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นาย จักรพงษ์ ไทยเจริญ

สถาบนวิทยบริการ

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DESIGN OF CONTROL STRUCTURE FOR ENERGY-INTEGRATED HYDRODEALKYLATION (HDA) PROCESS

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สถาบนวิทยบริการ

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การออกแบบโครงสร้างควบคุมแบบแพลนท์ไวด์ สำหรับกระบวนการทางเคมีที่มีสาร ้ ป้อนกลับและพลังงานเบ็คเสร็จเป็<mark>นสิ่งที่สำคัญอย่างมากในการบรรลุเป้าหมายของการออกแบบ</mark> กระบวนการ งานวิจัยนี้นำเสนอโครงสร้างการควบคุมแบบใหม่สำหรับกระบวนการไฮโครคิแอลคิลเล ้ชั้นโทลูอื่นที่พลังงานเบ็คเสร็จแบบที่3 5โครงสร้างควบคุมได้ถูกออกแบบ ทคสอบ และเปรียบเทียบ สมรรถนะกับโครงสร้างอ้างอิงของลูเบน (โครงสร้างที่1) ผลการจำลองแสดงว่ากระบวนการไฮโครคิ แอลกิลเลชันโทลูอื่นที่พลังงานเบ็คเสร็จสามารถลดก่าใช้จ่ายด้านพลังงานและยังสามารถดำเนิน กระบวนการได้อย่างปกติโดยการใช้กลยุทธ์ของแพลนท์ไวด์เพื่อออกแบบโครงสร้างการควบคุม ซึ่ง ้โครงสร้างการควบคุมที่ออกแบบนี้ให้ผลการตอบสนองทางพลวัตรได้ใกล้เคียงกับโครงสร้างการ ้ควบคุมอ้างอิง โครงสร้างการควบคุมที่2 มีข้อจำกัดเนื่องจากการใช้บายพาสทำให้สามารถรองรับต่อ ้สิ่งรบกวนระบบได้ไม่สูง โครงสร้างการควบคุมที่3 พัฒนาโครงสร้างการควบคุมที่2เพื่อให้สามารถ รองรับสิ่งรบกวนระบบได้มากขึ้นโดยการใช้หน่วยให้ความร้อนแทนการใช้บายพาสในการควบคุม อุณหภูมิหอเสถียร โครงสร้างการควบคุมที่4 ให้ผลตอบสนองของลูฟควบคุมอุณหภูมิในหอป้อนกลับ ต่อสิ่งรบกวนได้ดีกว่าโครงสร้างทั้ง 3 เนื่องจากใช้พลังงานหม้อต้มซ้ำในการควบคุมอุณหภูมิซึ่งมี ประสิทธิภาพการต่อควบคุมได้คึกว่าการปรับอัตราไหลของสารที่ออกจากก้นหอ โครงสร้างการ มีข้อคีในการกำหนดอัตราการผลิต ซึ่งสามารถกำหนดการผลิตขั้นปลายได้โดยตรง ควบคุมที่5 ้โครงสร้างการควบคุมที่6 สามารถทำให้กระบวนการประหยัคพลังงานมากกว่าโครงสร้างอ้างอิง และ สามารถรองรับสิ่งรบกวนระบบได้มากกว่าโครงสร้างการควบคุมที่2

จุฬาลงกรณ์มหาวิทยาลย

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| ลายมือชื่อนิสิต |
|----------------------------|
| ลายมือชื่ออาจารย์ที่ปรึกษา |

##4670251321 : MAJOR CHEMICAL ENGINEERING

KEY WORD: HDA / PLANTWIDE / CONTROL STRUCTURE DESIGN / HEAT INTEGRATED PROCESS / CONTROL

CHAKKRAPHONG THAICHAROEN: DESIGN OF CONTROL STRUCTURE FOR ENERGY-INTEGRATED HYDRODEALKYLATION (HDA) PROCESS. THESIS ADVISOR: MONTREE WONGSRI, D.Sc., 152 pp. ISBN 974-17-6866-4.

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

Department Chemical Engineering Field of study Chemical Engineering Academic year 2004 Student's signature..... Advisor's signature.....

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|---|
| reaction rate of side reaction of hydrodealkylation of toluene reaction |
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| the partial pressure of hydrogen, psia |
| the partial pressure of benzene, psia |
| the partial pressure of diphenyl, psia |
| reactor volume |
| temperature |
| pressure |
| reference control structure |
| design control structure I |
| design control structure II |
| design control structure III |
| design control structure IV |
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| |

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CHAPTER I

INTRODUCTION

This chapter introduces the importance and reasons for research, research objectives, scope of research, procedure and method, expected result, and the research contents.

1.1Importance and reasons for research

One of the most common, important, and challenging control tasks confronting chemical engineer is: How do we design the control loops and system needed to run our processes? Typically processes in many industrials have a complicated process flowsheet containing several recycle streams, energy integration, and many different unit operation.

In an industrial environment, a plant's control strategy should be simple enough, so that everyone from the operator to the plant manager can understand how it works. The more complex the process, the more desirable it is to have a simple control strategy. This view differs radically from much of current academic thinking about process control, which suggests that a complex process demands complex control. Plantwide process control involves the system and strategies required to control an entire chemical plant consisting of many interconnected unit operations.

Most industrial processes contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. The economic can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. Therefore, strategies for plantwide control are required to operate an entire plant safely and achieve its design objectives. Hydrodealkylation (HDA) process of toluene to benzene consists of a reactor, furnace, vapor-liquid separator, recycle compressor, heat exchangers and distillations. This plant is a realistically complex chemical process. It is considering that the energy integration for realistic and large processes is meaningful and useful, it is essential to design a control strategy for process associate with energy integration, so it can be operated well. So the main objective of this study is to use plantwide control strategies to develop the new control structures for the HDA process with energy integration schemes that are designed by Terrill and Douglas (i.e. alternative 1 and 3). In this work, the commercial software HYSYS is chosen to carry out both steady state and dynamic simulations.

1.2 Research objectives

- 1. To design control structures for energy-integrated hydrodealkylation (HDA) process.
- 2. To assess performance of the designed control structures.

1.3 Scope of research

- 1. Simulation of the hydrodealkylation (HDA) of toluene process is performed by using a commercial process simulator –HYSYS.
- Description and data of hydrodealkylation (HDA) of toluene process is obtained from Douglas, J. M. (1988), William L. Luyben, Bjorn D. Tyreus, and Michael L. Luyben (1998), and William L. Luyben (2002). And the energy integrated hydrodealkylation (HDA) process is obtained from Terrill and Douglas 1987 (alternative 3) or Ploypaisansang A. (2004).
- 3. The design control structures are design using Luyben's method.

1.4 Contribution of Research

New control structures of the HDA process with heat integration of alternative 3 (Terrill and Douglas 1987)

1.5 Procedure Plan

- 1. Steady state modeling and simulation of HDA process with heat integration (alternative3).
- 2. Dynamic modeling and simulation.
- 3. Design of control structures of the HDA process.
- 4. Simulation of the HDA process with control structures design.
- 5. Assessment of the performance of the control structure.
- 6. Analysis of the design and simulation results.
- 7. Conclusion of the thesis.

This thesis is divided into five 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, Control Structure Design and heat integrated processes.

Chapter III covers some background information of plantwide and theory concerning with plantwide control fundamentals, plantwide control design procedure, and control structure evaluation.

Chapter IV describes the designed control structures and dynamic simulation results and compares with control structures of Luyben.

Chapter V 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 Graph

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CHAPTER II

LITERATURE REVIEW

2.1 Plantwide Control

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

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

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

Luyben and Tyreus (1997) constructed nine steps of the proposed procedure center around the fundamental principles of plantwide control: energy management; production rate; product quality; operational, environmental and safety constrain; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, the Eastman plantwide control process, and the HDA process.

McAvoy (1999) presented an approach to synthesizing plantwide control architectures that made use of steady-state models and optimization. The optimization problem solved was a mixed-integer linear programming (MILP) problem that aimed at minimizing the absolute value of valve movements when a disturbance occurs. Results were presented for its application to the Tennessee Eastman process.

Wang and McAvoy (2001) discussed an optimization-based approach to synthesizing plantwide control architectures. The plantwide controller was synthesized in three stages involving fast and slow safety variables to be controlled, followed by product variables. In each stage a mixed integer linear program was solved to generate candidate architectures. The objective function involved a tradeoff between manipulated variable moves and transient response area. Controlling component balances and adding unit operation controls completed the plantwide control system design. The Tennessee Eastman process was used to illustrate the synthesis procedure.

Vasbinder and Hoo (2003) presented plantwide method based on a modified version of the decision-making methodology of the analytic hierarchical process (AHP). The decomposition utilized a series of steps to select among a set of competing modules. The control structure for each of the individual modules was developed using Luyben's nine steps approach. The decomposition served to make

the plantwide control problem tractable by reducing the size of the problem, while the AHP guarantees consistency. The modular decomposition approach was applied to the dimethyl ether (DME) process, and the results were compared to a traditional plantwide design approach. Both methods produced the same control structure that was shown to be adequate for the process. Satisfactory disturbance rejection was demonstrated on the integrated flowsheet.

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

2.2 Control Structure Design

For control structure design Luyben et al. (1995) presented two workable control structures for a system with a reactor, two distillation columns, and two recycle streams. The reaction $A + B \rightarrow C$ occurred in a reactor, the two distillation columns recycled components A and B back to the reactor process. One fixed the flow rates of the two recycle streams and brought in makeup fresh feeds of components A and B on level control. The other control structure fixed the reactor effluent flow rate, controlled the composition of one reactant in the reactor by manipulating one fresh feed, and brought in the other fresh feed on reactor level control. These two structures have the undesirable feature of not being able to set directly the production rate and, in the second structure, requiring a reactor composition measurement, which can be difficult due to the hostile environment and can require expensive instrument maintenance. After that in 1996 they modified control structure for this process by designed control structures in which one fresh feed is fixed and no reactor composition is measured. Their results show that these control structures can work if modifications are made. By changing in reactor holdup and recycle flow rates away from their values in the economically optimal design improve the ability of this control strategy to handle large disturbances.

Luyben (2000) studied process which had exothermic, irreversible, gas phase reaction $A + B \rightarrow C$ occurring in an adiabatic tubular reactor. A gas recycle returned unconverted reactants from the separation section. Four alternative plantwide control structures for achieving reactor exit temperature control were explored. 1 the set point of the reactor inlet temperature controller was changed (CS1), 2 the recycle flow rate was changed, 3 the flow rate of one of the reactant fresh feeds was changed (CS3) and 4 used an "on-demand" structure. Manipulation of inlet reactor temperature appeared to be the last attractive scheme. Manipulation of recycle flow rate gave the best control but may be undesirable in some system because of compressor limitations. The on demand structure provided effective control in the face of feed composition disturbances. And in the same year he considered the design and control aspects of a ternary system with the gas phase reversible, exothermic reaction $A + B \leftrightarrow C$ occurring in an adiabatic tubular reactor packed with solid catalyst. He designed different control structure by fresh feed control pressure. The inlet reactor temperature is fixed. The recycle flowrate is used to indirectly set the production rate (CS1). Pressure was controlled by recycle flowrate and the production rate was directly set by the fresh feed flowrate (CS2). Given a control structure where the recycle flowrate was fixed (CS3). If process had inerts, the additional control loop added is the control of composition of the inert component in recycle and purge gas. Effective control was obtained in the face of quite large disturbances.

Geroenendijk et al. (2000) proposed a systematic approach that involves the combination of steady state and dynamic simulations. Several controllability measures (relative gain array, singular value decomposition, closed loop disturbance gain, etc.) are employed to develop the final control structure and to assess its performance. The systems approach is illustrated with a vinyl chloride monomer (VCM) plant.

Shinnar et al. (2000) introduced the concept of partial control, the identification of a dominant subset of variables to be controlled such that, by

controlling only these variables, a stabilizing affects on the entire system results. The methodology to find the dominant partial control set relies predominantly on process experience. The approach was demonstrated on a fluid catalytic cracker unit, not on an entire plant.

Reyes and Luyben (2001) studied adiabatic tubular reactor systems with liquid recycles and distillation column used in the separation section. Irreversible and reversible reaction cases have been explored. Both steady-state economics and dynamic controllability have been considered in the design. For the numerical case studied, which is typical of many real chemical system, the liquid recycle system is more expensive because of the high cost of the distillation column and the need to vaporize the recycle. The liquid recycle process is also more difficult to control because the large holdup in the recycle loop produces slow composition changes. For irreversible reactions, the activation energy is shown to slightly affect the steady-state design but to drastically impact the dynamic controllability. Steady state economic designs are shown to very difficult to control because of the severe temperature sensitivity with high activation energies. Changes in the design conditions and changes in the control structure can be used to produce a more easily controlled process. For reversible reactions, the steady-state design is more difficult because of the additional degrees of freedom, but the dynamic controllability is much better because of the inherent self-regulation of exothermic reversible reactions as they encounter chemical equilibrium constraints.

Costin S. Bildea (2002) analyzed the non linear behavior of several recycle systems involving first-and second-order reaction. The result, presented in term of dimensionless number, explain some control difficulties. It is shown that conventional control structure, fixing the flow rate of fresh reactants and relying on self-regulation, can lead to parametric sensitivity, unfeasibility, state multiplicity, or instability, particularly at low conversions. These problems can be solved by fixing the flowrate in the recycle loop, as stated by Luyben's rule. They was demonstrated that a particular location for fixing the recycle flow rate is advantageous, i.e. the reactor inlet. This decouples the reactor from the rest of the plant and avoids undesired phenomena due to mass recycles. For example, the unstable closed-loop behavior

observed with non-isothermal PFRs disappears. The HDA plant case study illustrates the proposed strategy.

Design a process control structure for complex process was a complicate task. The designed control loop would affect the operation significantly. Poothanakul (2002) used plantwide control strategies for designed control structures of butane isomerization process to achieved impurity of normal butane in product and desired production rate. First control structure controlled quality of product by fix product flow, second control structure concerned about reduction of effected of recycle by controlled temperature inside the distillation which could be controlled by adjusted distillate rate of column. And the last wanted to reduce effect of recycle indirectly by controlled temperature inside the distillation with outlet flow of bottom.

Kietawarin (2002) designed 3 control structures for reduced effect from disturbances that caused production rate change. 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 ratio of hydrogen and toluene within the process. These three control structures was compared with reference on plantwide process control book, Luyben (1999), the result was performance of these structure higher than reference.

Larsson, Govatsmark, Skogestead (2003) considered control structure selection for a simple plant with a liquid phase reactor, a distillation column, and recycle of unreacted reactants. To optimized economics, they needed to control active constraints. For the cased of both minimizing operating costs (case1) and maximizing production rate (case2), it was optimal to keep the reactor holdup at its maximum. For the unconstrained variable, they looked for self-optimizing variables where constant setpoints gave acceptable economic loss. To avoid the snowball effect, it had been proposed to fix a flow in a liquid recycle loop. But it had a limit because it could handle only small feed-rate changes or result in large variations in the reactor holdup.

In process which there are three reactions producing components M, D, and T in Kapilakarn and Luyben L (2003). research. Both steady-state design and dynamic control are explored for this three product process, which features one reactor, four distillation columns, and two recycle streams. Several conventional control structures are studied in which the flow rates of the fresh feed streams are fixed or manipulated by level or composition/temperature controllers and the production rates are not directly set. An alternative "on-demand" control structure for "agile" manufacturing is also developed in which all three product streams are flow-controlled. The control system adjusts the conditions in the plant and the fresh feed streams to achieve the set product flow rates. The ratio of the fresh feeds is adjusted to give the desired production rates of M and T, and the recycles of D and T are adjusted to give the desired production rate of D.

Qiu, Rangaiah and Krishnaswamy (2003) presented a rigorous model for the hydrodealkylation of toluene (HDA) process was developed using the commercial software, HYSYS.PLANT. After reviewing the reported methods for plantwide 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 show that the CCD method successfully yields workable base-level regulatory control structures for the HDA process.

