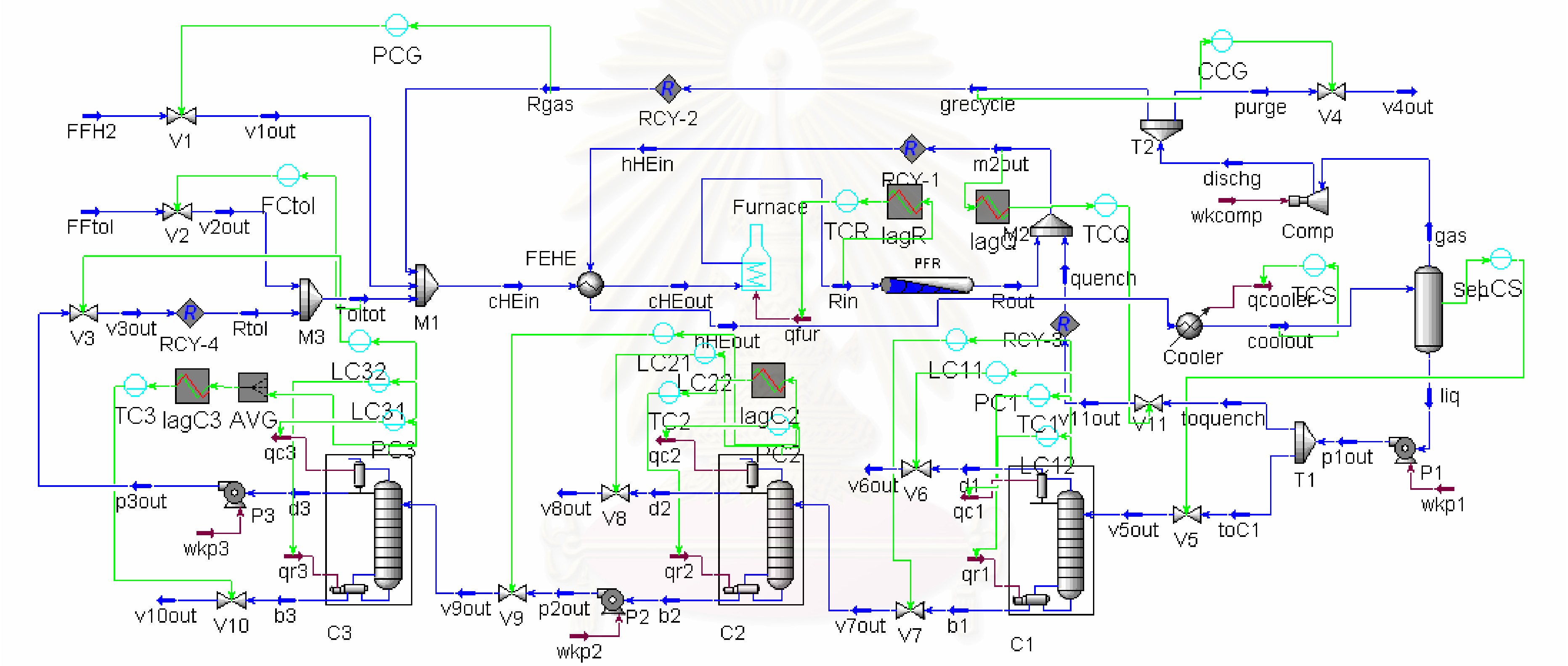


Figure C.6: The hysys flowsheet of HDA process (alt.1) with control scheme (CS1).

