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PLANTWIDE CONTROL STRUCTURE DESIGN FOR AMMONIA PRODUCTION PROCESS

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A Thesis Submitted in Partial Fulfillment of the Requirements
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บุญเสริม โสภณอุดมทรัพย์ : การออกแบบโครงสร้างการควบคุมแบบแพลนไวท์สำหรับกระบวนการผลิตแอมโมเนีย.(PLANTWIDE CONTROL STRUCTURE DESIGN FOR AMMONIA PRODUCTION PROCESS) อ. ที่ปรึกษาวิทยานิพนธ์หลัก: ผศ.ดร.มนตรี วงศ์ศรี, 73 หน้า.

งานวิจัยนี้เสนอการประยุกต์ใช้การออกแบบโครงสร้างการควบคุมแบบแพลนไวท์ของวงศ์ศรี 2012 สำหรับกระบวนการผลิตแอมโมเนีย ซึ่งโครงสร้างการควบคุมใหม่ 2 โครงสร้างที่ได้จากการออกแบบโดยวิธีของวงศ์ศรีจะถูกนำมาประเมินผลและเปรียบเทียบกับโครงสร้างการควบคุมที่ออกแบบโดย Skogestad ซึ่งในการประเมินผลจะใช้ตัวแปรรบกวนคือ การเปลี่ยนแปลงของอัตราการไหลของสารขาเข้า การเปลี่ยนแปลงของอุณหภูมิของสารขาเข้า และการเปลี่ยนแปลงของความเข้มข้นของมีเทนในสายขาเข้า ผลการวิจัยพบว่าโครงสร้างการควบคุมที่ 2 ให้ประสิทธิภาพการควบคุมที่ดีสำหรับการทดสอบการเปลี่ยนแปลงของตัวแปรรบกวนอัตราการไหลของสารขาเข้าและอุณหภูมิของสารขาเข้า และสำหรับการเปลี่ยนแปลงความเข้มข้นของมีเทนในสายขาเข้า ทุกโครงสร้างการควบคุมให้ผลการควบคุมที่ใกล้เคียงกัน

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This thesis presents the application of the plantwide control design procedure of Wongsri (2012) to the ammonia production process. Two new control structures obtained are evaluated and compared with the control structure of Skogestad (2008).The disturbances used in the evaluation are gas feed flowrate, feed temperature, and methane composition in feed changes. The new control structure, CS2, resulted in good dynamic performance for the feed flowrate and feed temperature changes. For methane composition in feed change, all control structures give comparable good performances.

Department : Chemical Engineering Student's Signature ....
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CONTENTS

PAGE

CHAPTER

CHAPTER PAGE

CHAPTER PAGE

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

INTRODUCTION

1.1 Importance and Reasons for Research

Presently, most industries are developed of more efficient production process, the development has to use the energy integration and recycle stream in the process. For the control of energy integration and recycle stream, the control section technique can be carried out difficultly since feedbacks of material and energy affect to upstream and downstream units. Therefore, the strategies of plantwide control are used to control the production process, achieving the objectives of design and safety.

Plantwide control design research has been active in the process control communities for decades. There have been many published contribution on plantwide control design. The design approaches can be arbitrarily grouped into two main schools, heuristics and optimization. The pioneer in the heuristic school is Luyben *et al*. (1998); he presents the nine-step design procedure which makes use of chemical engineering and process knowledge and experiences. The followers are Konda and co-worker (2005); they presented the design procedure that used heuristic to design the control structures and evaluated them using a dynamic simulator. Some researchers used optimization technique to find the plantwide control structures. Skogestad (2004) who used self-optimizing control to find a set of self-optimizing variable ; Cao and Saha (2005) who used “branch and bound” method for control structure screening; and Kookos and Perkins (2001) who used mixed-integer nonlinear programming in a mixed approach to minimize overall sensitivity of the control system to disturbances. Morari *et al*. (1980) presented a unified formulation for the problem of synthesizing control structures for chemical processes based on a hierarchical partition of the process system and feasibility analysis of the control structures. Each methodology has its own advantages and drawbacks. For example, rigorous optimization methodologies can be computationally expensive and subject to model accuracies, while heuristics-based methodologies normally require experience and insight.

In this research, the plantwide control structure for the ammonia production process is designed by Wongsri Procedure (2012). It is compared with the control structure that is proposed by Skogestad. Both of control structures are evaluated by Integral Absolute Error (IAE) and carried out using HYSYS dynamic simulator (Version 7.0). The simulation result indicates that the control structure designed of Wongsri (2012) in a good dynamic performance is achieved. Moreover, it has better performance comparing with Skogestad model.

1.2 Research Objectives

To design and evaluate the plantwide control structures of ammonia production process by using the procedure of Wongsri (2012).

1.3 Scopes of Research

1. The dynamic simulation of ammonia production process is performed by using the Aspen Hysys simulator.
2. The detail of ammonia production process is obtained by Araújo and Skogestad (2008).
3. To design two new control structures of ammonia production process using Wongsri procedure (2012).

1.4 Contributions of Research

1. Simulated a flowsheet diagram of the ammonia production process in steady state and dynamic modules.

2. The new plantwide control structures of the ammonia production process are designed using Wongsri procedure (2012) and compared with the work given by Araújo and Skogestad (2008).
3. Evaluation of the new plantwide control structures design procedure.