Tangsombutvisit (2003) developed rigorous model for the hydrodealkylation of toluene (HDA) process by using the commercial software, HYSYS.PLANT. Steady-state and dynamic simulations are combined with controllability analysis tools, both stead-state and in the frequency domain, which extracts more value from simulation than the usual sensitivity studies. The case of HDA process, the two control structures designed by Kietawarin (2002) are considered. The steady-state analysis is confirmed that the second control structure should be used. For using the controllability analysis it appeared that the problems mainly came from the interaction between the different units in the flowsheet. Controllability analysis described the control structure2 could give the result into satisfied bound. That means the effect of changing setpoint is less than the first one. However, results shown the reference structure and the control structure1 can reject the disturbance better than the second one.

Kasemchainun (2003) applied plantwide control strategy for designing control structures of a Vinyl Acetate Monomer plant. Three alternative plantwide control structures was designed, tested and compared the performance with Luyben's structure (1999). For the result, the first control structure used the fresh acetic fed to manipulated the total acetic feed in vaporizer and controlled the water composition in overhead column. In the azeotrope column was high boilup ratio so the second designed control structure modified from the first in column temperature loop. This scheme measured the tray temperature and adjusted the bottom flowrate to control the vinyl acetate composition and the level was controlled by changing the reboiler heat input. The last structure; when the reactant comes from upstream unit, the production rate was set by changing the fresh ethylene feed. Results shown that all of control structures achieved a good controllability.

Distillation columns which large temperature differences between the condenser and reboiler; the base temperature of this type of column was often quite high. It required the use of expensive high-pressure steam. Luyben L (2004) presented method to reduce energy costs by using two reboilers. One at the base of the column used high-pressure steam. A second was at an intermediate tray in the stripping section. His paper compared the steady-state design and the dynamic control of a conventional single-reboiler distillation column with a column having both intermediate and base reboilers. Result shown consumption of high-pressure heat could be reduced, and the column diameter was also reduced. The economic effect is a reduction in both energy and capital costs. Dynamic controllability is just as good in the intermediate reboiler column as it is in the standard column. Average temperature control should be used in both because of the very sharp temperature profile.

2.3 Heat Integrated Process

Terrill and Douglas (1987) 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.

Kunlawaniteewat (2002) presented rules and procedure for design control structure of heat exchanger network using heuristic approach. The rules devised in this work were categorized as following: generals, match pattern, loop placement, bypass placement, and split fraction rules. In this research, 6 alternative control structures of 3 networks were designed. It shown that the network with control structure designed using their procedure gave minimum the integral time absolute error, compared to the other network found in the literature, while maintained maximum energy recovery and achieved outlet temperature targets.

Ploypaisansang A. (2003)designed resilient network for the Hydrodealkylation process (HDA Process). The match pattern heuristic, shift approach and the heat load propagation technique were essential approach. Six alternatives for the HDA process were redesign to be the resiliency networks for maintain target temperature and also reached maximum energy recovery (MER). The Resiliency Parameters of resilient networks were required to compare and selected the best resilient network. In order to receive resilient network, a trade-off between cost and resilient may be needed. The auxiliary unit should be added in the network for cope safely with variations and easy to design control structure to the network.

In 2003, the controllability of a complex heat-integrated reactor has been studied by Yih and Yu. In their work the parameter, the ultimate effectiveness, was defined to indicate the amount of heat that can be recovered via a feed-effluent heat exchanger (FEHE) before the overall open-loop system becomes unstable. First, a systematic approach is proposed to model the reactor, the controllability of a particular flowsheet can then be evaluated on the basis of the stability margin of design. With the evaluated controllability, implications for design are further explored. Since the loss of controllability comes from the positive feedback loop, several design parameters are studied, and design heuristics are proposed to improve the controllability of heat-integration schemes. Two examples, a simple two-FEHE example and an HDA example, were used to assess the controllability of different designs. The results show that, contrary to one's intuition, some of the complex heatintegrated reactor design alternatives are indeed more controllable than the simpler schemes.

Shih-Wen Lina, Cheng-Ching Yu (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.

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CHAPTER III

THEORY

A typical chemical plant flowsheet has a mixture of multiple units connected both in series and parallel that consist of reaction sections, separation sections and heat exchanger network. So Plantwide Process Control involves the system and strategies required to control entire plant consisting of many interconnected unit operations.

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: the effect of material recycle, the effect of energy integration, and the need to account for chemical component inventories.



Figure 3.1 Integrated Process flowsheet

3.1.1 Material recycle

Material is recycled for six basic and important reasons.

1. Increase conversion.

For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints.

Therefore the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.

2. Improve economics.

In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than it is to reach the necessary conversion level in one reactor or several in series. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

3. Improve yields.

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

4. Provide thermal sink

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

5. Prevent side reactions.

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

6. Control properties.

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

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.

3.1.3 Chemical component inventories

In chemical processes 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 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.

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

3.2 Effects of Recycle

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

3.2.1 Snowball effect

Snowball effect is high sensitivity of the recycle flowrates to small disturbances. When feed conditions are not very different, recycle flowrates increase drastically, usually over a considerable period of time. Often the equipment cannot handle such a large load. It is a steady-state phenomenon but it does have dynamic implications for disturbance propagation and for inventory control.

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

3.3 Plantwide Control Design Procedures

In plantwide control design procedure satisfies the two fundamental chemical engineering principles, namely the overall conservation of energy and mass. Additionally, the procedure accounts for nonconserved entities within a plant such as chemical components (produced and consumed) and entropy (produced).

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.

3.3.1 Basic Concepts of Plantwide Control

3.3.1.1 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.

3.3.1.2 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.

3.3.1.3 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.

3.3.1.4 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.

3.3.1.5 Richardson rule

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

3.3.1.6 Shinskey schemes

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

3.3.1.7 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:

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

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.

3.3.2 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. The "best" control structure for a plant depends upon the design and control criteria established.

These objectives include reactor and separation yields, product quality specification, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine control degrees of freedom

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

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

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 functions

- 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 removal in exothermic reactors is crucial because of the potential for thermal runaways. In endothermic reactions, failure to add enough heat simply results in the reaction slowing up. If the exothermic reactor is running adiabatically, the control system must prevent excessive temperature rise through the reactor.

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

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

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)

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. 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)

Proportional-only control should be used in nonreactive level loops for cascade units in series. Even in reactor level control, proportional control should be considered to help filter flowrate disturbances to the downstream separation system.

Step 7: Check component balances

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).

In process, we don't want reactant components to leave in the product streams because of the yield loss and the desired product purity specification. 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. Hightemperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor.

Step 9: Optimize economics or improve dynamic controllability

After 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.

3.4 Control Issues for Distillation Column.

Distillation is the most frequently used separation technique in the chemical and petroleum industries. The design and control of this important unit operation is vital for safe and profitable operation of many plants.

Distillation columns are fairly complex units. They have several inputs and outputs, so they can present challenging multivariable control problems. Their dynamics are a mixture of very fast vapor flowrate changes, moderately fast liquid flowrate changes, slow temperature changes and very slow composition changes. The manipulated variables often have constraints because of column flooding limitations or heat exchanger limitations. Developing an effective control system for an individual column is not a trivial job. There are at last six loop involved on even the most simple column.

3.4.1 Typical Control Schemes of Distillation Column.

A number of alternative structures are used to control distillation columns. This section presents some of the most commonly employed strategies and discusses when they are appropriate. The standard terminology is to label a control structure with the two manipulated variables that are employed to control compositions. For example, the "R-V" structure refers to a control system in which reflux and vapor boilup are used to control two composition (or temperature). The "D-V" structure means distillate and vapor boilup are used.

The simultaneous control of two compositions or temperatures is called dual composition control. This is ideally what we would like to do in a column because it provides the required separation with the minimum energy consumption. However, many distillation columns operate with only one composition controlled, not two. This is called single-end composition control.

This is due to a variety of reasons. Dual requires two controllers that interact, making them more difficult to tune. Often the difference in energy consumption between dual and single-end composition control is quite small and is not worth the additional complexity. Frequently direct measurement of composition is difficult, expensive and unreliable, so temperatures must be used. The column temperature profile may permit only one temperature to be used for control because of the nonuniqueness of temperature in a multicomponent system, resulting in a lack of sensitivity to changes in column conditions. Perhaps the most important reason that most columns operate with single-end control is that just one tray temperature is a dominant variable for column behavior. The dominant temperature usually occurs either in the stripping or rectifying section where there is a significant variable generally provides partial control of both product compositions in the column. Therefore we often use the R-V structure, for example, with reflux flow controlled and reboiler heat input used to control an appropriate tray temperature.

Figure 3.2 shows a number of control configurations for simple two product distillation columns.

- 1. R-V: Reflux flow controls distillate composition. Heat input controls bottoms composition. By default, the inventory controls use distillate flowrate to hold reflux drum level and bottoms flowrate to control base level. This control structure (in its single-end control version) is probably the most widely used. The liquid and vapor flowrates in the column are what really affect product compositions, so direct manipulations of these variables make sense. One of the strengths of this system is that it usually handles feed composition changes quite well. It also permits the two products to be sent to downstream process on proportional-only level control so that plantwide flow smoothing can be achieved.
- 2. D-V: If the column is operating with a high reflux ratio (RR>4), the D-V structure should be used because the distillate flowrate is too small to control reflux drum level. Small changes in vapor to the condenser would require large changes in the distillate flowrate if it is controlling level. When the D-V structure is used, the tuning of the reflux drum level controller should be tight so that the changes in distillate flowrate result in immediate changes in reflux flowrate. If the dynamics of the level loop are slow, they slow down the composition loop. One way to achieve this quick

response is to ratio the reflux to the distillate and use the level controller to change the ratio.

- 3. RR-V: Reflux ratio is used to control distillate composition and heat input controls bottoms composition.
- 4. R-B: When the boilup ratio is high (V/B), bottoms flow should be used to control bottoms composition and heat input should control base level. However, in some columns potential inverse response (The dynamic behavior of certain process deviates drastically from what we have seen so far. Initial response is in the opposite direction to where it eventually end up) may create problems in controlling base level with boilup.
- 5. RR-BR: Reflux ratio controls distillate composition and boilup ratio controls bottoms composition.



Figure 3.2 Common control structures for distillation column. (a) Reflux-boilup; (b) distillate-boilup; (c) reflux ratio-boilup; (d) reflux-bottoms; (e) reflux ratio-boilup ratio.



Figure 3.2 (continue)

Figure 3.3 shows typical control structures for two special types of column. Figure 3.3a is for a column whose feed contains a small amount of a component that is much more volatile than the main component. The distillate product is small fraction of feed stream. It is removed from the reflux drum as a vapor to hold column pressure. Reflux flow is fixed, and reflux drum level is controlled by manipulating condenser coolant. In the petroleum industry, this type of column is called a stabilizer.

Figure 3.3b shows a column that is separating a mixture with a low relative volatility, so the column has a large number of trays and operates with a high reflux ratio. This type of column is called a superfractionator. Because of the high reflux

ratio, reflux should be used to control reflux drum level. For the same reason, vapor boilup should be used to control base level. Therefore the two manipulators left to control composition are distillate and bottoms flowrates. Obviously these two flows cannot be set independently for a given feed under steady-state conditions. Dynamically, however, they can be adjusted independently. This D-B control structure works well on this type of column. It should be noted that it is quite "fragile" because if either of the two composition loops is put on manual, the other cannot work. Override controls must be used to recognize that this situation has occurred and switch the control structure. For example, if the bottoms composition analyzer fails, the control structure should be switched so that overhead composition is controlled by distillate flow, base level is controlled by bottoms flow, and reboiler heat input is a constant.



Figure 3.3 Common types of columns and controls. (a) Stabilizer (small distillate flow); (b) superfractionator with distillate-bottoms control structure.

3.4.2 Heat-Integrated Distillation Columns

Distillation columns are major energy consumers in many petroleum and chemical plants. One commonly used method to reduce the energy requirements in distillation systems is heat-integration. The basic idea is to use the overhead vapor from one column as a heat source in another column. Multiple-effect evaporators use the same technique.

The pressure in the two columns are adjusted so that there is a reasonable differential temperature driving force for heat transfer in the heat exchanger serving as the condenser for the high-temperature column and the reboiler for the low-temperature column. A small temperature difference results in lower temperature heat source in the high-temperature column but a larger heat-transfer area in the reboiler/condenser. Typical temperature differentials are about 30 to 50 °F, depending on the relative cost of heat-exchanger area and energy. There are interesting designs optimization trade-offs that involve the many design degree of freedom: number of trays in each column, reflux ratios and pressures. The typical system has the low-pressure column pressure set by the use of cooling water in the condenser. Then the pressure in high-pressure column is set to a reasonable temperature differential in the condenser/reboiler.

Heat integration can be used in systems where two columns separating different chemical components have the required temperature levels. The reflux-drum temperature of the high-temperature column must be sufficiently higher than the base temperature of the low-temperature column to give reasonable heat-exchanger area. Of course, the heat duties of the two columns must be similar. Any differences between these duties the use of auxiliary condenser and/or reboilers. Even if the duties are perfectly balanced, auxiliary heat exchangers may be required to improve dynamic controllability.

Heat integration can also be used to separate a single feed stream. Instead of using one column with a reboiler and a condenser, two columns are used. One operates at high pressure and the other column operates at low pressure so that the appropriate temperatures are achieved in the coupled condenser/reboiler heat exchanger. This type of system is normally limited to

- 1. Binary systems with no lighter or heavier components. The effect of lighter-than-light or heavier-than-heavy key components is to lower or elevate reflux-drum and base temperatures, respectively.
- 2. Systems in which the components have boiling point those are not very different.

Systems that do not have these properties may require excessive pressure differences between the two columns, so the heat-integration economics become unfavorable.

A typical heat-integrated distillation system may involve somewhat higher capital investment, but the savings in energy costs can usually justify this investment.

There are a number of alternative heat-integration flowsheets. Two of more widely used are:

- 1. Feed split: Fresh feed is split between two columns that operate at different pressures to provide the specified ΔT in the condenser/reboiler. Specification products are produced at the ends of both columns.
- 2. Light split: All the fresh feed is introduced into one column. The distillate from this column contains about half of the lighter component in the feed. The bottom contains the rest of the lighter component and all of the heavy component. This is fed into the second column where the lighter component goes overhead in the distillate and all of the heavy component goes out in the bottoms. The heat integration can be in the direction of flow (the first column run at high pressure). One of the factors that influence this choice is the temperature level of the available heating medium. The direct scheme has a lower base temperature in the high-pressure column because the bottoms composition is a mixture of light and heavy components.

3.4.3 Plantwide control issues for distillation column

3.4.3.1 Reflux drum and base level control

When considering a column in isolation, we typically select heat input to control temperature on an appropriate column tray to achieve good, tight control composition control. Then we fix the reflux flowrate or ratio it to the feed flowrate. Finally, we control the level in the reflux drum by manipulating distillate flowrate and control the level in the column base by manipulating bottoms flowrate. This structure works well for the column and also fits nicely into a plantwide context because the proportional-only level controller setting both products provide gradual smooth flowrate changes to downstream sections of the plant. This type of control scheme would be used for a column with a liquid distillate product and with a low to moderate reflux ratio (less than 4).

However, for columns with higher reflux ratios, Richardson's rule dictates that we control reflux drum level with reflux, not distillate. The flowrate of distillate would be used (1) to control distillate product composition or (2) to control a constant reflux ratio. If the former strategy is used (distillate controls composition or temperature), there may be significant fluctuations in the distillate flowrate as the tightly tuned composition controller attempts to achieve good quality control. With this structure the reflux drum level loop must be tightly tuned (PI control) so that we do not introduce an additional lag in the composition loop; i.e., changes in distillate flowrate will result in immediate changes in reflux flowrate.

If the distillate is fed to a downstream unit, the variability in flowrate will be disturbance. So what can we do? We can make use of feedforward control to anticipate the required changes in reflux and distillate flowrates (ratio distillate to feed with the ratio reset by the composition controller).

In the second case (manipulate distillate to control reflux ratio), the variability of the distillate flow would be greatly reduced. The reflux drum level controller, manipulating reflux flowrate, is made P-only to get slow change in reflux flowrate and this give slow change in distillate flowrate in the reflux-ratio control structure. So from a plantwide control perspective, setting distillate flowrate to control reflux ratio is a better strategy than using distillate to control composition. Of course similar arguments can be made about bottoms flowrate in the case of a column with a high boilup ratio.

3.4.3.2 On-demand product

Suppose our plantwide control system requires "on-demand" products. The fourth step in the plantwide control design procedure is to establish where production rate is set. If the flowrate of one of product streams leaving the column is fixed by a down stream unit or customer, the column control structure must be set up in an appropriate way.