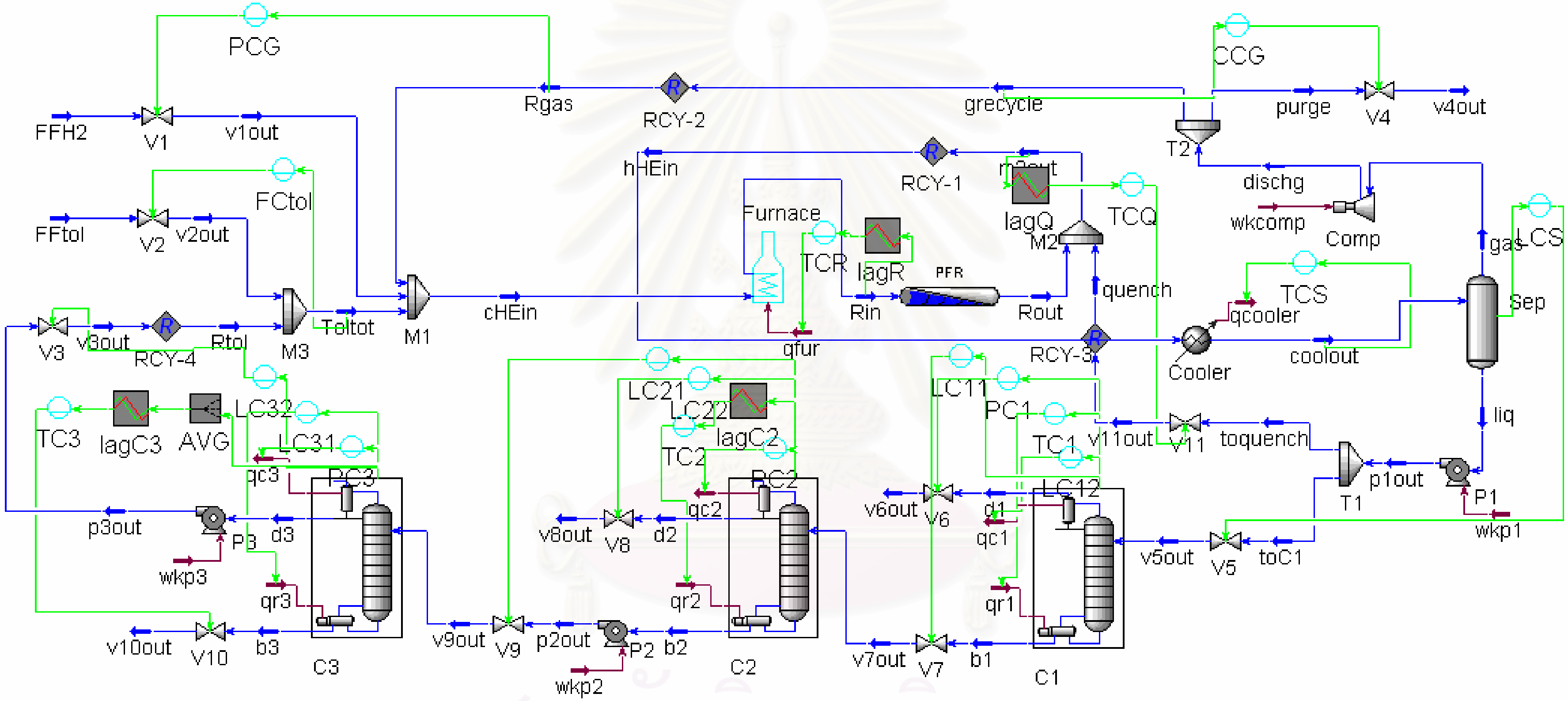


Figure C.7: The hysys flowsheet of HDA process (NO FEHE) with control scheme (CS1).