1.5 Research Procedures

1. Study the data of plantwide control theory and the ammonia production process.
2. Simulation of the ammonia production process at steady state and dynamic modules via HYSYS dynamic simulator (Version 7.0).
3. Study of the new control structures design procedure.
4. Designing of the new plantwide structures using Wongsri procedure (2012).
5. Simulation and evaluation of the new plantwide control structures at dynamic and compare with the base case.
6. Analyzation of the design and simulation results
7. Conclusion of the research studied.

1.6 Research Framework

This thesis is divided into six chapters as followed:

Chapter I is an introduction of this research. This chapter consists of an importance and reason, objective, scopes, contributions and procedure of the research.

Chapter II Review the earlier worked carried out on plantwide control and control structure design.

Chapter III covers some background information of Luyben plantwide control theory and plantwide control structure design procedure of Wongsri, 2012.

Chapter IV describes the ammonia production process, steady state and dynamic simulation and the new control structures design procedure.

Chapter V describes the design of control structures, dynamic simulation results and the comparison of the control structure of Araújo and Skogestad (2008) to the new design control structures (Wongsri, 2012).

Chapter VI presents the conclusion of this research and gives out the recommendations for future work.

CHAPTER II

LITERATURE REVIEWS

This chapter presented the literature reviews of this process which illustrated the previous work on plantwide control procedure and control structure design.

2.1 Plantwide control

Luyben (1996) presented the number of parameters or variables that must be specified to complete the defined steady-state process, called design degree of freedom (DOF). DOF can be calculated by subtracting the number of equations from the number of the number of variables. For complex process DOF equal to the number of manipulated variables (the number of control valves in the process). The complexity of the phase equilibrium and the physical properties does not affect DOF.

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

Skogestad (2000) presented the method is related to finding a simple and robust way of implementing the economically optimal operating policy. The goal is to find a set of controlled variables which, when kept at constant setpoints, indirectly lead to near-optimal operation with acceptable loss. Since the economics are determined by the overall plant behavior, it is necessary to take a plantwide perspective. A systematic procedure for finding suitable controlled variables based on only steady-state information is presented. Important steps are degree of freedom analysis, definition of optimal operation (cost and constraints), and evaluation of the loss when the controlled variables are kept constant rather than optimally adjusted. A case study yields very interesting insights into the control and maximum throughput of distillation columns. The focus in this paper has not been on finding the optimal operation policy, but rather on how to implement it in a simple manner in the control system. The idea is to find a set of controlled variables *c* which, when kept at constant setpoints, indirectly lead to near-optimal operation (with acceptable loss). This is denoted “self-optimizing” control.

Skogestad (2004) proposed two main systematic procedures for control structure design of complete chemical plants (plantwide control); top-down analysis and bottom-up design. Top-down analysis is used to determine definition of operational objectives, manipulated variables and degrees of freedom, primary controlled variables and production rate. While, bottom-up design is used to identify regulatory control layer, supervisory control layer, optimization layer and validation. The studied also presented inventory and production rate control, decentralized versus multivariable control, loss in performance by bottom-up design and a definition of a “complexity number”

Suntisrikomol (2008) used “Fixture Point Theorem” to develop the Hydrodealkylation process (HDA) by Selected the suitable set of controlled variable. The theorem states that the most disturbed points must be controlled before other controlled variables. The manipulate variables were selected and paired controlled variables by maximum gain. The performance of design process was illustrated in the IAE values. The Result compared with 2 reference structures (Araújo *et al.*, 2006, Luyben, 1998) which the design control structure via Fixture Point Theorem give responded faster and more effective.

Detjareansri (2009) used Wongsri (2009) procedure for designed control structure and developed the alkylation process. The dynamic performance of the design control structures are evaluated and compared with Luyben (2002) by inserted two types of disturbances; material and thermal disturbances. The designed control structures has good performance and economic.

2.2 Control structure design

Konda, Rangaiah and Krishnaswamy (2005) presented a simple effective procedure to find control degree of freedom (CDOF). The key idea is to define ‘restraining number’ (i.e., the minimum number of flows that cannot be manipulated along with others in a unit, which is also an inherent characteristic of that unit) of a unit. The study show that the restraining number is equal to the number of independent and overall material balances with no associated inventory in that particular unit. The concept of restraining number is then used to find CDOF of not only simple units but also highly integrated processes.

B.V. Babu, Rakesh Angira (2005) presented the simulation and optimal design of an auto-thermal ammonia synthesis reactor. The main objective in the optimal design of an auto-thermal ammonia synthesis reactor is the estimation of optimal length of reactor for different top temperatures with the constraints of energy and mass balance of reaction and feed gas temperature and mass flow rate of nitrogen for ammonia production. The result ammonia synthesis reactor did not stable even at high top temperature of 800 K.

Dorneau, Bildea and Grievink (2007) proposed a new approach exploiting advantage of fundamental structure that fit in a chemical plant in the form of units or groups of units connected together via material and energy streams. The recommended procedure is to employ model reduction, then to link these reduced-order models. The procedure is flexible and accurate due to its algorithm and variation from one unit to another. The time for solving solution is drastically reduced. The performance of the approach is verified by means of a case study.

Antonio Araújo, Skogestad (2008) proposed the control structure design for complete chemical plants to the ammonia synthesis process. The studied also presented three modes of operation: (I) given feed rate, (IIa) maximum throughput, and (IIb) “optimized” throughput. Two control structures, one for Mode I and another for Mode IIb, are proposed. In Mode I, it is proposed to keep constant purge rate and compressor powers. There is no bottleneck in the process, and thus there is no Mode

IIa of operation. In Mode IIb, the compressors are at their maximum capacity and it is proposed to adjust the feed rate such that the inert concentration is constant. The final control structures result in good dynamic performance.