3.5 Heat Exchanger and Energy Management

3.5.1 Heat recovery

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

3.5.2 Control of utility exchangers

Control of Utility Exchangers

Armed with the thermodynamic fundamentals of heat management, we now take a closer look at the unit operation control loops for heat exchangers. We start with utility exchangers. These are used when heat is supplied to, or removed from, the process. Examples are steam heated reboilers, electric heaters, fuel-fired furnaces, water-cooled condensers, and refrigerated coolers.

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 the utility. A PI-controller is adequate in most instances although derivative action can be used to compensate for the lag introduced by thermowell. The location of the temperature measurement depends upon the purpose of the heat exchange. For example, when reaction heat is dissipated through a water cooler, the controlled temperature is in the reactor. Similarly, when the utility exchanger delivers heat to a separation system, the control point should be located the effects of the added energy are felt the most. Control of a tray temperature in a distillation column by manipulation of reboiler stream is a good example. Finally, when the utility exchanger is used for stream heated or cooled.

3.5.3 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. We can control the two exit temperatures provided we can independently manipulate the two inlet flowrates. However, these flowrates are normally unavailable for us to manipulate and we therefore give up two degrees of freedom for temperature control. We can restore one of these degrees of freedom fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Fig. 3.4a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig 3.4b.



Figure 3.4 Control of P/P heat exchangers: (a) Use of bypass; (b) use of auxiliary utility exchanger.

When the bypass method is used for unit operation control, we have several choices about the bypass location and the control point. Figure 3.5 shows the most common alternatives. We may ask "Which option is the best? It depends on how we define "best". As with many other examples, it boils down to a trade-off between design and control. Design considerations might suggest we measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than it is for high-temperature service. Cost considerations would also suggest a small bypass flow to minimize the exchanger and control valve sizes. From a control standpoint we should measure the most important stream, regardless of temperature, and bypass on the same side as we control. This minimizes the effects of exchanger dynamics in the loop. We should also want to bypass a large fraction of the controlled stream since it improves the control range. This requires a large heat exchanger.



Figure 3.5 Bypass control of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

There are several general heuristic guidelines for heat exchanger bypass systems. However, this very much remains an open research area since these guidelines are not always adequate to deal with all of the issues for bypass systems. We typically want to bypass the flow of the stream whose temperature we want to control. The bypass should be about 5 to 10 percent of flow to be able to handle disturbances. Finally, we must carefully consider the fluid mechanics of the bypass design for the pressure drops through the control valves and heat exchanger.

Use of auxiliary utility exchangers

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

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

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

3.6 Process Control

3.6.1 Cascade Control

One of the most useful concepts in advanced control is cascade control. A cascade control structure has two feedback controllers with the output of the primary (or master) controller changing the setpoint of the secondary (or slave) controller. The output of the secondary goes to the slave.

There are two purposes for cascade control: (1) to eliminate the effects of some disturbances, and (2) to improve the dynamic performance of the control loop.

To illustrate the disturbance rejection effect, consider the distillation column reboiler. Suppose the steam supply pressure increases. The pressure drop over the control valve will be larger, so the steam flow rate will increase. With the single-loop temperature controller, no correction will be made until the higher steam flow rate increases the vapor boilup and the higher vapor rate begins to rise the temperature on tray. Thus the whole system is disturbed by a supply-steam pressure change.



Figure 3.6 Cascade control in distillation-column-reboiler.

With the cascade control system, the steam flow controller will immediately see the increase in steam flow and will pinch back on the steam valve to return the steam flow rate to its setpoint. Thus the reboiler and the column are only slightly affected by the steam supply-pressure disturbance.

Figure shows another common system where cascade control is used. The reactor temperature controller is the primary controller; the jacket temperature controller is the secondary controller. The reactor temperature control is isolated by the cascade system from disturbances in cooling-water inlet temperature and supply pressure.

3.6.2 Valve Position Control

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

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

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

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

controller. Since the valve is AC, the setpoint of VPC is about 5 percent of scale so as to keep the cooling water valve almost wide open.

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

Luyben show another of the application of VPC to optimize a process as figure 3.7. We want to control the temperature of a reactor. The reactor is cooled by both cooling water flowing through a jacket surrounding the reactor and by condensing vapor that boil off the reactor in a heat exchanger that is cooled by a refrigerant. This form of cooling is called "autorefrigeration".



Figure 3.7 Use of VPC to minimize energy cost.

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

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



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CHAPTER IV

HYDRODEALKYLATION PROCESS

4.1 Process Description

The hydrodealkylation HDA of toluene process (alternative 1) by Douglas (1988) on conceptual design as in Fig. 4.1 contain nine basic unit operations: reactor, furnace, vapor-liquid separator, recycle compressor, two heat exchangers, and three distillation columns. Two raw materials, hydrogen, and toluene, are converted into the benzene product, with methane and diphenyl produced as by-products. The two vapor-phase reactions are

Toluene + $H_2 \rightarrow benzene + CH_4$

2BenZene \leftrightarrow diphenyl + H₂

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:

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

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

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.

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

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



Fig. 4.1 Hydrodealkylation HDA of toluene process (alternative 1)

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

4.2 Control Structure Design Consideration

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

In alternative 3 part of the heat in the reactor effluent stream is used to drive the stabilizer reboiler, recycle column was pressure shifted to be above the pinch temperature, and the condenser for the recycle column is used to drive the product column reboiler as in Fig. 4.2



Fig. 4.2 HDA process –alternative 3

Table 4.1 TAC and Utilities Usage of HEN Alternatives of the HDA Process

| | Alternative | | | | | | |
|---|-------------|------|------|------|------|------|--|
| | 1 | 2 | 3 | 4 | 5 | 6 | |
| utilities usage for alternatives with base-case design values, MW | 9.06 | 7.68 | 7.39 | 7.30 | 7.30 | 7.30 | |
| energy savings from new HEN, % | 29 | 40 | 42 | 43 | 43 | 43 | |
| TAC for alternatives with base- case design values, \$106/year | 6.40 | 6.45 | 6.38 | 6.11 | 6.04 | 6.03 | |
| improvement from new HEN, % | -0.3 | -1 | 0 | 4 | 5 | 5 | |

4.3 Steady-State Modeling

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Douglas (1988); Luyben et al. (1998) . Table A.1, 4 presents the data and specifications for the equipment employed other than the three columns. For this 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).

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 choose reflux ratio and overhead benzene mole fraction for the stabilizer column. For the remaining two columns, bottom and overhead composition mole fractions are specified to meet the required purity of products given in Douglas (1988). The detailed design data and specifications for the columns are summarized in Table A.3. This table also includes details of trays, which are required for dynamic modeling. The simulated HDA process at steady-state by HYSYS is showed in figure 4.3.

In addition, in alternative 3 some data are change from reference due to heat integration. This alternative has 4 P/P heat exchangers: two heat exchangers for preheat feed, heat in the reactor effluent stream is used to drive the stabilizer reboiler, and heat from the top of recycle column is used to drive the product column reboiler. Recycle column is pressure shifted to be above the pinch temperature. For this alternative, the three columns have only one specification. We choose overhead composition mole fraction for the stabilizer column. Product column overhead composition mole fraction is specified. And bottom composition mole fraction is specified in recycle column. Table A.2-4 shows the data and specification of this process. The simulated HDA process (alt. 3) at steady-state by HYSYS is showed in figure 4.4.



Figure 4.3 The simulated HDA process (alt.1) at steady-state by HYSYS



Figure 4.4 The simulated HDA process (alt.3) at steady-state by HYSYS

4.4 Plantwide control design procedure

Step 1. Establish Control Objectives.

For this process, the essential is to produce pure benzene while minimizing yield losses of hydrogen and diphenyl. The reactor effluent gas must be quenched to 1150 °F. The design a control structures for process associate with energy integration can be operated well.

Step 2. Determine Control Degree of Freedom.

There are 21 control degrees of freedom in HDA alternative 3. They include: two fresh feed valves for hydrogen and toluene, purge valve, separator base and overhead valves, cooler cooling water valve, liquid quench valve, furnace fuel valve, stabilizer column steam; reflux; cooling water; and vapor product valves, product column steam ; bottoms; reflux; distillate; and cooling water valves, and recycle column steam; bottoms; reflux; and distillate.

Step 3. Establish Energy management system.

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

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

Step 4. Set Production Rate.

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

- Pressure is not a variable choice for production rate control because of the compressor has to operate at maximum capacity for yield purposes.
- Reactor inlet temperature is controlled by specify the reactant fresh feed rate and reactant composition into the reactor constant. The reactor temperature is constrained below 1300 °F for preventing the cracking reaction that produce undesired byproduct.
- Toluene inventory can be controlled in two ways. Liquid level at the top of recycle column is measured to change recycle toluene flow and total toluene feed flow in the system is measured for control amount of fresh toluene feed flow.

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

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

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

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

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

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

For liquid control loops, there are a separator and two receivers in each column (base and overhead). The most direct way to control separator level is with the liquid flow to the stabilizer column. The stabilizer column overhead level is controlled with cooling water flow and base level is controlled with bottom flow. In

several cases of this research; the product column, distillate flow controls overhead receiver level but on demand control structure condenser level is controlled by cascade the total flow rate of the toluene and bottom flow controls base level. In the recycle column manipulate the total toluene flow to control level. The base level of recycle column in the reference is controlled by manipulating the column steam flow because it has much larger effect than bottoms flow. But the column steam flow does not obtain a good controllability, so base level is controlled with bottom flow.

Step 7. Check Component Balances.

Component balances control loops consists of:

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

Step 8. Control Individual Unit Operations.

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

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

| | Input | +Generation | -Output | -Consumption | =Accumulation |
|---------------------------------|------------|-------------------------------|----------------|-------------------------------|--|
| Component | | | | | Inventory Controlled by |
| H ₂ | Fresh Feed | $0.5V_{R}r_{2}$ | Purge stream | $V_R r_1$ | Pressure control of recycle gas loop |
| CH ₄ | 0 | V _R r ₁ | Purge stream | 0 | Composition control of recycle gas loop |
| C ₆ H ₆ | 0 | V _R r ₁ | Product stream | $2V_Rr_2$ | Temperature control in product column |
| C ₇ H ₈ | Fresh Feed | 0 | 0 | V _R r ₁ | Level control in recycle column reflux drum |
| C ₁₂ H ₁₀ | 0 | $0.5V_{R}r_{2}$ | Purge stream | 0 | Temperature control in recycle column |

Table 4.2 Component Material Balance

| Where $V_R = reac$ | tor v | volume |
|--------------------|-------|--------|
|--------------------|-------|--------|

 r_1 = first reaction rate

 \mathbf{r}_2 = second reaction rate

Step 9. Optimize Economics or Improve Dynamic Controllability.

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



Figure 4.5 Reference control structure (CS1) of HDA process



Figure 4.6 Designed control structure (CS2) of HDA process



Figure 4.7 Enlarged designed control structure (CS2) of HDA process



Figure 4.7 Enlarged designed control structure (CS2) of HDA process (cont.)



Figure 4.8 Designed control structure (CS3) of HDA process


Figure 4.9 Enlarged designed control structure (CS3) of HDA process



Figure 4.10 Designed control structure (CS4) of HDA process



Figure 4.11 Enlarged designed control structure (CS4) of HDA process



Figure 4.12 Designed control structure (CS5) of HDA process



Figure 4.13 Enlarged designed control structure (CS5) of HDA process



Figure 4.14 Designed control structure (CS6) of HDA process



Figure 4.15 Enlarged designed control structure (CS6) of HDA process

4.5 Control Structure Alternatives

For HDA process alternative 1, Kietawarin (2002) designed 3 control structures to reduce the effects of disturbances in order to achieve a desired production rate. 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 adding a cooling unit to control the outlet temperature of the reactor. In the third scheme, a ratio control was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process. These three control structures were compared with reference on plantwide process control book by Luyben (1998), the result show that performances of Kietawarin's structures were better than Luyben's structures.

4.5.1 Comparison dynamic responses between this work with reference

The disturbance testing is used to compare the dynamic response of this simulation (HYSYS) with Kietawarin (2002; Aspen plus) and Luyben (1998; TMODS, 2002; HYSYS). By step change in reactor inlet temperature setpoint (increase 5 °F) and step change in total toluene flowrate (decrease 15%).



Figure 4.16 Comparison dynamic responses of step change in total toluene flowrate (decrease 15%) between: (A) this work, (B) Kietawarin, (C) Luyben



Figure 4.16 Comparison dynamic responses of step change in total toluene flowrate (decrease 15%) between: (A) this work, (B) Kietawarin, (C) Luyben (cont.)



Figure 4.17 Comparison dynamic responses of step change in reactor inlet temperature setpoint (increase 5 °F) between: (A) this work, (B) Luyben

In this current work, we apply the first control structure of Kietawarin (2002), namely control structure 1 (CS1) to the HDA process alternative 1 as shown in Figure 4.5. The new plantwide control structures CS2 to CS6 are designed for the HDA process alternative 3 as shown in Figure 4.6 to 4.15 respectively. In all of these control structures, the same loops are used as follows:

- Valve V1 is manipulated to control separator pressure.
- Valve V2 is manipulated to control total toluene flow.
- Valve V3 is manipulated to control quench temperature.
- Valve V4 is manipulated to control methane in the recycle gas.
- Valve V5 is manipulated to control separator level.
- Valve V6 is manipulated to control column1 pressure.
- Valve V8 is manipulated to control column2 condenser level.
- Valve V10 is manipulated to control column3temperature.
- Cooler duty is manipulated to control separator temperature.
- Furnace duty is manipulated to control reactor inlet temperature.
- Column1 condenser duty is manipulated to control level of column1 condenser.
- Column2 condenser duty is manipulated to control column2 pressure.
- Column3 reboiler duty is manipulated to control level of column3 reboiler. The main difference between CS1, CS2 to CS6 are explained below:

4.5.2 Reference control structure (CS1)

Based on Fig. 4.5, valve V7 is manipulated to control column1 reboiler level, column1 reboiler duty is manipulated to control column1 temperature; valve V9 is manipulated to control column2 reboiler level; column1 reboiler duty is manipulated to control column2 temperature; valve V11 is manipulated to control column3 condenser level; column3 condenser duty is manipulated to control column3 pressure.

• Increase temperature

The starting conditions are the base-case design where reactor inlet temperature is 1150 °F. Step change of 10 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.



Figure 4.18a Dynamic response of increase 10 °F in reactor inlet temperature of CS1



Figure 4.18b Dynamic response of increase 10 °F in reactor inlet temperature of CS1



Figure 4.18c Dynamic response of increase 10 °F in reactor inlet temperature of CS1

Figure 4.18a gives simulation result for decreasing the reactor inlet temperature. The temperature response is oscillatory and it comes to new setpoint within 20 minutes. Effect from the temperature increase, the rate of reaction of HDA increase because of increasing temperature can raise the reaction rate. Figure 4.18b show the fresh feed H₂, toluene, benzene product flow, and toluene impurity in product responses. Fresh feed H₂, toluene, benzene product flow are slowly increased about 120 minute to new steady-state due reaction rate increasing. But toluene impurity in product is slowly decreased because of increasing temperature increase of increase because of increase because of increased because of increasing.

Figure 4.18c show the temperature control in 3 distillation columns. The temperature response of stabilizer column is oscillatory and it comes to setpoint within 50 minutes. The temperature response of product column does not see the changing. But recycle column takes long time to achieve setpoint.

• Decrease total toluene flowrate

Step change of 15 % decreasing at time 10 minute is made in the setpoint of the total toluene flowrate controller.



Figure 4.19a Dynamic response of decrease 15 % in total toluene flowrate of CS1



Figure 4.19b Dynamic response of decrease 15 % in total toluene flowrate of CS1



Figure 4.19b Dynamic response of decrease 15 % in total toluene flowrate of CS1 (cont.)



Figure 4.19c Dynamic response of decrease 15 % in total toluene flowrate of CS1

Figure 4.19a gives the dynamic response of the process for a 15% decrease in the total toluene flowrate. This flow quickly responses within 10 minute. This step change affects to the fresh feed H_2 , toluene, benzene product flow, and toluene impurity in product. They slowly decrease because decrease total toluene flowrate affect to the production rate and toluene impurity in product decrease due to reduction toluene in the process as show in figure 4.19b.