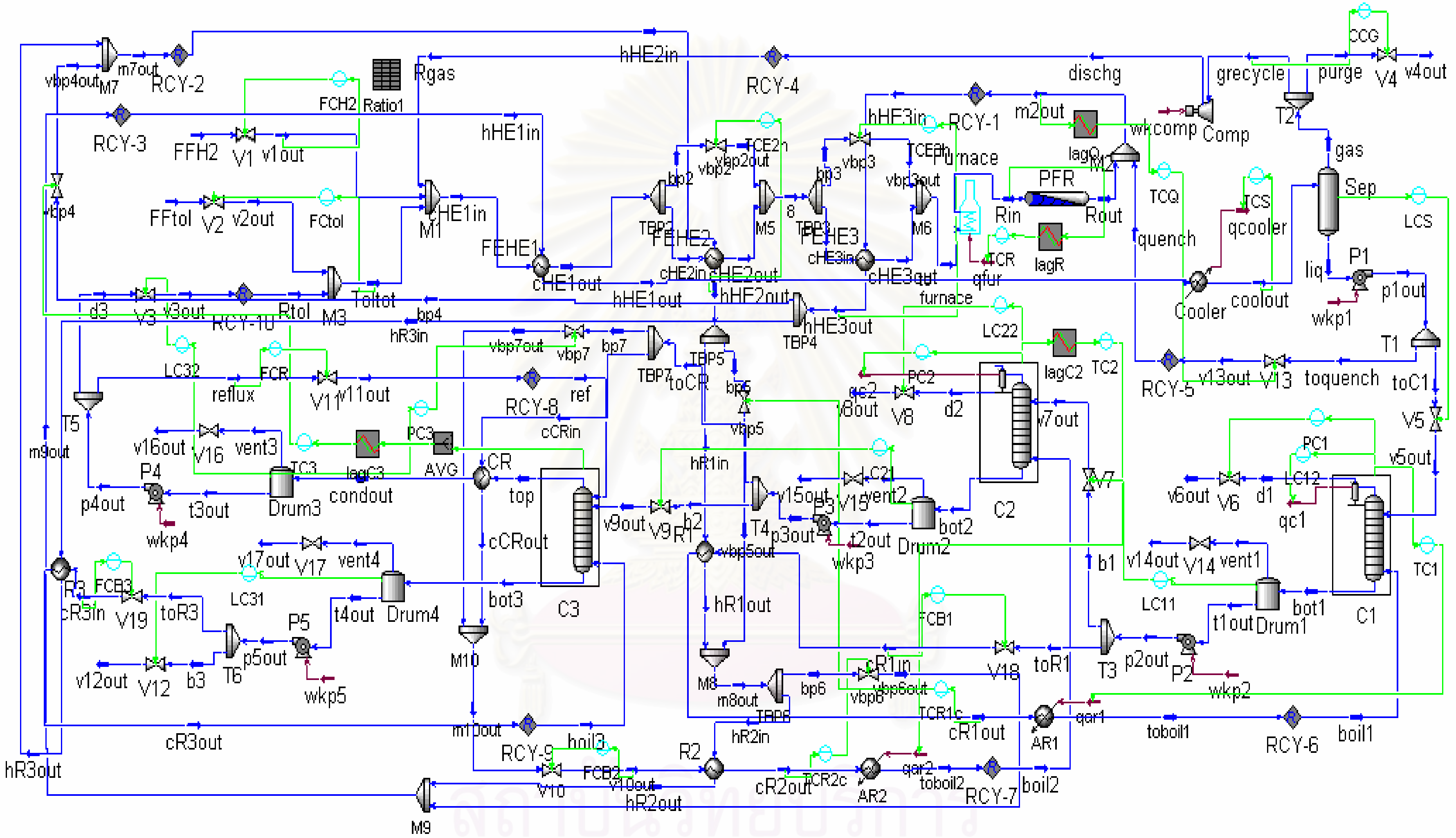


Figure C.8: The hysys flowsheet of HDA process (alt.6) with control scheme (CS2).

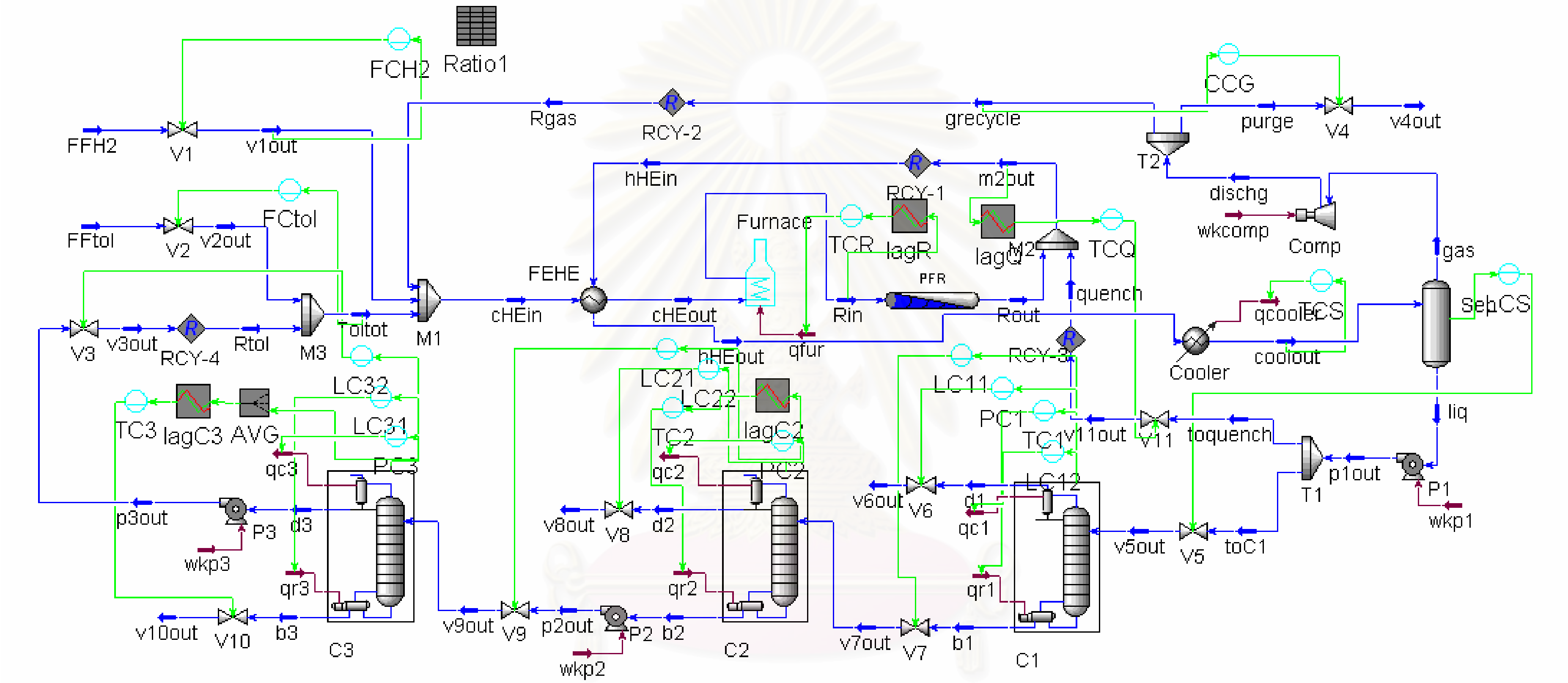


Figure C.9: The hysys flowsheet of HDA process (alt.1) with control scheme (CS2).