James J. Downs, Skogestad (2011) presented the concept of process control design based on a holistic, the variety of procedures and approaches to the design problem has illustrated the difficulty of a unified approach. Using examples, the need and advantages of using a systematic approach based on considering the plant economics are highlighted. The examples deal with disturbance rejection, throughput maximization and economic optimization of plants consisting of parallel units.

CHAPTER III

THEORY

The chemical processes consist of many unit operation are connected by material and energy recycle stream. The control section technique can be carried out difficultly. Therefore, strategies for plantwide control are used to control process for achieve design objective and safety. This chapter is present about of plantwide control fundamentals.

3.1 Integrated Processes

There are three fundamental basic of integrated processes:

(1) The effects of material recycle.
(2) The effects of energy integration.
(3) The need to account for chemical component inventories.

3.1.1 Material recycles

Material is recycled for six basic and important reasons.

1. Increase conversion: The conversion of reactants to products of chemical processes is limited by thermodynamic equilibrium constraints. Therefore the separation and recycle of reactants are essential for adjusting the economic process.

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. The simple little process discussed in Sec. 2.6 illustrates this for a binary system with one reaction (A→B). A reactor

followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

3. Improve yields: In reaction systems such as A→B→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 raise the temperature of the excess material in the stream flowing through the reactor.

5. Prevent side reactions: A large excess of one the reactant 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. There 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 thermodynamic efficiency of the process. This translates into a reduction in utility cost. For energy-intensive processes, the savings can be quite significant.

3.1.3 Chemical Component Inventories

We can characterize a plant’s chemical species into three types: reactants, products and inerts. A material balance for each of these components must be satisfied. This is typically not a problem for products and inerts. However, the real problem usually arises when 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 via reaction or leave as an impurity or purge. Because of their value, we want to minimize the loss of reactants exiting the process since this represents a yield penalty. So we prevent reactants form leaving. This means we must ensure that every mole of reactant fed to the process is consumed by the reactions.

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

Plants are not necessarily self-regulating in terms of reactants. We might expect that the reaction rate will increase as reactant composition increases. However, in system with several reactants (e.g., $A + B \rightarrow$ products), increasing one reactant composition will decrease the other reactant composition with an uncertain net effect on reaction rate.

3.2 Plantwide Control Problems

3.2.1 Units in Series

If process units are arranged in a purely series configuration, where the products of each unit feed downstream units and there is no recycle of material or energy, the plantwide control problem is greatly simplified. It is not had to worry about the issues discussed in the previous section and it can be simply configure the control scheme on each individual unit operation to handle load disturbances.

If production rate is set at the front end of the process, each unit will only see load disturbances coming from is upstream neighbor. If the plant is set up for “on-demand” production, changes in throughput will propagate back through the process. So any individual unit will see load disturbances coming from both its downstream neighbor (flowrate changes to achieve different throughputs) and its upstream neighbor (composition changes as the upstream units adjust to the load changes they see).

Figure 3.1 compares these two possible configurations for a simple plant. A fresh feed stream containing a mixture of chemical components A, B, and C is fed into a two-column distillation train. The relative volatilities are $\alpha_A > \alpha_B > \alpha_{C,}$ and the “direct” (or “light-out-first”) separation sequence is selected: A is taken out the top of the first column and B out the top of the second column.

Figure 3.1 (a) shows the situation where the fresh feed stream is flow-controlled into the process. The inventory loops (liquid levels) in each unit are controlled by manipulating flows leaving that unit. All disturbances propagate from unit to unit down the series configuration. The only disturbances that each unit sees are changes in its feed conditions.

Figure 3.1 (b) shows the on-demand situation where the flow rate of product C leaving the bottom of the second column is set by the requirements of a downstream unit.