Figure 4.19c show the temperature control in 3 distillation columns. The temperature response of stabilizer column is oscillatory and it comes to setpoint within 100 minutes. The temperature response of product column is slight change. But recycle column takes long time to achieve setpoint.

4.5.3 Design Control Structure I (CS2)

This control structure uses bypass method to control the tray temperature in column1 (Figure 4.6-7). We measure column1 temperature and bypass on the cold side of heat exchanger since this side has flowrates less than the hot side. That small bypass flow has minimized the exchanger and control valve size. Valve V7 is manipulated to control column1 accumulate tank level; valve on the bypass line of E3 valve is manipulated to control column1 temperature; V9 is manipulated to control column2 tank level, auxiliary E4 duty is manipulated to control column2 temperature, valve V11 is manipulated to control column3 tank level, bypass valve of E5 is manipulated to control pressure in column3. In order to accommodate the liquid from the bottoms of stabilizer and product column, and the condensed vapor from the top of recycle column, three tanks are installed in the HDA process alternative 3.

• Increase temperature

Step change of 5 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.

Figure 4.20a gives simulation result for decreasing the reactor inlet temperature. This control structure can handle the changing of step change in inlet temperature only 5 °F due to limiting of bypass. The temperature response is oscillatory and it comes to new setpoint within 30 minutes. Effect from the temperature increase, the rate of reaction of HDA increase because of increasing temperature can raise the reaction rate. Figure 4.20b show the fresh feed H₂, toluene, benzene product flow, and toluene impurity in product responses. Fresh feed H₂, toluene, benzene product flow are slowly increased about 200 minute to new steady-state due reaction rate increasing. But toluene impurity in product is slowly decreased because of increasing temperature increasing temperature increasing temperature increasing.

Figure 4.20c show the temperature control in 3 distillation columns. The temperature response of these three columns like as CS1 but stabilizer column can handle disturbance only 5 $^{\circ}$ F.

| <u>۱</u> | | | | | | | _ | | | |
|----------|------|-----|-----|-----|----|------|------|-----|-----|-----|
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| ٢. | 1155 | | ha. | ~~~ | | | | | | |
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| F | 0.00 | 000 |) | 50. | 00 | 100 | D.O | 150 | 0.0 | 200 |
| | | | | | | Minu | utes | | | |

Figure 4.20a Dynamic response of increase 5 °F in reactor inlet temperature of CS2



Figure 4.20b Dynamic response of increase 5 °F in reactor inlet temperature of CS2



Figure 4.20c Dynamic response of increase 5 °F in reactor inlet temperature of CS2

• Decrease total toluene flowrate

Step change of 10 % decreasing at time 10 minute is made in the setpoint of the total toluene flowrate controller.



Figure 4.21a Dynamic response of decrease 10 % in total toluene flowrate of CS2

Figure 4.21a gives the dynamic response of the process for a 10% decrease in the total toluene flowrate. This flow quickly responses within 10 minute. This step change affects to the fresh feed H_2 , toluene, benzene product flow, and toluene impurity in product. They slowly decrease because decrease total toluene flowrate affect to the production rate and toluene impurity in product decrease due to reduction toluene in the process as show in figure 4.19b.

Figure 4.19c show the temperature control in 3 distillation columns. The temperature response of stabilizer column is oscillatory and it slowly comes to setpoint within 100 minutes. The temperature response of product column is slight change. But recycle column takes long time to achieve setpoint.



Figure 4.21b Dynamic response of decrease 10 % in total toluene flowrate of CS2



Figure 4.21b Dynamic response of decrease 10 % in total toluene flowrate of CS2 (cont.)



Figure 4.21c Dynamic response of decrease 10 % in total toluene flowrate of CS2

4.5.4 Design Control Structure II (CS3)

This control structure adopts Ploypaisansang's study (2003); the auxiliary reboiler is additionally installed in the stabilizer to control its tray temperature (Figure 4.8-9). The other control structures are the same as CS2.

• Increase temperature

Step change of 10 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.

Figure 4.22 show the dynamic response of the process for 10 °F increase. The dynamic response of these control structure same as CS2 but can handle more disturbance and faster than CS2.



Figure 4.22a Dynamic response of increase 10 °F in reactor inlet temperature of CS3



Figure 4.22b Dynamic response of increase 10 °F in reactor inlet temperature of CS3.



Figure 4.22c Dynamic response of increase 10 °F in reactor inlet temperature of CS3



Figure 4.22c Dynamic response of increase 10 °F in reactor inlet temperature of CS3 (cont.)

• Decrease total toluene flowrate

Step change of 15 % decreasing at time 10 minute is made in the setpoint of the total toluene flowrate controller.

Figure 4.22 show the dynamic response of the process for 15 % decrease. The dynamic response of these control structure same as CS2 but can handle more disturb and faster than CS2.

| 0.00 | 000 | 50. | .00 | 100 Mine | D.O Jiles | 150 | 0.0 | 200 |
|-----------|-----|-----|-----|-------------|--------------|-----|-----|-----|
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| ± 336.0- | | | | | | | - | - |
| § 350.0∙ | | | | | | | | |
| g 364.0- | | | | 11 | | | | |
| § 378.0- | 5 | | | | | | | |

Figure 4.23a Dynamic response of decrease 15 % in total toluene flowrate of CS3



Figure 4.23b Dynamic response of decrease 15 % in total toluene flowrate of CS3



Figure 4.23b Dynamic response of decrease 15 % in total toluene flowrate of CS3 (cont.)

249.0 317.2 248.8 314.6 e 248.6 VI - 001-00 312.0 248.4 309.4 248.2 306.8 248.0 0.0000 50.00 100.0 150.0 200 50.00 100.0 150.0 200 0.0000 Minules Minules 520.0 518.4 516.8 515.3 515.2 513.6 5 0.0000 100.0 200.0 300.0 400.0 Moules

Figure 4.23c Dynamic response of decrease 15 % in total toluene flowrate of CS3

4.5.5 Design Control Structure III (CS4)

This control structure develops from CS3. Due to both column3 reboiler duty which is manipulated to control level of column3 reboiler and valve V10 which is manipulated to control column3 temperature obtain poor performance. Because of boilup ratio is not high enough. So this control structure switches these two variables as show in figure 4.10-11.

• Increase temperature

Step change of 10 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.

Figure 4.24 show the dynamic response of the process for 10 °F increase in reactor inlet temperature. The dynamic response of these control structure same as CS3 except temperature control in recycle column. The dynamic response of this control loop is faster than others because column reboiler can control the column temperature more effective than bottom flow.



Figure 4.24a Dynamic response of increase 10 °F in reactor inlet temperature of CS4



Figure 4.24b Dynamic response of increase 10 °F in reactor inlet temperature of CS4



Figure 4.24c Dynamic response of increase 10 °F in reactor inlet temperature of CS4



Figure 4.24c Dynamic response of increase 10 °F in reactor inlet temperature of CS4 (cont.)

• Decrease total toluene flowrate

Step change of 15 % decreasing at time 10 minute is made in the setpoint of the total toluene flowrate controller.

Figure 4.25 show the dynamic response of the process for 15 % decrease in total toluene flowrate. The dynamic response of these control structure same as CS3 except temperature control in recycle column. The dynamic response of this control loop faster than others.

| 0.00 | n | 50.0 | nn | 100 | 0 | 150 | 0.0 | 200 |
|-------------------------|---|------|----|-----|---|-----|-----|-----|
| 는 330.0 한 316.8 | L | | | | | | | _ |
| ≥ 366.4 ≥ 4 343.2 | | | | | | | | |
| 2 369.6 | 1 | | | | | _ | | 2 |

Figure 4.25a Dynamic response of decrease 15 % in total toluene flowrate of CS4



Figure 4.25b Dynamic response of decrease 15 % in total toluene flowrate of CS4



Figure 4.25b Dynamic response of decrease 15 % in total toluene flowrate of CS4 (cont.)



Figure 4.25c Dynamic response of decrease 15 % in total toluene flowrate of CS4

4.5.6 Design Control Structure IV (CS5)

In this control structure, the distillate flow of column3 is flow controlled, which can set production rate by on demand. This on-demand structure might be used when the downstream customer desires immediate responses in the availability of the product stream from this unit. The level of colum3 condenser is controlled by cascade to the total toluene flow controller as show in figure 4.12-13.

• Increase temperature

Step change of 10 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.



Figure 4.26a Dynamic response of increase 10 °F in reactor inlet temperature of CS5

Figure 4.26a gives simulation result for decreasing the reactor inlet temperature. The temperature response is oscillatory and it comes to new setpoint within 20 minutes. Effect from the temperature increase, the rate of reaction of HDA increase because of increasing temperature can raise the reaction rate. But this control structure fix production rate, so this disturbance does not affect to benzene product flow. Figure 4.18b show the fresh feed H₂, toluene, benzene product flow, and toluene impurity in product responses. Fresh feed H₂, and toluene are slightly increased about 1% at new steady-state due reaction rate increasing but production rate of benzene is fixed. And toluene impurity in product is more decreased than other control structure because of increasing temperature increase conversion of toluene to benzene at almost constant feed.



Figure 4.26b Dynamic response of increase 10 °F in reactor inlet temperature of CS5



Figure 4.26c Dynamic response of increase 10 °F in reactor inlet temperature of CS5

• Decrease production rate

Step change of 25 % decreasing at time 10 minute is made in the setpoint of the column3 distillate flow controller.

Figure 4.27 gives simulation result for decreasing the column3 distillate flow. This flow quickly responses within 10 minute. This step change affects to the fresh feed H_2 , toluene, benzene product flow, and toluene impurity in product. They slowly decrease because less production rate consume less feed rate and toluene impurity in product more decrease due to reduction toluene in the process at constant reactor inlet temperature as show in figure 4.27b.



Figure 4.27a Dynamic response of decrease 25 % in column3 distillate flow of CS5

| <u>ē</u> | | | | | | | | | | |
|--------------|---------|-----|--|-----|-----|-----|-----|-----|--|--|
| Ĕ 440.0 | | | | | | | | | | |
| € 385.0 | | | | | | | | | | |
| > 4 330.0 | | | | | | | | | | |
| ± 275.0 | | ~ | | | | | | | | |
| ti 270.0 | | | | | | | | | | |
| | 200 | 50 | | 400 | 2.0 | AEC | 2.0 | | | |
| ⊖ 0.00 | 000 | 50. | | 100 | 0.0 | 190 | 0.0 | 200 | | |
| ш. | Minutes | | | | | | | | | |

Figure 4.27a Dynamic response of decrease 25 % in column3 distillate flow of CS5 (cont.)



Figure 4.27b Dynamic response of decrease 25 % in column3 distillate flow of CS5



Figure 4.27c Dynamic response of decrease 25 % in column3 distillate flow of CS5

Figure 4.27c show the temperature control in 3 distillation columns. The temperature response of stabilizer column and recycle are oscillatory and it slowly comes to setpoint within 200 minutes as a result of slowly change in total flowrate (cascade from level control of product column). The temperature response of product column is slight change.

4.5.7 Design Control Structure V (CS6)

This control structure used valve position control concept Luyben (1990) which can reduce energy-cost of utility. In this control structure both valve bypart of column1 heat exchanger and column1 auxiliary heater is used to control tray temperature of stabilizer column. When valve bypart decrease to 5% open but temperature cannot achieve to its setpoint the auxiliary will operate to control temperature as show in figure 4.14-15.

• Increase temperature

Step change of 10 °F increasing at time 10 minute is made in the setpoint of the reactor inlet temperature controller.



Figure 4.28a Dynamic response of increase 10 °F in reactor inlet temperature of CS6



Figure 4.28b Dynamic response of increase 10 °F in reactor inlet temperature of CS6



Figure 4.28b Dynamic response of increase 10 °F in reactor inlet temperature of CS6 (cont.)



Figure 4.28c Dynamic response of increase 10 °F in reactor inlet temperature of CS6

• Decrease total toluene flowrate

Step change of 15 % decreasing at time 10 minute is made in the setpoint of the total toluene flowrate controller.

| 2 369.6 356.4 343.2 330.0 316.8 0 0000 50.00 400.0 450.0 205 | | | | | |
|--|-----------------------|-------|-------|-------|-----|
| 343.2 50.0 100.0 150.0 200 316.8 50.00 100.0 150.0 200 | 0 2 369.6 🗖 – | | | | |
| | ≣ 356.4 ≥ 343.2 | | | | |
| | 5 330.0 | | | | _ |
| | 5 316.8 | 50.00 | 400.0 | 450.0 | 200 |

Figure 4.29a Dynamic response of decrease 15 % in total toluene flowrate of CS6



Figure 4.29b Dynamic response of decrease 15 % in total toluene flowrate of CS6



Figure 4.29c Dynamic response of decrease 15 % in total toluene flowrate of CS6 (cont.)

Figure 4.28 and 4.29 show the dynamic responses of the process for 10 $^{\circ}$ F increase in reactor inlet temperature and 15 % decrease in total toluene flowrate. The dynamic response of these control structure same as CS4. Because this control structure modifies CS2 and CS4 to optimize energy cost.

The integral absolute error (IAE) for the six control structures are summarized in table 4.3.

| | D | ecrease Tota | al Toluene Fl | owrate5% | |
|----------|----------|--------------|---------------|-----------|----------|
| | CS1 | CS2 | CS3 | CS4 | CS6 |
| f_tottol | *16.7046 | 16.8467 | 17.0188 | 16.9606 | 16.782 |
| t_col1 | 33.8958 | *31.4283 | 41.8548 | 46.1904 | 41.7358 |
| t_col2 | *0.0573 | 0.083 | 0.1113 | 0.1147 | 0.0761 |
| t_col3 | 123.6263 | 130.6594 | 134.1722 | 0.7981 | *0.7705 |
| t_quench | *3.6525 | 4.7158 | 3.71 | 3.7017 | 4.0008 |
| t_reacin | *5.7933 | 8.2733 | 6.49 | 6.5133 | 7.63 |
| t_sep | 25.3622 | 18.6854 | *17.0026 | 17.0501 | 18.1923 |
| x_gasre | *0.5583 | 0.835 | 0.837 | 0.837 | 0.8242 |
| total | 209.6503 | 211.5269 | 221.1967 | 92.1659 | *90.0117 |
| | | | | | |
| | De | ecrease Tota | l Toluene Flo | owrate10% | |
| | CS1 | CS2 | CS3 | CS4 | CS6 |
| f_tottol | 32.5632 | *32.4208 | 33.4078 | 33.2332 | 32.7979 |
| t_col1 | *63.3114 | 111.7511 | 76.3328 | 74.9459 | 83.8908 |
| t_col2 | *0.102 | 0.1326 | 0.1536 | 0.1627 | 0.1357 |
| t_col3 | 233.5163 | 245.7238 | 252.7919 | 1.5478 | *1.5442 |
| t_quench | *6.9958 | 8.19 | 7.2383 | 7.2283 | 7.8375 |
| t_reacin | *11.4442 | 14.6075 | 12.6792 | 12.6758 | 14.7333 |
| t_sep | 50.5375 | 35.1886 | 33.9293 | *33.8712 | 36.3393 |
| x_gasre | *1.1253 | 1.6839 | 1.6931 | 1.693 | 1.6735 |
| total | 399.5957 | 449.6983 | 418.226 | *165.3579 | 178.9522 |
| | | | | | |
| | De | ecrease Tota | l Toluene Flo | owrate15% | |
| | CS1 | CS2 | CS3 | CS4 | CS6 |
| f_tottol | *47.5824 | - | 49.3356 | 49.0594 | 48.0783 |
| t_col1 | 108.1415 | - | 102.1855 | *101.2128 | 124.6101 |
| t_col2 | *0.1378 | 00701 | 0.1856 | 0.1925 | 0.1683 |
| t_col3 | 330.1441 | 1415 | 357.2563 | 2.2746 | *2.2712 |
| t_quench | *10.1958 | ~ | 10.3275 | 10.3175 | 11.1308 |
| t_reacin | *16.9225 | | 18.7 | 18.7183 | 21.305 |
| t_sep | 75.6252 | | 50.8318 | *50.747 | 55.135 |
| x_gasre | 1.7033 | - | 2.5696 | 2.5695 | 2.5532 |
| total | 590.4526 | _ | 591.3919 | *235.0916 | 265.2519 |

Table 4.3a Integral absolute error of the five control structures when decrease total toluene flowrate.