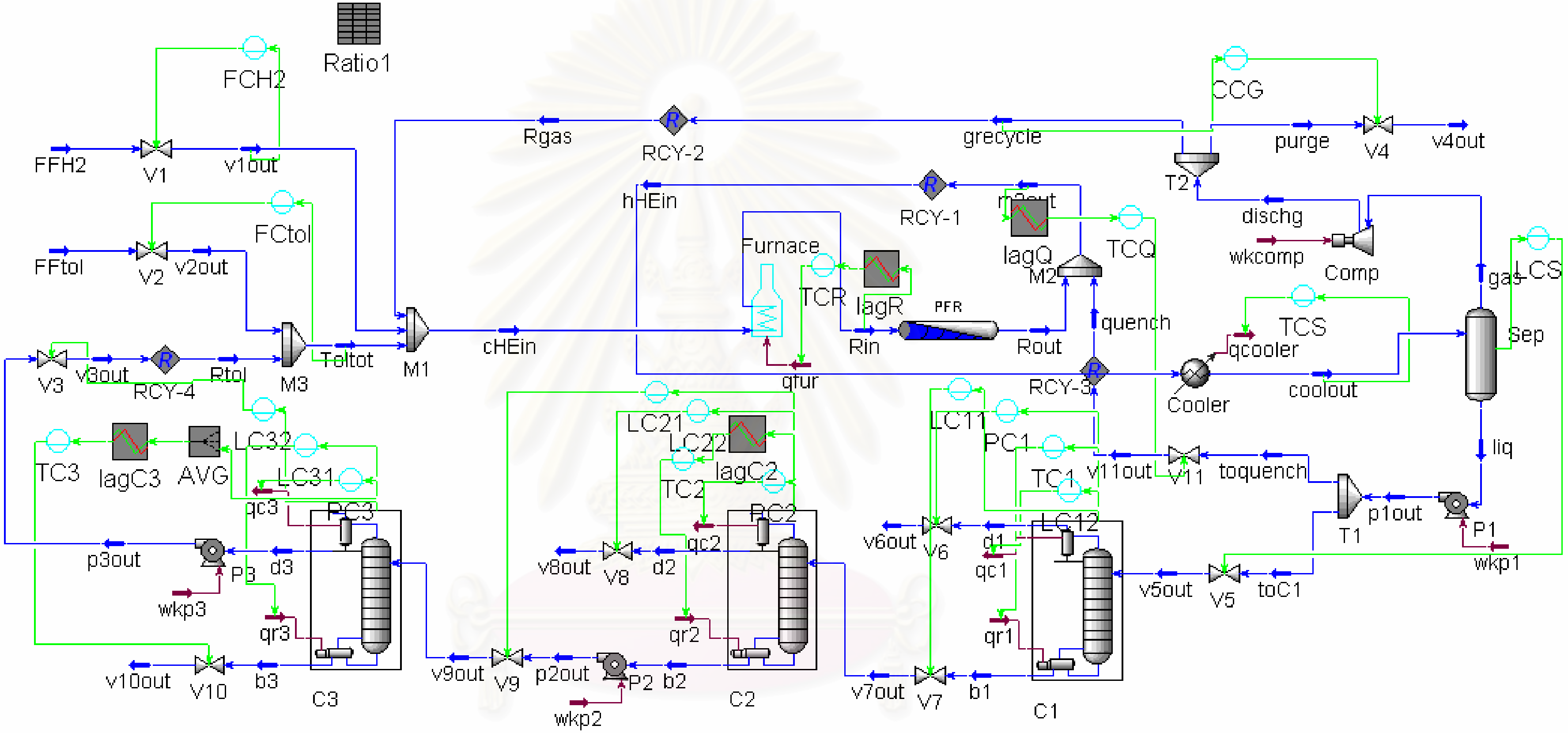


Figure C.10: The hysys flowsheet of HDA process (NO FEHE) with control scheme (CS2).

VITA

Miss Patcharee Kunsawad was born in Bangkok on September 20, 1983. She graduated Bachelor Degree in Science of department of Chemical Technology from Chulalongkorn University in 2004. After that she studied for Master Degree in Chemical Engineering, Chulalongkorn University in 2005.