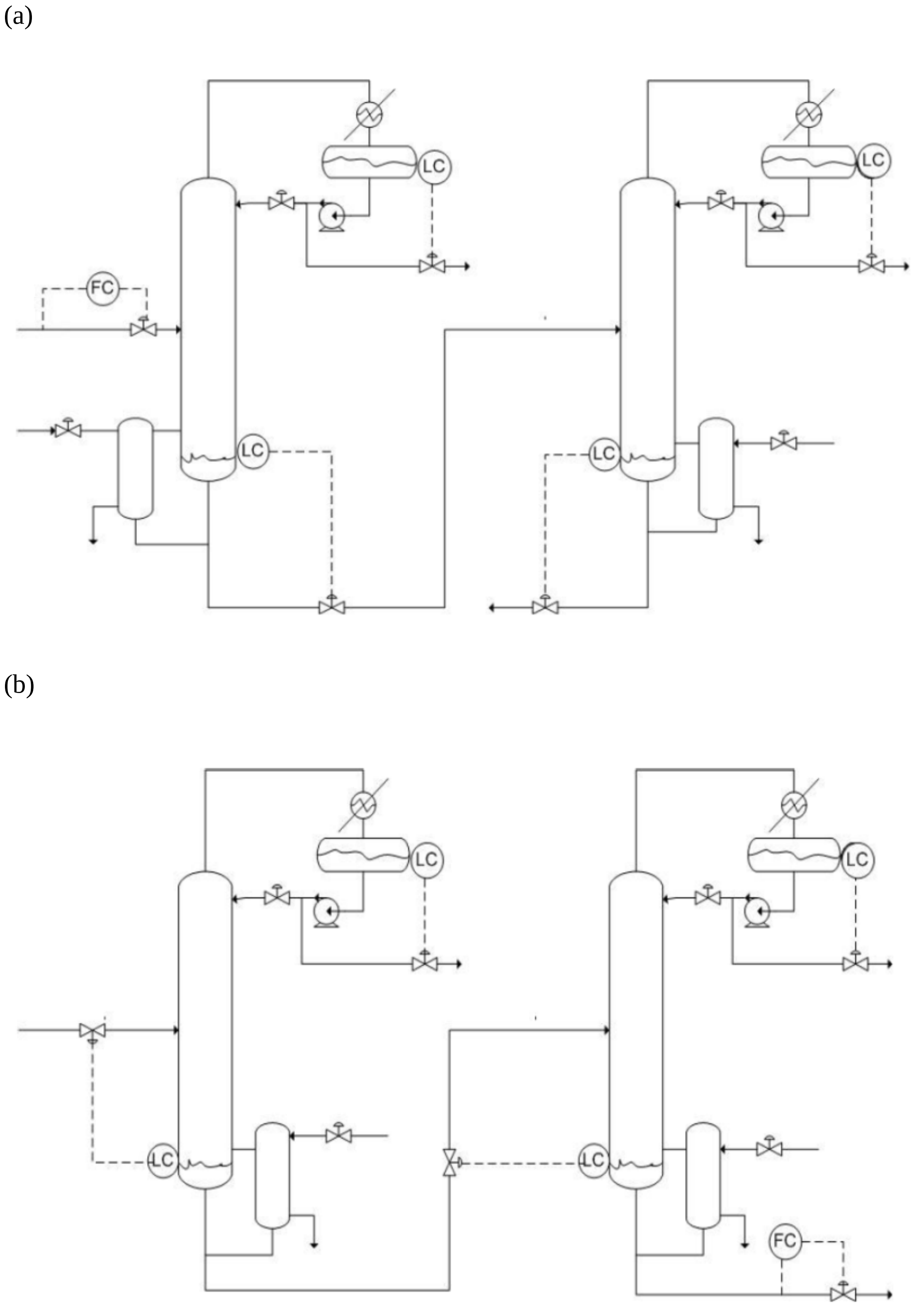


Figure 3.1 Unit in series. (a) Level controls in direction of flow; (b) level control in direction opposite flow.

Now some of the inventory loops (the base of both columns) are controlled by manipulating the feed into each column.

When the units are arranged in serried with no recycles, the plantwide control problem can be effectively broken up into the control of each individual unit operation. There is no recycle effect, no coupling, and no feedback of material from downstream to upstream units. The plant’s dynamic behavior is governed by the individual unit operations and the only path for disturbance propagation is linear along the process.

3.2.2 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex and its solution is not intuitively obvious. The presence of recycle streams profoundly alters the plant’s dynamic and steady-state behavior. To gain an understanding of these effects, some very simple recycle systems are looked. The insight they are obtained from these idealized, simplistic system can be extended to the complex flowsheet of typical chemical processes. First the groundwork must be laid and had some feel for the complexities and phenomena that recycle streams produce in a plant.

There are two basic effects of recycle:

(1) 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 individual units.

(2) Recycle leads to the “snowball” effect. This has two manifestations, one steady state and one dynamic. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flow rates. These disturbances can lead to even larger dynamic changes in flows, which propagate around the recycle loop. Both effects have implications for the inventory control of components.

3.2.3 Snowball Effects

Another interesting observation that has been made about recycle systems is their tendency to exhibit large variations in the magnitude of the recycle flows. Plant operators report extended periods of operation when very small recycle flows occur. It is often difficult to turn the equipment down to such low flow rates. Then, during other periods when feed conditions are not very different, recycle flow rates increase drastically, usually over a considerable period of time. Often the equipment cannot handle such a large load.

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

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

3.3 Basic Concepts of Plantwide Control

3.3.1. Buckley Basics

Page Buckley (1964), a true pioneer with DuPont in the field of process control, was the first to suggest the idea of separating the plantwide control problem into two parts: material balance control and product quality control. He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loops is established, using the flow rates of the liquid and gas process streams. No controller tuning or inventory sizing is done at this step. The idea is to establish the inventory control system by setting up this “hydraulic” control structure as the first step.

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

Then the inventory loops are revisited. The liquid holdups in surge volumes are calculated so that the time constants of the liquid level loops (using proportional-only controllers) are a factor of 10 large than the product-quality time constants. This separation in time constants permits independent tuning of the material-balance loops and the product-quality loops. Note that most level controllers should be proportional-only (P) to achieve flow smoothing.

3.3.2 Douglas doctrines

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Although he primarily considers the steady-state aspects of process design, he has developed several useful concepts that have control structure implications. He 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 the two douglas doctrines:

1. Minimize losses of reactants and products.
2. Maximize flowrate through gas recycle system.

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

3.3.3 Downs drill

Jim Downs (1992) of Eastman Chemical Company has insightfully 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. The concepts of overall component balances go back to our first course in chemical engineering, where we learned how to apply mass and energy balances to any system, microscopic or macroscopic. We did these balances for individual unit operations, for sections of a plant, and for entire processes.