| | - 1 | | | | | | | |
|-------------------------|------------------------|---------------|---------------|-----------|-----------|--|--|--|
| | I | ncrease Tota | l Toluene Flo | wrate 5% | | | | |
| | CS1 | CS2 | CS3 | CS4 | CS6 | | | |
| f_tottol | 17.6216 | 18.5244 | 17.6693 | 17.5872 | *17.4712 | | | |
| t_col1 | *31.2903 | 32.1093 | 36.2457 | 37.141 | 34.9958 | | | |
| t_col2 | 0.0654 | 0.063 | 0.0989 | 0.0945 | *0.0593 | | | |
| t_col3 | 138.4164 | 145.0308 | 150.473 | 0.8162 | *0.7933 | | | |
| t_quench | *3.7617 | 6.3492 | 4.01 | 4.0058 | 4.6 | | | |
| t_reacin | *5.9883 | 9.9975 | 6.4458 | 6.4442 | 7.7133 | | | |
| t_sep | 25.4712 | *18.364 | 16.8936 | 16.8804 | 18.0287 | | | |
| x_gasre | *0.553 | 0.8106 | 0.824 | 0.8239 | 0.8112 | | | |
| total | 223.1679 | 231.2488 | 232.6603 | *83.7932 | 84.4728 | | | |
| | T | Total | Taluara Elar | | | | | |
| | | crease Total | | | 000 | | | |
| <u> </u> | CSI | CS2 | CS3 | CS4 | CS6 | | | |
| f_tottol | 36.1991 | 37.8617 | 36.2349 | *36.0877 | 36.123 | | | |
| t_col1 | *62.5587 | 62.6406 | 73.9282 | 74.02 | 68.8108 | | | |
| t_col2 | 0.1079 | 0.0987 | 0.1429 | 0.1384 | *0.0915 | | | |
| t_col3 | 292.7522 | 306.8865 | 318.7847 | 1.6536 | *1.6299 | | | |
| t_quench | *7.725 | 13.2742 | 8.1475 | 8.1575 | 10.1 | | | |
| t_reacin | *12.2783 | 20.4533 | 13.2408 | 13.2167 | 16.3017 | | | |
| t_sep | 51.08 <mark>9</mark> 4 | 35.8922 | 33.8655 | *33.8014 | 35.9378 | | | |
| x_gasre | *1.1038 | 1.6114 | 1.6401 | 1.6401 | 1.6194 | | | |
| total | 463.8144 | 478.7186 | 485.9846 | *168.7154 | 170.6141 | | | |
| | I, | noransa Total | Toluene Flor | wrata15% | | | | |
| | CS1 | | | | CS6 | | | |
| f_tottol | 55 779 | 0.52 | 55 6679 | *55 /633 | 55 9842 | | | |
| $\frac{1-00001}{1-001}$ | *94 9682 | | 115 128 | 115 2549 | 104 372 | | | |
| t_{col2} | 0 1449 | 0000 | 0 1537 | 0 162 | *0 1192 | | | |
| t_{col3} | 463 4428 | | 504 9943 | *2 5165 | 2 5192 | | | |
| t_cuench | *11 9392 | | 12 6158 | 12 5808 | 16 1333 | | | |
| t reacin | *18 7442 | | 20 1783 | 20 1658 | 25 3567 | | | |
| t sen | 76 6733 | | 50 7173 | *50 6305 | 51 2618 | | | |
| x gasre | *1 6545 | | 2 4517 | 2 4516 | 2 4379 | | | |
| total | 723 3461 | _ | 761 907 | 259 2254 | *258 1843 | | | |
| lotai | 123.3401 | - | /01.70/ | 237.2234 | 250.1045 | | | |

Table 4.3b Integral absolute error of the five control structures when increase total toluene flowrate.

| | Incre | Increase Reactor Inlet Temperature 5°F | | | | | | | |
|------------|----------|--|----------|----------|---------|---------|--|--|--|
| | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | | | |
| f_tottol | 11.3743 | 11.8757 | 11.3033 | 11.279 | *8.2041 | 11.7472 | | | |
| t_col1 | *18.3802 | 20.9747 | 25.6221 | 24.4173 | 42.3365 | 22.3318 | | | |
| t_col2 | 0.0777 | 0.0781 | 0.0987 | 0.0936 | 0.1051 | *0.0601 | | | |
| t_col3 | 193.6085 | 225.3952 | 220.9563 | *2.3495 | 2.6826 | 2.4425 | | | |
| t_quench | *4.2833 | 5.75 <mark>75</mark> | 4.7575 | 4.7575 | 6.7183 | 5.1808 | | | |
| t_reacin | *5.8017 | 8.1208 | 6.7033 | 6.7042 | 7.46 | 7.2808 | | | |
| t_sep | 12.7603 | 12.0404 | 8.1426 | *8.1333 | 12.5813 | 11.4847 | | | |
| x_gasre | *0.4778 | 0.7112 | 0.6841 | 0.684 | 0.9777 | 0.7152 | | | |
| total | 246.7638 | 284.9536 | 278.2679 | *58.4184 | 81.0656 | 61.2431 | | | |
| f_ondemand | | | | | 0.0278 | | | | |

Table 4.3c Integral absolute error of the six control structures when increase reactor inlet temperature.

| | | Increase l | Reactor Inle | t Temperati | ure 10°F | |
|------------|----------|----------------|--------------|-------------|----------|---------|
| | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 |
| f_tottol | 21.6659 | 11-11= | 21.3589 | 21.3457 | *14.5601 | 22.0922 |
| t_col1 | *34.4289 | 1 5 10 | 44.3785 | 44.4793 | 74.6809 | 41.5913 |
| t_col2 | *0.1163 | - 200 | 0.1362 | 0.1448 | 0.1489 | 0.1195 |
| t_col3 | 408.6362 | 100 | 456.6059 | *4.4048 | 4.9342 | 4.5653 |
| t_quench | *8.0275 | | 9.1833 | 9.1825 | 12.36 | 9.7017 |
| t_reacin | *11.2908 | <u> </u> | 12.8183 | 12.82 | 15.1842 | 13.9633 |
| t_sep | 24.8781 | Math And In | *15.8785 | 15.8924 | 23.9971 | 22.6201 |
| x_gasre | *0.9139 | | 1.3009 | 1.3009 | 1.8799 | 1.3556 |
| total | 509.9576 | 20 <u>9</u> 97 | 561.6605 | *109.5704 | 147.7453 | 116.009 |
| f_ondemand | 12 | | | | 0.0665 | |

Table 4.3d Integral absolute error of the six control structures when decrease reactor inlet temperature.

| | | Decrease Reactor Inlet Temperature 5°F | | | | | | | | |
|------------|----------|--|----------|---------|----------|----------|--|--|--|--|
| 3 | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | | | | |
| f_tottol | 12.0154 | 12.6961 | 12.1178 | 12.092 | *10.6842 | 11.7472 | | | | |
| t_col1 | *21.3976 | 25.9986 | 32.977 | 33.3353 | 57.2377 | 28.2545 | | | | |
| t_col2 | *0.0771 | 0.1663 | 0.1833 | 0.1878 | 0.1682 | 0.1608 | | | | |
| t_col3 | 168.2273 | 197.8495 | 195.2698 | *2.5865 | 3.0717 | 2.6952 | | | | |
| t_quench | *5.0433 | 6.635 | 5.5808 | 5.5817 | 7.4933 | 6.1 | | | | |
| t_reacin | *6.1458 | 8.7333 | 7.06 | 7.0517 | 7.8517 | 7.8242 | | | | |
| t_sep | 13.2486 | 11.4269 | *8.5515 | 8.5528 | 13.7829 | 11.3132 | | | | |
| x_gasre | *0.5142 | 0.783 | 0.745 | 0.7449 | 1.0455 | 0.7853 | | | | |
| total | 226.6693 | 264.2887 | 262.4852 | 70.1327 | 101.3352 | *68.8804 | | | | |
| f_ondemand | | | | | 0.0302 | | | | | |

Note * = Minimum IAE value

The energy consumption at steady state of the six control structures are summarized in table 4.4.

| Heat Flow (Btu/hr) | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 |
|------------------------|----------|----------|----------|----------|----------|----------|
| Furnace Duty | 3.14E+06 | 5.52E+06 | 5.33E+06 | 5.33E+06 | 5.33E+06 | 5.51E+06 |
| Cooler Duty | 9.03E+06 | 7.43E+06 | 8.08E+06 | 8.08E+06 | 8.06E+06 | 7.46E+06 |
| Column1 Condenser Duty | 3.86E+05 | 3.86E+05 | 3.86E+05 | 3.86E+05 | 3.87E+05 | 3.86E+05 |
| Column1 Reboiler Duty | 4.30E+06 | | - | - | - | |
| Column2 Condenser Duty | 1.36E+07 | 1.36E+07 | 1.37E+07 | 1.37E+07 | 1.37E+07 | 1.36E+07 |
| Column2 Reboiler Duty | 1.16E+07 | 1.03E+07 | 1.03E+07 | 1.03E+07 | 1.03E+07 | 1.03E+07 |
| Column3 Condenser Duty | 1.52E+06 | ANA CANA | <u> </u> | - | - | |
| Column3 Reboiler Duty | 1.62E+06 | 1.86E+06 | 1.84E+06 | 1.84E+06 | 1.84E+06 | 1.85E+06 |
| Auxiliary Duty | - | | 8.20E+05 | 8.19E+05 | 8.19E+05 | 4.57E+04 |
| Total | 4.52E+07 | 3.91E+07 | 4.04E+07 | 4.05E+07 | 4.04E+07 | 3.92E+07 |

Table 4.4 The energy consumption of the six control structures



CHAPTER V

CONCLUSIONS AND RECCOMMENDATIONS

5.1 Conclusion

Most industrial processes contain a complex flowsheet with several recycle streams, energy integration, and many different unit operations. The economic can be improved by introducing recycle streams and energy integration into the process. However, the recycle streams and energy integration introduce a feedback of material and energy among units upstream and downstream. Therefore, strategies for plantwide control are required to operate an entire plant safely and achieve its design objectives. Hydrodealkylation (HDA) process of toluene to benzene consists of a reactor, furnace, vapor-liquid separator, recycle compressor, heat exchangers and distillations. This plant is a realistic complex chemical process. It is considering that the energy integration for realistic and large processes is meaningful and useful, it is essential to design a control strategy for process alternative 1, three control structures designed by Kietawarin (2002) were compared with Luyben (1998), the effects of disturbances could be reduced in order to keep the production rate as desired value.

This work presents five plantwide designed control structures, the control results of these alternative structures are compared with reference structure (Kietawarin; 2002, Luyben; 1998 and 2002). The dynamic simulation of this process with various disturbances is made to evaluate performance of each control structures: increasing and decreasing the reactor inlet temperature, increasing and decreasing total toluene flowrate, increasing and decreasing benzene production rate.

The result shows that the dynamic performance of hydrodealkylation of toluene process deteriorates when the process incorporates complex heat integration. However it can reduce energy cost and can be operated well by use plantwide methodology to design control structure. The dynamic responses of the proposed control structures compared with the reference are similar. CS2 has been limited in bypass, so it can handle in small disturbance. CS3 which is improved from CS2 is able to handle more disturbances by using auxiliary instead of bypass valve to control stabilizer column temperature. CS4 obtain faster response of temperature of recycle column than the other column because the column temperature is able to be controlled via using reboiler duty more effectively than the bottom flow rate. CS5 on-demand structure advantage when the downstream customer desires immediate responses in the availability of the product stream from this unit. For CS6, the dynamic responses are same as other but it use energy less than CS1 and CS4. Because this control structure, CS6, is modified from CS2 and CS4 to optimize energy cost.

The performance of these control structures can be arranged from the best to lowest performance (error of controllability point of view) as the following sequences: CS4, CS6, CS5, CS1, CS3, and CS2. For Kietawarin's control structures performance of her structures are S2, S3, and S1 respectively.

Nowadays, hydrodealkylation of toluene process (HDA) is out of date; some industry use disproportionation to produce benzene because this new process achieves more economically. However control structures of this work still have usefulness because they can be applied to any heat integrated-process.

5.2 Recommendations

- 1. Study and design the control structure of other complex heat-exchange network of HDA or other process in plantwide control point of view.
- 2. Study and improve the methodology of MPC plantwide control of HDA process.

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สถาบันวิทยบริการ จุฬาลงกรณ์มหาวิทยาลัย

APPENDICES

สถาบันวิทยบริการ จุฬาลงกรณ์มหาวิทยาลัย

APPENDIX A

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

| Name | FFH2 | v1out | FFtol | v2out | Tottol | Regas | cout | hin | hout |
|---|---|---|---|--|--|---|--|--|---|
| Vapour Fraction | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0000 | 1.0000 | 1.0000 | 0.9521 |
| Temperature [°F] | 86.0000 | 85.9936 | 86.0000 | 86.4137 | 136.7109 | 148.7124 | 1106.0765 | 1149.8994 | 228.7425 |
| Pressure [psia] | 605.0000 | 575.0000 | 635.0000 | 575.0000 | 575.0000 | 575.0000 | 512.9964 | 486.0030 | 480.0028 |
| Molar Flow [lbmole/hr] | 490.3800 | 490 <mark>.3</mark> 800 | 288.9999 | 288.9999 | 373.4282 | 3519.2000 | 4383.0082 | 4492.3479 | 4492.3479 |
| Comp Mole Frac (Hydrogen) | 0.970000 | 0.970000 | 0.000000 | 0.000000 | 0.000000 | 0.401969 | 0.431274 | 0.357993 | 0.357993 |
| Comp Mole Frac (Methane) | 0.030000 | 0.030000 | 0.000000 | 0.000000 | 0.000000 | 0.586840 | 0.474542 | 0.528375 | 0.528375 |
| Comp Mole Frac (Benzene) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000146 | 0.009989 | 0.008033 | 0.086641 | 0.086641 |
| Comp Mole Frac (Toluene) | 0.000000 | 0.000000 | 1.000000 | 1.000000 | 0.999850 | 0.001201 | 0.086151 | 0.025194 | 0.025194 |
| Comp Mole Frac (BiPhenyl) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000005 | 0.000000 | 0.000000 | 0.001796 | 0.001796 |
| Name | reacin | condout | gas | liq | purge | gasre | v3out | v5out | d1 |
| Vapour Fraction | 1.0000 | 0.8910 | 1.0000 | 0.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0297 | 1.0000 |
| Temperature [°F] | 1150.0000 | 113.0000 | 113.0000 | 113.0000 | 113.0000 | 113.0000 | 113.8318 | 114.7485 | 123.8687 |
| Pressure [psia] | 503.0000 | 476.8033 | 476.8033 | 476.8033 | 476.8033 | 476.8033 | 485.9992 | 150.2591 | 150.0000 |
| Molar Flow [lbmola/br] | | | | | | | | | |
| | 4383.0082 | 4492.3479 | 4002.5994 | 489.7485 | 483.3964 | 3519.2030 | 108.4994 | 381.2491 | 19.7295 |
| Comp Mole Frac (Hydrogen) | 4383.0082 0.431274 | 4492.3479 0.357993 | 4002.5994 0.401225 | 489.7485 0.004670 | 483.3964 0.401225 | 3519.2030 0.401225 | 108.4994 0.004670 | 381.2491 0.004670 | 19.7295 0.090237 |
| Comp Mole Frac (Hydrogen) Comp Mole Frac (Methane) | 4383.0082 0.431274 0.474542 | 4492.3479 0.357993 0.528375 | 4002.5994 0.401225 0.587533 | 489.7485 0.004670 0.044890 | 483.3964 0.401225 0.587533 | 3519.2030 0.401225 0.587533 | 108.4994 0.004670 0.044890 | 381.2491 0.004670 0.044890 | 19.7295 0.090237 0.867428 |
| Comp Mole Frac (Hydrogen) Comp Mole Frac (Methane) Comp Mole Frac (Benzene) | 4383.0082 0.431274 0.474542 0.008033 | 4492.3479 0.357993 0.528375 0.086641 | 4002.5994 0.401225 0.587533 0.010071 | 489.7485 0.004670 0.044890 0.712431 | 483.3964 0.401225 0.587533 0.010071 | 3519.2030 0.401225 0.587533 0.010071 | 108.4994 0.004670 0.044890 0.712431 | 381.2491 0.004670 0.044890 0.712431 | 19.7295 0.090237 0.867428 0.041999 |
| Comp Mole Frac (Hydrogen) Comp Mole Frac (Methane) Comp Mole Frac (Benzene) Comp Mole Frac (Toluene) | 4383.0082 0.431274 0.474542 0.008033 0.086151 | 4492.3479 0.357993 0.528375 0.086641 0.025194 | 4002.5994 0.401225 0.587533 0.010071 0.001170 | 489.7485 0.004670 0.044890 0.712431 0.221539 | 483.3964 0.401225 0.587533 0.010071 0.001170 | 3519.2030 0.401225 0.587533 0.010071 0.001170 | 108.4994 0.004670 0.044890 0.712431 0.221539 | 381.2491 0.004670 0.044890 0.712431 0.221539 | 19.7295 0.090237 0.867428 0.041999 0.000336 |