But somehow these basics are often forgotten or overlooked in the complex and intricate project required to develop a steady-state design for a large chemical plant and specify its control structure. Often the design job is broken up into pieces. One person will design the reactor and its control system and someone else will design the separation section and is control system. The task sometimes falls through the cracks to ensure that these two sections operate effectively when coupled together. Thus it is important that we perform the Downs drill.

We must ensure that all components (reactants product, and inerts) have a way to leave or be consumed within the process. The consideration of inerts is seldom overlooked. Heavy inerts can leave the system in the bottoms product from a distillation column. Light inerts can be purged form a gas recycle stream or form a partial condenser on a column. Intermediate inerts must also be removed in some way, for example in sidestream purges or separate distillation columns.

Most of the problems occur in the consideration of reactants, particularly when several chemical species are involved. All of the reactants fed into the system must either be consumed via reaction or leave the plant as impurities in the exiting streams. Since 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. This is due to the fact that we prevent reactants from leaving the process though composition controls in the separation section. Any imbalance in the number of moles of reactants involved in the reactions, no matter how slight, 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 flow rates so that exactly the right amounts of the two reactants are fed in.

3.3.4 Luyben laws

Luyben (1998) presented three laws have been developed as a result of a number of case studies of many types of systems:

1. A stream somewhere in all recycle loops should be flow controlled. This is to prevent the snowball effect

2. A fresh reactant feed stream cannot be flow-controlled unless there is essentially complete one-pass conversion of one of the reactants. This law applies to systems with reactions types such as A + B → product .In systems with consecutive reactions such as A + B → M + C and M + B → D + C, the fresh feeds can be flow-controlled into the system because any imbalance in the ratios of reactants is accommodated by shift in the two products (M and D) that are generated. An excess of A will result in the production of more M and less D. An excess of B results in the production of more D and less M.

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). Changes in feed flow rate or feed composition have less of a dynamic effect on distillate composition than they do on bottoms composition if the feed is saturated liquid. The reverse is true if the feed is saturated vapor: bottom is less affected than distillate. If our primary goal is to achieve tight product quality control, the basic column design should consider the dynamic implications of feed thermal conditions.

3.3.5 Richardson rule

Bob Richardson (1988) proposed the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense because it provides more muscle to achieve the desired control objective. An analogy is that it is much easier to maneuver a large barge with a tugboat than with a life. The point is that the bigger the handle you have to affect a process, the better you can control it. This is why there are often fundamental conflicts between steady-state design and dynamic controllability.

3.3.6 Shinskey schemes

Greg Shinskey (1988), over the course of a long and productive career at Foxboro, has proposed a number of “advanced control” structures that permit improvements in dynamic performance. These schemes are not only effective, but they are simple to implement in basic control instrumentation. Liberal use should be made of ratio control, cascade control, override control, and valve-position (optimizing) control. These strategies are covered in most basic process control textbooks.

3.3.7 Tyreus tuning

One of the vital steps in developing a plantwide control system, once both the process and the control structure have been specified, is to determine the algorithm to be used for each controller (P, PI, or PID) and to tune each controller. We strongly recommend the use of P-only controllers for liquid levels (even in some liquid reactor applications). Tuning of a 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 (assuming the stream flowing out of the vessel is manipulated to control liquid level; if the level is controlled by the inflowing stream the action of the controller is reverse instead of direct).

For other control loops, we 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 settings (for very tight control with a closed-loop damping coefficient of about 0.1) or the Tyreus-Luyben (1992) settings (for more conservative loops where a closed-loop damping coefficient of 0.4 is more appropriate) can be used:

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

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

The use of PID controllers should be restricted to those loops where two criteria are both satisfied: 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. The classical example of the latter is temperature control in an irreversible exothermic chemical.

3.4 Step of Plantwide Process Control Design Procedure.

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

Step 1: Establish control objectives

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

This is probably the most important aspect of the problem because different control objectives lead to different control structures. The “best” control structure for a plant depends upon the design and control criteria established.

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

Step 2: Determine control degrees of freedom

Count the number of control valves available.

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

(1) Set production rate
(2) Maintain gas and liquid inventories
(3) Control product qualities
(4) 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., minimizes 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.

The term energy management is used to describe two functions:

(1) To provide a control system that removes exothermic heats of reaction form 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) To provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled.

Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

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

Heat transfer between process streams can create significant interaction. In the case of reactor feed/effluent heat exchangers it can lead to positive feedback and even instability. Where there is partial condensation or partial vaporization in a process-to-process heat exchanger, disturbances can be amplified because of heat of vaporization and temperature effects.

Step 4: Set production rate

Establish the variables that dominate the productivity of the reactor and determine the most appropriate manipulator to control production rate.

Throughput changes can be achieved only by altering, either directly or indirectly, conditions in the reactor. To obtain higher production rates, the overall reaction rates must be increased. This can be accomplished by raising temperature (higher specific reaction rate), increasing reactant concentrations, increasing reactor holdup (in liquid-phase reactors), or increasing reactor pressure (in gas-phase reactors).

Our first choice for setting production rate should be to alter one of these variables in the reactor. The variable that is selected must be dominant for the reactor. Dominant reactor variables always have significant effects on reactor performance. For example, temperature is often a dominant reactor variable. In irreversible reactions, specific rates increase exponentially with temperature. As long as reaction rates are not limited by low reactant concentrations, temperature can be increased to increase production rate in the plant. In reversible exothermic reactions, where the equilibrium constant decreases with increasing temperature, reactor temperature may still be a dominant variable. If the reactor is large enough to reach chemical equilibrium at the exit, the reactor temperature can be decreased to increase production.

There are situations where reactor temperature is not a dominant variable or cannot be changed for safety or yield reasons. In these cases, another dominant variable must be found, such as the concentration of the limiting reactant, flow rate of initiator or catalyst to the reactor, reactor residence time, reactor pressure, or agitation rate.

Once the dominant variables must be identified, the manipulators (control valves) must also be identified that are most suitable to control them. The manipulators are used in feedback control loops to hold the dominant variables at setpoint. The setpoints are then adjusted to achieve the desired production rate, in addition to satisfying other economic control objectives.

Whatever variable is chosen, it can provide smooth and stable production rate transitions and to reject disturbances. 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 is often wanted select.

When the setpoint of a dominant variable is used to establish plant production rate, the control strategy must ensure that the tight amounts of fresh reactants are brought into the process. This is often accomplished through fresh reactant makeup control based upon liquid levels or gas pressures that reflect component inventories.

However, design constraints may limit our ability to exercise this strategy concerning fresh reactant makeup. An upstream process may establish the reactant feed flow sent to the plant. A downstream process may require on-demand production, which fixes the product flow rate from the plant. In these cases, the development of the control strategy becomes more complex because the setpoint of the dominant variable on the basis of the production rate that has been specified externally must be somehow adjusted. The production rate with what has been specified externally must be balanced. This cannot be done in an open-loop sense. Feedback of information about actual internal plant conditions is required to determine the accumulation or depletion of the reactant components.

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

Select the "best" valves to control each of the product-quality, safety, and environmental variables.

The tight control of these important quantities for economic and operational reasons is wanted. Hence the manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and deadtimes and large steady-state gains should be selected. The former gives small closed-loop time constants and the latter prevents problems with the range ability of the manipulated variable (control valve saturation).

It should be noted that establishing the product-quality loops first. Before the material balance control structure, is a fundamental difference between our plantwide control design procedure and Buckley's procedure, since product quality considerations have become more important is recent year, this shift in emphasis follows naturally.

The magnitudes of various flowrate also come into consideration. For example, temperature (or bottoms product purity) in a distillation column is typically controlled by manipulating stem flow to the reboiler (column boilup) and base level is controlled with bottoms product flowrate. However, in columns with a large boilup ratio and small bottoms flowrate, these loops should be reversed because boilup has a larger effect on base level than bottoms flow (Richardson rule). However, inverse response problems in some columns may occur when base level is controlled by heat input. High reflux ratios at the top of a column require similar analysis in selecting reflux or distillate to control overhead product purity.

Step 6: Control inventories (pressures and levels) and fix a flow in every recycle loop

Determine the valve to control each inventory variable. These variables include all liquid levels and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit.

Proportional-only control should be used in nonreactive level loops for cascaded units in series. Even in reactor-level control, proportional control should be considered to help filter flow-rate disturbances to the downstream separation system. There is nothing necessarily sacred about holding reactor level constant.

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

Step 7: Check component balances

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

Ensure that the overall component balances for each chemical species can be satisfied either through reaction or exit streams by accounting for the component's composition or inventory at some point in the process. Light, intermediate, and heavy inert components must have an exit path from the system. Reactant must be consumed in the reaction section or leave as impurities in the product streams. Fresh reactant makeup feed streams can be manipulated to control reactor feed composition or a recycle stream composition (or to hold pressure or level as noted in the previous step). Purge streams can also be used to control the amount of high- or low-boiling impurities in a recycle stream.

Component balances can often be quite subtle. They depend upon the specific kinetics and reaction paths in the system. They often affect what variable can be used to set production rate or rate in the reactor.

Step 8: Control individual unit operations

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

Many effective control schemes have been established over the years for chemical units. For example, a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust fuel flow rate to a furnace supplying energy to the reactor. Crystallizers require manipulation in the stack gas from a furnace is controlled to prevent excess fuel usage. Liquid solvent feed flow to an absorber is controlled as some ratio.

Step 9: Optimize economics or improve dynamic controllability

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

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

Additional considerations

Certain quantitative measures from linear control theory may help at various steps to assess relationships between the controlled and manipulated variables. These include steady-stat process gains, open-loop time constants, singular value decomposition, condition numbers, eigenvalue analysis for stability, etc. these techniques are described in detail in most process control textbooks. The plantwide control strategy should ultimately be tested on a nonlinear dynamic model that captures the essential process behavior.

3.5 New Plantwide Control Structure Design Procedure

New design procedure of Wongsri (2009) presented the eight step of plantwide control design procedure which analyzed by mathematical-based and heuristic-based. The priority of control variables is established in the procedure. The major disturbance are handled explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method) to cover the material disturbances. The propose procedure for selection the best set of control structure is perceptive, simple and straightforward. The new design procedures of Wongsri (2009) are:

Step 1: Establish of Control Objectives.

Step 2: Selection of Controlled Variables (CVs) to achieve Product Quality, Safety, Operational and Environmental Constrains using The Fixture Point Theorem.

Step 3: Selection of Manipulated Variables and Measurements by DOF Analysis.

Step 4: Energy Management via Heat Exchanger Networks (HENs).

Step 5: Selection of Control Configuration using Various Tools available.

Step 6: Completing Control Structure Design by Checking the Component Balances.