| Name | fquence | f1 | d2 | b2 | p2out | v8out | v9out | cin | reactout |
|---------------------------|----------|----------|----------|-----------|----------|-----------|----------|-----------|-----------|
| Vapour Fraction | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.1162 | 0.0177 | 0.9086 | 1.0000 |
| Temperature [°F] | 113.4559 | 113.4559 | 221.9900 | 290.8027 | 290.9465 | 177.5349 | 286.1634 | 140.8752 | 1230.9282 |
| Pressure [psia] | 551.5992 | 551.5992 | 30.0000 | 32.2600 | 52.2607 | 15.0000 | 30.3274 | 575.0000 | 486.0030 |
| Molar Flow [lbmole/hr] | 108.4994 | 381.2491 | 270.8122 | 90.7074 | 90.7074 | 270.8122 | 90.7074 | 4383.0082 | 4383.0083 |
| Comp Mole Frac (Hydrogen) | 0.004670 | 0.004670 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.431274 | 0.366857 |
| Comp Mole Frac (Methane) | 0.044890 | 0.044890 | 0.000001 | 0.000000 | 0.000000 | 0.000001 | 0.000000 | 0.474542 | 0.540387 |
| Comp Mole Frac (Benzene) | 0.712431 | 0.712431 | 0.999699 | 0.000600 | 0.000600 | 0.999699 | 0.000600 | 0.008033 | 0.071023 |
| Comp Mole Frac (Toluene) | 0.221539 | 0.221539 | 0.000300 | 0.930176 | 0.930176 | 0.000300 | 0.930176 | 0.086151 | 0.020305 |
| Comp Mole Frac (BiPhenyl) | 0.016470 | 0.016470 | 0.000000 | 0.069224 | 0.069224 | 0.000000 | 0.069224 | 0.000000 | 0.001428 |
| Name | v10out | Retol | v11out | tot | quench | discharge | v4out | plout | p3out |
| Vapour Fraction | 0.3592 | 0.0000 | 0.0000 | 1.0000 | 0.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0000 |
| Temperature [°F] | 498.9020 | 286.1792 | 287.1636 | 1149.8441 | 113.8318 | 148.7032 | 112.2715 | 113.4559 | 286.1792 |
| Pressure [psia] | 16.0000 | 875.0000 | 575.0000 | 486.0030 | 486.0030 | 575.0020 | 446.8033 | 551.5992 | 875.0000 |
| Molar Flow [lbmole/hr] | 6.2791 | 84.4283 | 84.4283 | 4492.1083 | 109.1000 | 3519.2030 | 483.3964 | 489.7485 | 84.4283 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 | 0.358060 | 0.004670 | 0.401225 | 0.401225 | 0.004670 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000000 | 0.000000 | 0.000000 | 0.528353 | 0.044890 | 0.587533 | 0.587533 | 0.044890 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.000000 | 0.000645 | 0.000645 | 0.086601 | 0.712422 | 0.010071 | 0.010071 | 0.712431 | 0.000645 |
| Comp Mole Frac (Toluene) | 0.000260 | 0.999335 | 0.999335 | 0.025193 | 0.221549 | 0.001170 | 0.001170 | 0.221539 | 0.999335 |
| Comp Mole Frac (BiPhenyl) | 0.999740 | 0.000020 | 0.000020 | 0.001794 | 0.016469 | 0.000000 | 0.000000 | 0.016470 | 0.000020 |
| | จุฬา | ลงก | รณ | าหา | ามยา | าลย | | | |

| Name | b1 | v6out 📕 | v7out | d3 | b3 |
|---------------------------|----------|-------------------------|----------|----------|----------|
| Vapour Fraction | 0.0000 | 1.0000 | 0.4501 | 0.0000 | 0.0000 |
| Temperature [F] | 373.0749 | 122. <mark>246</mark> 4 | 239.8926 | 279.7473 | 558.8265 |
| Pressure [psia] | 150.5432 | 120.0000 | 31.0400 | 30.0000 | 31.0000 |
| Molar Flow [lbmole/hr] | 361.5196 | 19.7295 | 361.5196 | 84.4283 | 6.2791 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.090237 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000001 | 0.867428 | 0.000001 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.749019 | 0.041 <mark>999</mark> | 0.749019 | 0.000645 | 0.000000 |
| Comp Mole Frac (Toluene) | 0.233611 | 0.000336 | 0.233611 | 0.999335 | 0.000260 |
| Comp Mole Frac (BiPhenyl) | 0.017369 | 0.000000 | 0.017369 | 0.000020 | 0.999740 |

| Name | fuel | q1 | wk1 | wk2 | qr1 | | qc1 | qr2 | qc2 | wk3 |
|--------------------|------------|------------|------------|------------|---------|------|------------|------------|------------|-----------|
| Heat Flow [Btu/hr] | 3125599.66 | 9050594.37 | 1007267.82 | 13645.1676 | 4297131 | 1.38 | 614094.503 | 11646761.3 | 13662444.3 | 905.47261 |
| Name | qc3 | qr3 | wk4 | | | | | | | |
| Heat Flow [Btu/hr] | 1450510.46 | 1601662.45 | 34560.4574 | | | | | | | |

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| Name | FFH2 | v1out | Toltol | cin | Regas | reacin | reactout | tot | quench |
|---------------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|
| Vapour Fraction | 1.0000 | 1.0000 | 0.0000 | 0.9094 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 0.0000 |
| Temperature [F] | 86.0000 | 85.9936 | 157.5732 | 146.0224 | 148.7100 | 1149.9980 | 1230.9399 | 1149.8646 | 113.8317 |
| Pressure [psia] | 605.0000 | 575.0000 | 575.0000 | 575.0000 | 575.0000 | 503.0000 | 486.0016 | 486.0016 | 486.0016 |
| Molar Flow [lbmole/hr] | 490.3800 | 490.3800 | 373.5522 | 4383.1351 | 3519.2030 | 4383.1351 | 4383.1352 | 4492.2352 | 109.1000 |
| Comp Mole Frac (Hydrogen) | 0.970000 | 0.970000 | 0.000000 | 0.431262 | 0.401969 | 0.431262 | 0.366833 | 0.358037 | 0.004670 |
| Comp Mole Frac (Methane) | 0.030000 | 0.030000 | 0.000000 | 0.474529 | 0.586841 | 0.474529 | 0.540383 | 0.528350 | 0.044889 |
| Comp Mole Frac (Benzene) | 0.000000 | 0.000000 | 0.000252 | 0.008042 | 0.009989 | 0.008042 | 0.071046 | 0.086623 | 0.712432 |
| Comp Mole Frac (Toluene) | 0.000000 | 0.000000 | 0.999659 | 0.086160 | 0.001201 | 0.086160 | 0.020305 | 0.025192 | 0.221538 |
| Comp Mole Frac (BiPhenyl) | 0.000000 | 0.000000 | 0.000090 | 0.000008 | 0.000000 | 0.000008 | 0.001433 | 0.001798 | 0.016472 |
| Name | condout | gasre | discharge | v4out | p1out | fquence | d1 | b1 | vбout |
| Vapour Fraction | 0.8910 | 1.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 1.0000 | 0.0000 | 1.0000 |
| Temperature [F] | 113.0000 | 113.0000 | 148.7072 | 112.2715 | 113.4559 | 113.4559 | 123.9116 | 372.9882 | 122.2895 |
| Pressure [psia] | 476.7934 | 476.7934 | 575.0020 | 446.7934 | 551.5894 | 551.5894 | 150.0000 | 150.5400 | 120.0000 |
| Molar Flow [lbmole/hr] | 4492.3510 | 3519.2030 | 3519.2030 | 483.4032 | 489.7447 | 108.4994 | 19.7223 | 759.6531 | 19.7223 |
| Comp Mole Frac (Hydrogen) | 0.357993 | 0.401225 | 0.401225 | 0.401225 | 0.004670 | 0.004670 | 0.090265 | 0.000000 | 0.090265 |
| Comp Mole Frac (Methane) | 0.528376 | 0.587533 | 0.587533 | 0.587533 | 0.044889 | 0.044889 | 0.867384 | 0.000019 | 0.867384 |
| Comp Mole Frac (Benzene) | 0.086641 | 0.010072 | 0.010072 | 0.010072 | 0.712432 | 0.712432 | 0.042002 | 0.749007 | 0.042002 |
| Comp Mole Frac (Toluene) | 0.025194 | 0.001170 | 0.001170 | 0.001170 | 0.221538 | 0.221538 | 0.000349 | 0.233604 | 0.000349 |
| Comp Mole Frac (BiPhenyl) | 0.001796 | 0.000000 | 0.000000 | 0.000000 | 0.016472 | 0.016472 | 0.000000 | 0.017370 | 0.000000 |
| 6 | จูฬา | ลงก | รณา | เหาว | ายา | າລຢ | | | |

| Name | v7out | d2 | v9out | d3 | b3 | p3out | v10out | v14out | toConR |
|---------------------------|----------|----------|----------|----------|----------|----------|-----------|-----------|----------|
| Vapour Fraction | 0.4498 | 0.0000 | 0.0000 | 1.0000 | 0.0000 | 0.0000 | 0.1847 | 1.0000 | 0.0000 |
| Temperature [F] | 239.8817 | 221.6034 | 291.2763 | 357.2290 | 656.3956 | 360.3198 | 631.0466 | 289.6320 | 291.2182 |
| Pressure [psia] | 31.0381 | 30.0000 | 75.7532 | 75.4196 | 76.4349 | 875.0000 | 61.4349 | 27.2600 | 96.0186 |
| Molar Flow [lbmole/hr] | 361.5231 | 270.7180 | 90.8051 | 106.5737 | 6.2484 | 106.5737 | 6.2484 | 0.0000 | 846.8800 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000019 | 0.000025 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.749007 | 0.999675 | 0.001052 | 0.001126 | 0.000000 | 0.001126 | 0.000000 | 0.002275 | 0.001052 |
| Comp Mole Frac (Toluene) | 0.233604 | 0.000300 | 0.929737 | 0.998435 | 0.000260 | 0.998435 | 0.000260 | 0.995902 | 0.929737 |
| Comp Mole Frac (BiPhenyl) | 0.017370 | 0.000000 | 0.069212 | 0.000439 | 0.999740 | 0.000439 | 0.999740 | 0.001823 | 0.069212 |
| Name | tov10 | v15out | boil1 | v13out | tov8 | toboil1 | tofur | hout2 | v13in |
| Vapour Fraction | 0.0000 | 0.0937 | 0.9321 | 0.0000 | 0.0000 | 0.9321 | 1.0000 | 1.0000 | 0.0000 |
| Temperature [F] | 291.2182 | 298.0462 | 396.8000 | 373.4298 | 372.9882 | 396.8000 | 1072.0802 | 502.0912 | 373.4855 |
| Pressure [psia] | 96.0186 | 35.1478 | 150.5400 | 164.1400 | 150.5400 | 150.5400 | 513.0000 | 484.0015 | 191.1506 |
| Molar Flow [lbmole/hr] | 90.8051 | 846.8800 | 398.1300 | 398.1300 | 361.5231 | 398.1300 | 4383.1351 | 4492.2352 | 398.1300 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.431262 | 0.358037 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000000 | 0.000000 | 0.000019 | 0.000019 | 0.000019 | 0.000019 | 0.474529 | 0.528350 | 0.000019 |
| Comp Mole Frac (Benzene) | 0.001052 | 0.001052 | 0.749007 | 0.749007 | 0.749007 | 0.749007 | 0.008042 | 0.086623 | 0.749007 |
| Comp Mole Frac (Toluene) | 0.929737 | 0.929737 | 0.233604 | 0.233604 | 0.233604 | 0.233604 | 0.086160 | 0.025192 | 0.233604 |
| Comp Mole Frac (BiPhenyl) | 0.069212 | 0.069212 | 0.017370 | 0.017370 | 0.017370 | 0.017370 | 0.000008 | 0.001798 | 0.017370 |
| 0 | าพ่า | ลงก' | ริณา | เทาว | ายก | າລຍ | | | |

| Name | toTop3 | hotout5 | cout5 | vent3 | v17out | boil2out | v16out | v11out | 2.0000 |
|---------------------------|----------|-------------------------|----------|-----------|-----------|-----------|-----------|----------|----------|
| Vapour Fraction | 0.0189 | 0.0000 | 0.0000 | 1.0000 | 0.0189 | 0.8861 | 1.0000 | 0.0000 | 0.0000 |
| Temperature [F] | 356.2950 | 352.6895 | 322.5725 | 352.6895 | 356.2983 | 330.0000 | 351.6682 | 360.6969 | 86.0000 |
| Pressure [psia] | 75.4200 | 72.5189 | 93.1178 | 72.5189 | 75.4200 | 32.2600 | 67.5189 | 575.0000 | 635.0000 |
| Molar Flow [lbmole/hr] | 22.0170 | 106.5737 | 846.8800 | 0.0000 | 22.0170 | 846.8800 | 0.0000 | 84.5522 | 289.0000 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.001113 | 0.001126 | 0.001052 | 0.002038 | 0.001126 | 0.001052 | 0.002038 | 0.001113 | 0.000000 |
| Comp Mole Frac (Toluene) | 0.998491 | 0.9 <mark>98435</mark> | 0.929737 | 0.997941 | 0.998435 | 0.929737 | 0.997941 | 0.998491 | 1.000000 |
| Comp Mole Frac (BiPhenyl) | 0.000396 | 0.000 <mark>4</mark> 39 | 0.069212 | 0.000020 | 0.000439 | 0.069212 | 0.000020 | 0.000396 | 0.000000 |
| Name | 222 | 333 | 444 | cout | hin2 | hout | gas | liq | purge |
| Vapour Fraction | 1.0000 | 1.0000 | 0.0000 | 1.0000 | 1.0000 | 0.9374 | 1.0000 | 0.0000 | 1.0000 |
| Temperature [F] | 357.2290 | 356.6400 | 324.0093 | 345.5600 | 1149.8646 | 211.9567 | 113.0000 | 113.0000 | 113.0000 |
| Pressure [psia] | 75.4196 | 72.5189 | 72.5189 | 543.9982 | 486.0016 | 480.0434 | 476.7934 | 476.7934 | 476.7934 |
| Molar Flow [lbmole/hr] | 10.6574 | 10.6574 | 95.9164 | 4383.1351 | 4492.2352 | 4492.3510 | 4002.6062 | 489.7447 | 483.4032 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 | 0.431262 | 0.358037 | 0.357993 | 0.401225 | 0.004670 | 0.401225 |
| Comp Mole Frac (Methane) | 0.000000 | 0.000000 | 0.000000 | 0.474529 | 0.528350 | 0.528376 | 0.587533 | 0.044889 | 0.587533 |
| Comp Mole Frac (Benzene) | 0.001126 | 0.001126 | 0.001126 | 0.008042 | 0.086623 | 0.086641 | 0.010072 | 0.712432 | 0.010072 |
| Comp Mole Frac (Toluene) | 0.998435 | 0.998435 | 0.998435 | 0.086160 | 0.025192 | 0.025194 | 0.001170 | 0.221538 | 0.001170 |
| Comp Mole Frac (BiPhenyl) | 0.000439 | 0.000439 | 0.000439 | 0.00008 | 0.001798 | 0.001796 | 0.000000 | 0.016472 | 0.000000 |
| | | | 99199 | | | 1610 | | | |
| | | | | | | | | | |

| Name | f1 | v3out | v5out | b2 | p2out | v8out | boil2 | vent2 | tankout |
|---------------------------|----------|-------------------------|----------|-----------|-----------|----------|----------|----------|----------|
| Vapour Fraction | 0.0000 | 0.0000 | 0.0297 | 0.0000 | 0.0000 | 0.1153 | 0.8861 | 1.0000 | 0.0000 |
| Temperature [F] | 113.4559 | 113.8317 | 114.7485 | 290.7607 | 291.2182 | 177.5225 | 330.0000 | 290.7607 | 290.7607 |
| Pressure [psia] | 551.5894 | 486.0068 | 150.2591 | 32.2600 | 96.0186 | 15.0001 | 32.2600 | 32.2600 | 32.2600 |
| Molar Flow [lbmole/hr] | 381.2454 | 108.4994 | 381.2454 | 937.6851 | 937.6851 | 270.7180 | 846.8800 | 0.0000 | 937.6851 |
| Comp Mole Frac (Hydrogen) | 0.004670 | 0.004670 | 0.004670 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.044889 | 0.044889 | 0.044889 | 0.000000 | 0.000000 | 0.000025 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.712432 | 0.712432 | 0.712432 | 0.001052 | 0.001052 | 0.999675 | 0.000983 | 0.002275 | 0.001052 |
| Comp Mole Frac (Toluene) | 0.221538 | 0.2215 <mark>3</mark> 8 | 0.221538 | 0.929737 | 0.929737 | 0.000300 | 0.929799 | 0.995902 | 0.929737 |
| Comp Mole Frac (BiPhenyl) | 0.016472 | 0.016 <mark>4</mark> 72 | 0.016472 | 0.069212 | 0.069212 | 0.000000 | 0.069218 | 0.001823 | 0.069212 |
| Name | vent1 | tank1out | v12out | hin1 | toE1 | to_p | Tout3 | v17in | toR4 |
| Vapour Fraction | 1.0000 | 0.0000 | 1.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Temperature [F] | 372.9882 | 372.9882 | 372.0431 | 427.3700 | 427.3700 | 372.9882 | 352.6895 | 360.3198 | 360.3198 |
| Pressure [psia] | 150.5400 | 150.5400 | 145.5400 | 482.0014 | 482.0014 | 150.5400 | 72.5189 | 875.0000 | 875.0000 |
| Molar Flow [lbmole/hr] | 0.0000 | 759.6531 | 0.0000 | 4492.3510 | 4492.2352 | 398.1300 | 106.5737 | 22.0170 | 84.5567 |
| Comp Mole Frac (Hydrogen) | 0.000010 | 0.000000 | 0.000010 | 0.357993 | 0.358037 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000686 | 0.000019 | 0.000686 | 0.528376 | 0.528350 | 0.000019 | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.843409 | 0.749007 | 0.843409 | 0.086641 | 0.086623 | 0.749007 | 0.001126 | 0.001126 | 0.001126 |
| Comp Mole Frac (Toluene) | 0.155217 | 0.233604 | 0.155217 | 0.025194 | 0.025192 | 0.233604 | 0.998435 | 0.998435 | 0.998435 |
| Comp Mole Frac (BiPhenyl) | 0.000678 | 0.017370 | 0.000678 | 0.001796 | 0.001798 | 0.017370 | 0.000439 | 0.000439 | 0.000439 |
| | | | 99199 | | | 1610 | | | |
| | | | | | | | | | |

| Name | V2out | Retol | 111 |
|---------------------------|----------|-------------------------|----------|
| Vapour Fraction | 0.0000 | 0.0000 | 1.0000 |
| Temperature [F] | 86.4137 | 360.3164 | 357.2290 |
| Pressure [psia] | 575.0000 | 875. <mark>00</mark> 00 | 75.4196 |
| Molar Flow [lbmole/hr] | 289.0000 | 84.5522 | 95.9164 |
| Comp Mole Frac (Hydrogen) | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Methane) | 0.000000 | 0.000000 | 0.000000 |
| Comp Mole Frac (Benzene) | 0.000000 | 0.001113 | 0.001126 |
| Comp Mole Frac (Toluene) | 1.000000 | 0.998491 | 0.998435 |
| Comp Mole Frac (BiPhenyl) | 0.000000 | 0.000396 | 0.000439 |

| Name | fuel | q1 | wk1 | wk2 | qc1 | qc2 | wk3 | qr3 |
|--------------------|-------------|------------|-------------|-------------|-------------|-------------|------------|-------------|
| Heat Flow [Btu/hr] | 5517949.756 | 7433657.42 | 1007381.919 | 13645.07811 | 614687.9938 | 13658547.23 | 29835.8334 | 1857622.929 |
| Name | wk4 | qb2 | wk5 | | 71 | | | |
| Heat Flow [Btu/hr] | 44208.62065 | 10268501 | 7755.245429 | | | | | |

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Equipment data and specifications

| | Stabilizer column | Product column | Recycle column |
|-------------------------------------|-------------------|------------------|---------------------|
| Number of theoretical | 6 | 27 | 7 |
| trays | | | |
| Feed tray | 3 | 15 | 5 |
| Diameter (ft) | 1 | 5.7 | 2.5 |
| Reboiler volume (ft ³) | 250 | 293 | 36 |
| Condenser volume (ft ³) | 7.5 | 316 | 46 |
| Reflux ratio | 1.57 | 3 | 0.32 |
| Specification 1 | Benzene fraction | Toluene fraction | Diphenyl fraction |
| | in overhead = | in distillate = | in distillate = |
| Specification 2 | 0.042 | 0.0003 | 0.00002 |
| | Methane fraction | Benzene fraction | Toluene fraction in |
| | in bottom $= 1$ | in bottom = | bottom = 0.00026 |
| | ppm | 0.0006 | |

Table A.3 Column specifications

Table A.4 Equipment data

| Peactor | Length [ft] | 57 |
|-------------|--------------------|---------|
| Reactor | Diameter [ft] | 9.53 |
| Furnace | Tube volume | 300 |
| Separator | Volume [ft3] | 80 |
| КПОК | Shell volume [ft3] | 500 |
| FEHE (E100) | Tube volume [ft3] | 500 |
| าลงกรถ | UA [Btu/F-hr] | 8.18E+5 |
| | Shell volume [ft3] | 500 |
| FEHE (E1) | Tube volume [ft3] | 500 |
| | UA [Btu/F-hr] | 2.11E+5 |
| | | |

 Table A.4 Equipment data (cont.)

| FEHE (E2) | Shell volume [ft3] | 500 |
|-----------|--------------------|------------|
| | Tube volume [ft3] | 500 |
| | UA [Btu/F-hr] | 4.1E+5 |
| FEHE (E3) | Shell volume [ft3] | 500 |
| | Tube volume [ft3] | 500 |
| | UA [Btu/F-hr] | 56290.3608 |
| FEHE (E5) | Shell volume [ft3] | 100 |
| | Tube volume [ft3] | 100 |
| | UA [Btu/F-hr] | 2.98E+4 |
| | | |



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APPENDIX B

Parameter Tuning of Control Structures

B.1 Tuning Controllers

Notice throughout this work use PI controllers. In theory, control performance can be improved by the use of derivative action. But in practice the use of derivative has some significant drawbacks:

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

B.1.1 Tuning Flow, Level and Pressure Loops

The dynamics of flow measurement are fast. The time constants for moving control valves are small. Therefore, the controller can be tuned with a small integral or reset time constant τ_I . A value of $\tau_I = 0.3$ minutes work 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.

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

Most pressure controllers can be fairly easily tuned. The process time constant is estimated by dividing the gas volume of the system by the volumetric flowrate of gas flowing through the system. Setting the integral time equal to about 2 to 4 times the process time constant and using a reasonable controller gain usually gives satisfactory pressure control. Typical pressure controller tuning constants for columns and tanks are $K_c = 2$ and $\tau_1 = 10$ minutes.

B.1.2 Relay-Feedback Testing

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

The method consists of merely inserting an on-off relay in the feedback loop. The only parameter that must be specified is the height of the relay h. This height is typically 5 to 10% of the controller-output scale. The loop starts to oscillate around the setpoint, with the controller output switching every time the process-variable (*PV*) signal crosses the setpoint. Figure shows the PV and OP signals from a typical relay-feedback test.

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

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

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

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

All these features make relay-feedback testing a useful identification tool.

Knowing the ultimate gain K_u and ultimate period P_u permits us to calculate controller setting. There are several methods that require only these two parameters. The Ziegler-Nichols tuning equations for a PI controller are

$$K_c = \frac{K_u}{2.2}$$
$$\tau_I = \frac{P_u}{1.2}$$

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

$$K_c = \frac{K_u}{3.2}$$
$$\tau_I = 2.2P_u$$

| Controller | Process Variable | Output | Control Action | Set point | Kc | τi (min) |
|------------|-----------------------------|--------------------------------|-------------------|------------------|-------|----------|
| PIC_Sep | separator pressure | fresh feed hydrogen valve (V1) | reverse | 476.8 psia | 2 | 10 |
| FIC_Tottol | total toluene flow rate | fresh feed toluene valve (V2) | reverse | 373.67 lbmole/hr | 0.2 | 0.1 |
| TIC_Reacin | reactor inlet temperature | furnace duty (fuel) | reverse | 1150 oF | 0.111 | 0.323 |
| TIC_Sep | separator temperature | cooler duty (q1) | direct | 113 oF | 0.129 | 0.776 |
| TIC_Quench | quenched temperature | quench valve (V3) | direct | 1150 oF | 0.383 | 0.148 |
| XIC_Gasre | methane purged fraction | purge valve (V4) | direct | 0.5875 | 0.342 | 11.7 |
| LIC_Sep | separator liquid level | column C1 feed valve (V5) | direct | 50% | 2 | - |
| LIC_Con1 | column C1 reflux drum level | column C1 condenser duty (qc1) | reverse | 50% | 1 | - |
| TIC_Col1 | column C1 tray temperature | column C1 reboiler duty (qr1) | reverse | 308.94 oF | 0.5 | 2.66 |
| PIC_Con1 | column C1 pressure | column C1 gas valve (V6) | direct | 150 psia | 1 | 10 |
| LIC_Re1 | column C1 base level | column C2 feed valve (V7) | direct | 50% | 2 | - |
| LIC-Con2 | column C2 reflux drum level | column C2 product valve (V8) | direct | 50% | 2 | - |
| LIC_Re2 | column C2 base level | column C3 feed valve (V9) | direct | 50% | 2 | - |
| TIC_Col2 | column C2 tray temperature | column C2 reboiler duty (qr2) | reverse | 248.5 oF | 15 | 0.803 |
| PIC_Con2 | column C2 pressure | column C2 condenser duty (qc2) | direct | 30 psia | 2 | 10 |
| LIC_Con3 | column C3 reflux drum level | toluene recycle valve (V11) | direct | 50% | 2 | - |
| LIC_Re3 | column C3 base level | column C3 reboiler duty (qr3) | direct | 50% | 3 | - |
| TIC_Col3 | output of AVG | column C3 bottom valve (V10) | direct | 412.6 oF | 1.7 | 24.5 |
| PIC_Con3 | column C3 pressure | column C3 condenser duty (qc3) | direct | 30 psia | 2 | 10 |

Table B.1 Parameter tuning of HDA process (reference, CS1)

| Controller | Process Variable | Output | | | Set point | Kc | τ_i (min) |
|------------|-----------------------------|--------------------------------|---------------------------------------|---------|------------------|----------|----------------|
| PIC_Sep | separator pressure | fresh feed hydrogen valve (V1) | | | 476.8 psia | 2 | 10 |
| FIC_Tottol | total toluene flow rate | t | fresh feed toluene valve (V2) | reverse | 373.67 lbmole/hr | 0.2 | 0.1 |
| TIC_Reacin | reactor inlet temperature | | furnace duty (fuel) | reverse | 1150 °F | 9.17E-02 | 0.374 |
| TIC_Sep | separator temperature | | cooler duty (q1) | direct | 113 °F | 0.121 | 0.783 |
| TIC_Quench | quenched temperature | | quench valve (V3) | direct | 1150 °F | 0.361 | 0.21 |
| XIC_Gasre | methane purged fraction | | purge valve (V4) | direct | 0.5875 | 0.328 | 17 |
| LIC_Sep | separator liquid level | | column C1 feed valve (V5) | direct | 50% | 2 | - |
| LIC_Con1 | column C1 reflux drum level | со | lumn C1 condenser duty (qc1) | reverse | 50% | 1 | - |
| FIC_Reb1 | column C1boilup flowrate | с | column C1 boilup valve (V13) | | 398.13 lbmole/hr | 3.92E-02 | 9.00E-03 |
| TIC_Col1 | column C1 tray temperature | CS2 | exchanger E3 hypart valve (V-hypart1) | direct | 309.04 °F | 6 | 2.91 |
| | | CS6 | uncer | 507.011 | 2.5 | 2.91 | |
| | | CS3, 4 | auxiliary duty (aux) | reverse | 309.04 °F | 5 | 3.25 |
| PIC_Con1 | column C1 pressure | | column C1 gas valve (V6) | direct | 150 psia | 1 | 10 |
| LIC_Tank1 | column C1 tank level | | column C2 feed valve (V7) | direct | 50% | 2 | - |
| LIC-Con2 | column C2 reflux drum level | CS2, 3, 4, 6 | column C2 product valve (V8) | direct | 50% | 2 | - |
| | | CS5 | FIC_Tottol | reverse | 50% | 1 | - |
| FIC_Reb2 | column C2boilup flowrate | c | olumn C2 boilup valve (V15) | reverse | 846.88 lbmole/hr | 1.56E-02 | 9.11E-03 |
| LIC_Tank2 | column C2 tank level | | column C3 feed valve (V9) | direct | 50% | 2 | _ |
| | 9 | | | | | | |

Table B.2 Parameter tuning of HDA process (CS2-6)

| Controller | Process Variable | | Output | Control Action | Set point | Kc | τ_i (min) |
|------------|----------------------------|--------------------------------|----------------------------------|-------------------|------------------|------|----------------|
| TIC_Col2 | column C2 tray temperature | heater E4 duty (qb2) | | | 248.62 °F | 25 | 0.96 |
| PIC_Con2 | column C2 pressure | column C2 condenser duty (qc2) | | | 30 psia | 2 | 10 |
| LIC_Tank3 | column C3 tank level | | toluene recycle valve (V11) | direct | 50% | 2 | - |
| LIC_Re3 | column C3 base level | CS2, 3 | column C3 reboiler duty (qr3) | direct | 50% | 3 | - |
| | | CS4 | column C3 bottom valve (V10) | direct | 50% | 2 | - |
| TIC_Col3 | output of AVG | CS2, 3 | column C3 bottom valve (V10) | direct | 515.5 °F | 1.5 | 24.5 |
| | | CS4 | column C3 reboiler duty (qr3) | reverse | 515.5 °F | 7 | 2.83 |
| PIC_Col3 | tank column C3 pressure | exe | changer E3 bypart valve (VLV100) | direct | 72.52 psia | 5 | 10 |
| FIC_100 | C2 production rate | | column C2 product valve (V8) | reverse | 270.72 lbmole/hr | 0.17 | 1.76E-02 |
| IC_100 | logic output | | auxilairy duty (aux) | direct | 0 | 0.1 | 5 |

Table B.2 Parameter tuning of HDA process (CS2-6) (cont.)



APPENDIX C

Dynamic Responses

C.1 Changing in Reactor Inlet Temperature

C.1.1 Control structure 1 (reference)

10 °F increase



Figure C.1 dynamic responses of CS1 to 10 °F increase in reactor inlet temperature at time equal 10 minutes.

5 °F decrease



Figure C.2 dynamic responses of CS1 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes



Figure C.2 dynamic responses of CS1 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes (cont.).

C.1.2Control structure 2



Figure C.3 dynamic responses of CS2 to 5 ^oF increase in reactor inlet temperature at time equal 10 minutes.



Figure C.3 dynamic responses of CS2 to 5 °F increase in reactor inlet temperature at time equal 10 minutes (cont.).

5 °F decrease



Figure C.4 dynamic responses of CS2 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes.

C.1.3 Control structure 3

10 °F increase



Figure C.5 dynamic responses of CS3 to 10 °F increase in reactor inlet temperature at time equal 10 minutes (cont.).

5 °F decrease



Figure C.6 dynamic responses of CS3 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes.



Figure C.6 dynamic responses of CS3 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes (cont.).