Step 7: Selection of Controller Type: Single loops or MPC.

Step 8: Validation via Rigorous Dynamic Simulation.

Wongsri (2008) propose the fixture point theorem that used to define the most sensitive CV. The steps of theorem analysis are:

1. Consider the process at dynamic mode until it's responses are at steady-state.
2. CVs are arranged to follow the most sensibility of the process variable by step change of the MV in open loop control (change only one MV, the other should be fixed than alternate to other until complete).
3. Evaluate the magnitude of integral absolute error (IAE) of all process variables that deviates from steady state.
4. Select CV by considering CV that gave the most deviation from steady state (high value score).

3.6 Plantwide energy management

Heat management is accomplished by controlling the flow of energy in various heat exchangers. We differentiate between utility exchangers and process-to-process heat exchangers. Utility exchangers allow us to import heat from heat sources or discard heat to the environment. Process-to-process exchangers, on the other hand, are used to transfer heat from one part of the process to another. We will look at the unit operation controls of both types of exchangers. The plantwide control issues around energy management. We need to identify the various pathways for heat and to devise a control strategy that allows effective delivery and removal of energy.

3.6.1 Heat Pathway

In the process, the most energy required for heating certain streams are matched by similar amount of energy required for cooling other streams. Heat recover from cooling a stream could be recycling back to the process to heat another stream. This is the proposed of heat integration and heat exchanger networks (HENs).

From a plantwide perspective, the heat pathways in the process can be separated to three different paths as illustrate in Fig. 3.2. The first pathway dissipates to the environment heat generated by exothermic reaction and by degradation of mechanical work. This pathway is from inside the process and flows out. It is also possible to convert some of the heat to work as it is removed from high temperature in the process.

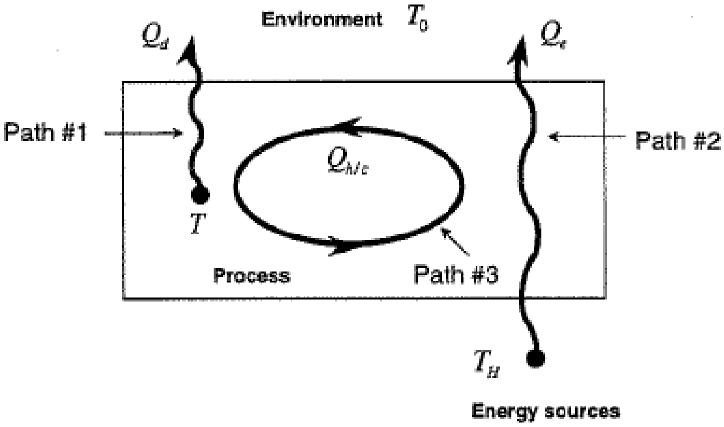


Figure 3.2 Heat Pathways.

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

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

3.6.2 Heat recovery

In the process, we can make great improvements in the plant's thermal efficiency by recycling much of the energy needed for heating and cooling process streams. It is also possible to introduce heat integration schemes for distillation columns to reduce the separation heat. And finally we can recover the reaction heat in waste heat boilers and use the steam for power generation. 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.

CHAPTER IV

AMMONIA PRODUCTION PROCESS AND NEW CONTROL STRUCTURES DESIGN PROCEDURE

4.1 Introduction

Ammonia is a widely used raw material in process industry for production of nitrogen containing chemicals, i.e. fertilizers, explosive materials, pharmaceuticals, polymers, acids and coolers. The annual world production of ammonia is extremely large, estimated at 131 million tons in 2010.

4.2 Process Description

The Haber-Bosch process links atmospheric nitrogen with hydrogen in a 1:3 stoichiometric ratio to give ammonia with no by product.

$$3H_2 + N_2 \leftrightarrow 2NH_3 \tag{4.1}$$

The reaction of ammonia is reversible and exothermic, and follows the Temkin-Pyzhev kinetics:

$$R_{NH_3} = \frac{2f}{\rho_{cat}}\left(k_1 \frac{P_{N_2}P_{H_2}^{1.5}}{P_{NH_3}} - \ k_{-1}\frac{P_{NH_3}}{P_{H_2}^{1.5}}\right) \tag{4.2}$$

$$k_1 = 1.79 \times 10^4 \exp\left(-\frac{87{,}090\frac{kJ}{kmole}}{RT}\right) \tag{4.3}$$

$$k_{-1} = 2.57 \times 10^{16} \exp\left(-\frac{198{,}464\frac{kJ}{kmole}}{RT}\right) \tag{4.4}$$

where T is the temperature in Kelvin. ρ_{cat} is the bulk density of the catalyst, ρ_i is the partial pressure of the gaseous reactant/product i in bars. k_1 And k_{-1} are the rate coefficients of the forward and reverse reactions. The multiplier factor *f* is used to correct for the catalyst activity, and we use the value of the *f* = 4.75 as given in Morud and Skogestad (1998).

The simplified reactor model as shown in Fig.4.1 consists of 3 adiabatic catalytic reactors in series with interstage cooling and preheating of the feed with the reactor output streams. Each interstage stream is cooled by direct mixing it with cooler reactor feed. The reactors are modeled in HYSYS dynamic simulator (Version 7.0) using its built-in catalytic plug-flow reactor model. The last reactor effluent is first cooled with the partial reactor feed stream at HX-001.Then it’s cooled down further by releasing its heat to generate low pressure stream via H-501 and exchanged its heat with the reactor feed stream at H-502. Next it’s condensed to liquid ammonia in H-583 and sent to the separator (V-502). The liquid ammonia is mixed with the H_2-N_2 feed before entering the flash separator.