C.1.4 Control structure 4



Figure C.7 dynamic responses of CS4 to 10 °F increase in reactor inlet temperature at time equal 10 minutes.

5 °F decrease



Figure C.8 dynamic responses of CS4 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes.

C.1.5 Control structure 5



Figure C.9 dynamic responses of CS5 to 10 °F increase in reactor inlet temperature at time equal 10 minutes.



Figure C.9 dynamic responses of CS5 to 10 °F increase in reactor inlet temperature at time equal 10 minutes (cont.).





Figure C.10 dynamic responses of CS5 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes.

C.1.6 Control structure 6



Figure C.11 dynamic responses of CS6 to 10 °F increase in reactor inlet temperature at time equal 10 minutes.



Figure C.12 dynamic responses of CS6 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes.



Figure C.12 dynamic responses of CS6 to 5 °F decrease in reactor inlet temperature at time equal 10 minutes (cont.).

C.2 Changing in Total Toluene Flowrate

C.2.1 Control structure 1 (reference)

15 % increase



Figure C.13 dynamic responses of CS1 to 15 % increase in total toluene flowrate at time equal 10 minutes (cont.).

15 % decrease



Figure C.14 dynamic responses of CS1 to 15 % decrease in total toluene flowrate at time equal 10 minutes.

C.2.2 Control structure 2

10 % increase



Figure C.15 dynamic responses of CS2 to 10 % increase in total toluene flowrate at time equal 10 minutes.



Figure C.15 dynamic responses of CS2 to 10 % increase in total toluene flowrate at time equal 10 minutes (cont.).



10 % decrease

Figure C.16 dynamic responses of CS2 to 10 % decrease in total toluene flowrate at time equal 10 minutes.

C.2.3 Control structure 3

15 % increase



Figure C.17 dynamic responses of CS3 to 15 % increase in total toluene flowrate at time equal 10 minutes.

15 % decrease



Figure C.18 dynamic responses of CS3 to 15 % decrease in total toluene flowrate at time equal 10 minutes



Figure C.18 dynamic responses of CS3 to 15 % decrease in total toluene flowrate at time equal 10 minutes (cont.).

C.2.4 Control structure 4

15 % increase



Figure C.19 dynamic responses of CS4 to 15 % increase in total toluene flowrate at time equal 10 minutes.

15 % decrease



Figure C.20 dynamic responses of CS4 to 15 % decrease in total toluene flowrate at time equal 10 minutes.

C.2.6 Control structure 6

15 % increase



Figure C.21 dynamic responses of CS6 to 15 % increase in total toluene flowrate at time equal 10 minutes.



Figure C.21 dynamic responses of CS6 to 15 % increase in total toluene flowrate at time equal 10 minutes (cont.).



15 % decrease

Figure C.22 dynamic responses of CS6 to 15 % decrease in total toluene flowrate at time equal 10 minutes.
C.3 Changing in Production Flowrate

C.3.1 Control structure 5

25 % increase



Figure C.23 dynamic responses of CS6 to 25 % increase in production flowrate at time equal 10 minutes.



Figure C.24 dynamic responses of CS6 to 25 % decrease in production flowrate at time equal 10 minutes.



Figure C.24 dynamic responses of CS6 to 25 % decrease in production flowrate at time equal 10 minutes (cont.).

C.4 Decrease reactor inlet temperature 10 °F

Due to reference data simulation is not designed to handle disturbance in decrease reactor inlet temperature. So the modification is made by increase size of valve of recycle column distillate.



Figure C.25 dynamic responses of CS6 to 10 °F decrease in reactor inlet temperature at time equal 10 minutes.



Figure C.25 dynamic responses of CS6 to 10 °F decrease in reactor inlet temperature at time equal 10 minutes (cont.).

| | Decrease Reactor Inlet Temperature 10°F | | | | | | |
|--------------------|---|----------|-------------|----------|----------|-----------|--|
| | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | |
| f_tottol | 24.6482 | - | 25.0562 | 24.7494 | *20.401 | 25.1539 | |
| t_col1 | *47.1492 | | 67.8173 | 67.5217 | 95.8613 | 55.6931 | |
| t_col2 | <mark>*0.1415</mark> | | 0.2648 | 0.2599 | 0.2339 | 0.2258 | |
| t_col3 | 308.5261 | 1-56 | 358.7453 | *5.3201 | 6.4412 | 5.4764 | |
| t_quench | *10.3567 | //- | 11.81 | 11.7883 | 15.2792 | 12.8533 | |
| t_reacin | *12.5067 | 1 5-16 | 14.325 | 14.2558 | 16.565 | 15.8783 | |
| t_sep | 26.6429 | - 160 | 17.3207 | *17.2808 | 28.0687 | 22.1431 | |
| x_gasre | *1.0553 | 3 500 | 1.5417 | 1.5414 | 2.1431 | 1.5836 | |
| total ⁺ | 122.5005 | TAIO | *138.1357 | 137.3973 | 178.5522 | 133.5311 | |
| total | 431.0266 | <u></u> | 496.881 | 142.7174 | 184.9934 | *139.0075 | |
| f_ondemand | | Massie P | P. C. C. C. | | 0.0744 | | |

Table C.1 Integral absolute error of the six plantwide control structures.

Increase reactor inlet temperature 10 °F

Table C.2 Dynamic responses of CS6 original and modify CS6 to 10 °F increase in reactor inlet temperature at time equal 10 minutes

| () | CS6 | CS6* |
|--------------------|---------|----------|
| f_tottol | 22.0922 | 21.929 |
| t_col1 | 41.5913 | 41.6203 |
| t_col2 | 0.1195 | 0.115 |
| t_col3 | 4.5653 | 4.5579 |
| t_quench | 9.7017 | 9.6908 |
| t_reacin | 13.9633 | 13.9542 |
| t_sep | 22.6201 | 22.4918 |
| x_gasre | 1.3556 | 1.3541 |
| total ⁺ | 111.444 | 111.1552 |
| total | 116.009 | 115.7131 |

* = modify CS6

APPENDIX D

Kietawarin Control Structure

Kietawarin (2002) designed 3 control structures to reduce the effects of disturbances in order to achieve a desired production rate. The first control scheme (S1) measured toluene flow rate in the process and adjusted the fresh toluene feed rate accordingly. The second (S2) was modified from the first scheme by adding a cooling unit to control the outlet temperature of the reactor. In the third (S3) scheme, a ratio control was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process.



Figure D.1 First control scheme of Kietawarin (S1).



Figure D.2 Second control scheme of Kietawarin (S2).



Figure D.3 Third control scheme of Kietawarin (S3).

Result of her study showed performance of control structure S2 was the best (minimum total IAE) because of utilize auxiliary unit instead of quench can reduce effect of disturbance from recycle stream.

To guarantee this work, all of Kietawarin's control structures are applied to my control structures. Result from disturbance test below shows this work get the same result as hers control structures.

Applications of S2 to HDA alternative 3 are showed in figure below.

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Figure D.4 Application of S2 of Kietawarin to CS2



Figure D.5 Application of S2 of Kietawarin to CS3



Figure D.6 Application of S2 of Kietawarin to CS4



Figure D.7 Application of S2 of Kietawarin to CS5



Figure D.8 Application of S2 of Kietawarin to CS6



Figure D.9 Application of S3 of Kietawarin to CS2



Figure D.10 Application of S3 of Kietawarin to CS3



Figure D.11 Application of S3 of Kietawarin to CS4



Figure D.12 Application of S3 of Kietawarin to CS5



Figure D.13 Application of S3 of Kietawarin to CS6



The dynamic responses of decrease 10% total toluene flowrate step test are as follow:

Figure D.14 Dynamic responses of CS1 with S1 to decrease 10% total toluene flowrate step test

CS1 with S2



Figure D.15 Dynamic responses of CS1 with S2 to decrease 10% total toluene flowrate step test.



Figure D.15 Dynamic responses of CS1 with S2 to decrease 10% total toluene flowrate step test (cont.).

CS1 with S3



Figure D.16 Dynamic responses of CS1 with S3 to decrease 10% total toluene flowrate step test.

The dynamic responses of decrease 5°F reactor inlet temperature step test are as follow:





Figure D.17 Dynamic responses of CS1 with S1 to decrease 5°F reactor inlet temperature step test.



Figure D.18 Dynamic responses of CS1 with S2 to decrease 5°F reactor inlet temperature step test.



Figure D.17 Dynamic responses of CS1 with S2 to decrease 5°F reactor inlet temperature step test (cont.).

CS1 with S3



Figure D.17 Dynamic responses of CS1 with S3 to decrease 5°F reactor inlet temperature step test.



Figure D.17 Dynamic responses of CS1 with S3 to decrease 5°F reactor inlet temperature step test (cont.).

Integral absolute error of dynamic responses of design control structures which are applied with Kietawarin's control structures to decrease 10% total toluene and decrease 5°F in reactor inlet temperature step tests are below:

Table D.1 IAE of design control structures when decrease total toluene flowrate.

| | Kietawarin's control structure 1 | | | | | | | |
|----------|----------------------------------|---------|---------|----------|---------|--|--|--|
| | CS1 | CS2 | CS3 | CS4 | CS6 | | | |
| f_tottol | 32.5632 | 32.4208 | 33.4078 | 33.2332 | 32.7979 | | | |
| t_col1 | 63.3114 | 111.751 | 76.3328 | 74.9459 | 83.8908 | | | |
| t_col2 | 0.102 | 0.1326 | 0.1536 | 0.1627 | 0.1357 | | | |
| t_col3 | 233.516 | 245.724 | 252.792 | 1.5478 | 1.5442 | | | |
| t_quench | 6.9958 | 8.19 | 7.2383 | 7.2283 | 7.8375 | | | |
| t_reacin | 11.4442 | 14.6075 | 12.6792 | 12.6758 | 14.7333 | | | |
| t_sep | 50.5375 | 35.1886 | 33.9293 | 33.8712 | 36.3393 | | | |
| x_gasre | 1.1253 | 1.6839 | 1.6931 | 1.693 | 1.6735 | | | |
| total | 399.596 | 449.698 | 418.226 | *165.358 | 178.952 | | | |

| | Kietawarin's control structure 2 | | | | | | |
|----------|----------------------------------|---------|---------|---------|---------|--|--|
| <u>র</u> | CS1 | CS2 | CS3 | CS4 | CS6 | | |
| f_tottol | 33.4313 | 33.1316 | 34.0017 | 33.7968 | 33.274 | | |
| t_col1 | 56.6742 | 168.125 | 75.2488 | 71.0568 | 79.4836 | | |
| t_col2 | 0.1009 | 0.1687 | 0.1514 | 0.1451 | 0.1456 | | |
| t_col3 | 230.126 | 234.141 | 244.182 | 1.4867 | 1.5292 | | |
| t_quench | 9.6833 | 6.3792 | 6.0875 | 6.0883 | 5.9583 | | |
| t_reacin | 16.115 | 14.4325 | 13.5792 | 13.4967 | 15.0767 | | |
| t_sep | 28.7128 | 21.6172 | 24.0072 | 23.8918 | 22.5537 | | |
| x_gasre | 1.0843 | 1.5845 | 1.5879 | 1.5879 | 1.5675 | | |
| total | 375.927 | 479.58 | 398.846 | *151.55 | 159.589 | | |

| | Kietawarin's control structure 3 | | | | | | | |
|----------|----------------------------------|------|---------|----------|---------|--|--|--|
| | CS1 | CS2 | CS3 | CS4 | CS6 | | | |
| f_tottol | 66.5975 | - | 72.4926 | 72.4918 | 69.4545 | | | |
| t_col1 | 56.5042 | - | 90.7374 | 89.7309 | 119.739 | | | |
| t_col2 | 0.1043 | - | 0.1749 | 0.1761 | 0.1793 | | | |
| t_col3 | 285.21 | | 309.395 | 1.7854 | 1.7532 | | | |
| t_quench | 9.7117 | -177 | 5.9342 | 5.9383 | 5.965 | | | |
| t_reacin | 17.6925 | - | 19.4758 | 19.4667 | 16.9158 | | | |
| t_sep | 30.6412 | | 24.6455 | 24.6492 | 26.7949 | | | |
| x_gasre | 1.7038 | | 1.91 | 1.9099 | 2.0758 | | | |
| total | 468.166 | 11- | 524.765 | *216.148 | 242.878 | | | |

 Table D.1 IAE of design control structures when decrease total toluene flowrate (cont.).

 Table D.2 IAE of design control structures when decrease reactor inlet temperature.

| | | Kietawarin's control structure 1 | | | | | | |
|----------|----------|----------------------------------|----------|---------|----------|---------|--|--|
| | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | | |
| f_tottol | 12.0154 | 12.6961 | 12.1178 | 12.092 | 10.6842 | 11.7472 | | |
| t_col1 | 21.3976 | 25.9986 | 32.977 | 33.3353 | 57.2377 | 28.2545 | | |
| t_col2 | 0.0771 | 0.1663 | 0.1833 | 0.1878 | 0.1682 | 0.1608 | | |
| t_col3 | 168.2273 | 197.8495 | 195.2698 | 2.5865 | 3.0717 | 2.6952 | | |
| t_quench | 5.0433 | 6.635 | 5.5808 | 5.5817 | 7.4933 | 6.1 | | |
| t_reacin | 6.1458 | 8.7333 | 7.06 | 7.0517 | 7.8517 | 7.8242 | | |
| t_sep | 13.2486 | 11.4269 | 8.5515 | 8.5528 | 13.7829 | 11.3132 | | |
| x_gasre | 0.5142 | 0.783 | 0.745 | 0.7449 | 1.0455 | 0.7853 | | |
| total | 226.6693 | 264.2887 | 262.4852 | 70.1327 | 101.3352 | 68.8804 | | |

| | 0. | | | | | | |
|----------|----------------------------------|----------|----------|---------|---------|---------|--|
| | Kietawarin's control structure 2 | | | | | | |
| 6 | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | |
| f_tottol | 13.1323 | 12.4414 | 12.5295 | 12.5065 | 11.5853 | 12.4662 | |
| t_col1 | 6.0022 | 8.3372 | 27.9997 | 25.3223 | 33.3554 | 9.5175 | |
| t_col2 | 0.0814 | 0.2015 | 0.18 | 0.1842 | 0.1612 | 0.1697 | |
| t_col3 | 164.0398 | 184.018 | 186.1523 | 2.5417 | 3.0072 | 2.5537 | |
| t_quench | 6.785 | 4.7917 | 4.55 | 4.5508 | 5.6117 | 4.5842 | |
| t_reacin | 8.7033 | 7.6158 | 7.2675 | 7.2683 | 9.5342 | 7.4858 | |
| t_sep | 6.353 | 5.2678 | 5.5962 | 5.5322 | 7.6298 | 5.1691 | |
| x_gasre | 0.4892 | 0.7051 | 0.6874 | 0.6873 | 0.9593 | 0.7027 | |
| total | 205.5862 | 223.3785 | 244.9626 | 58.5933 | 71.8441 | 42.6489 | |

| | Kietawarin's control structure 3 | | | | | | |
|----------|----------------------------------|----------|----------|---------|----------|---------|--|
| | CS1 | CS2 | CS3 | CS4 | CS5 | CS6 | |
| f_tottol | 19.902 | 20.7123 | 22.1749 | 22.1988 | 58.596 | 20.6953 | |
| t_col1 | 9.5785 | 18.2892 | 29.9684 | 26.0839 | 45.6693 | 18.0579 | |
| t_col2 | 0.0831 | 0.1855 | 0.1738 | 0.1674 | 0.1424 | 0.1593 | |
| t_col3 | 152.9937 | 168.9802 | 170.37 | 2.4711 | 2.4709 | 2.5373 | |
| t_quench | 7.065 | 3.865 | 4.9983 | 4.6133 | 5.7592 | 4.5408 | |
| t_reacin | 9.7258 | 8.5558 | 9.9567 | 10.0692 | 14.9033 | 8.8383 | |
| t_sep | 7.399 | 7.6887 | 6.7936 | 6.746 | 9.7001 | 7.3155 | |
| x_gasre | 1.5098 | 1.3234 | 1.4361 | 1.4361 | 1.5662 | 1.2871 | |
| total | 208.2569 | 229.6001 | 245.8718 | 73.7858 | 138.8074 | 63.4315 | |

Table D.2 IAE of design control structures when decrease reactor inlet temperature (cont.).

Note * = Minimum IAE value

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