The flash separator is adiabatic and used to disengage ammonia product and gaseous reactants. The inerts (CH_4 and Ar) are purged before sent to the reactor section.

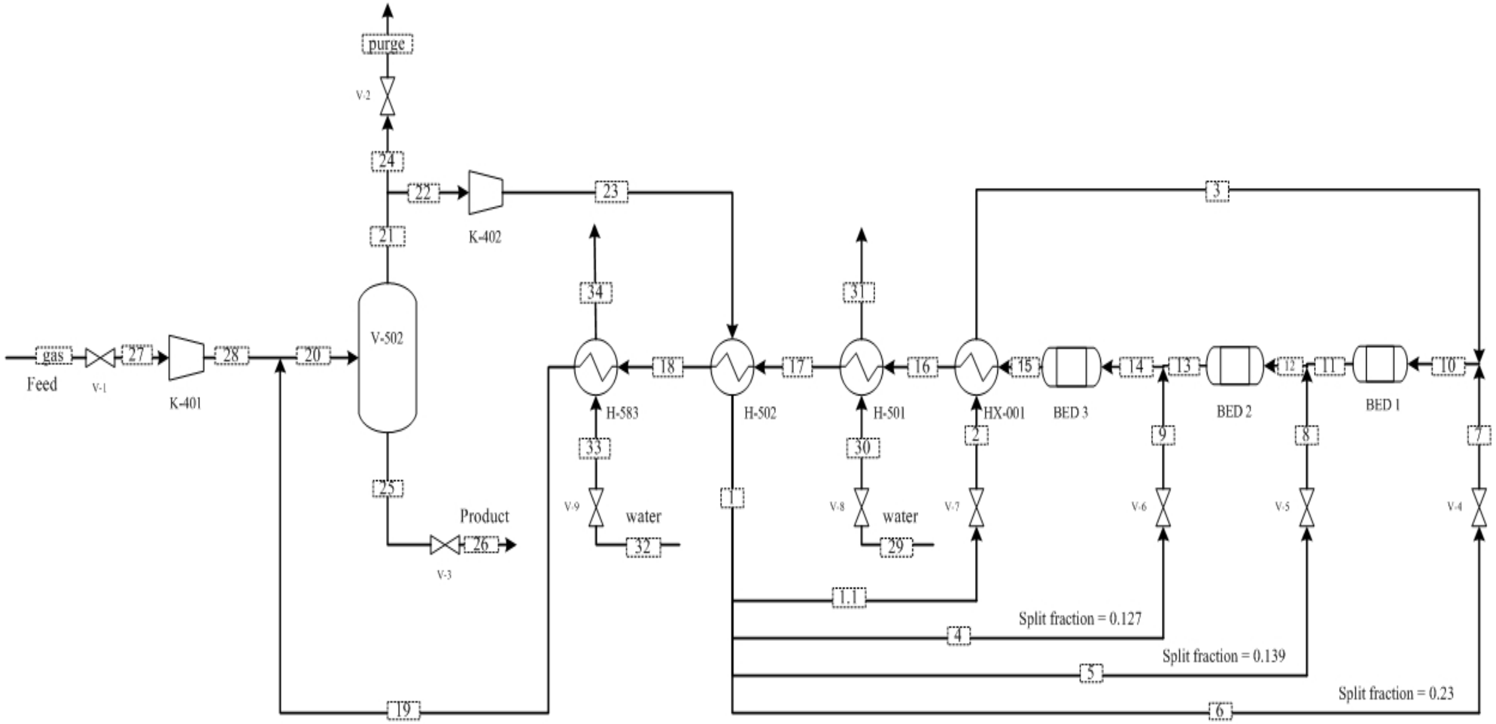


Figure 4.1 Ammonia production flowsheet (Araújo and Skogestad (2008))

4.3 Process modeling and steady state simulation

Our modeling and simulation are performed in HYSYS dynamic simulator program. Peng-Robinson equation of state is chosen for prediction of fluid properties**.**

The process condition and constraints are summarized in Table. 4.1-4.3

Table 4.1 Specifications for the heat exchangers model

Heat exchanger	**U (kJ/m^{2}hr-°C)**	**Heat transfers area (m^2)**
H-501	409	1,245.6
H-502	204.5	23,632
H-583	3066	3,042
HX-001	204.5	4,784

Note: The overall heat-transfer coefficients (U) are referred from Conceptual Design of Chemical Processes, James M. Douglas.

Table 4.2 Specifications for the ammonia reactor model and adiabatic flash separator

Specification	**Bed1**	**Bed2**	**Bed3**	**Separator**
Length/Height (m)	2.13	3.07	4.84	12
Diameter (m)	2	2	2	6
Bed voidage	0.33	0.33	0.33	-
Bulk density (kg/m^3)	2,200	2,200	2,200	-
Equipment heat capacity (J/kg-k)	1,100	1,100	1,100	-

Table 4.3 Constraints for the ammonia process

	Constraints	**Unit**
Reactor inlet pressure	≤ 250	bar
Operating temperature	< 500	˚C
Feed compressor power	≤ 25,000	kW
Recycle compressor power	≤ 3,500	kW
Cooling water flow rate of H-501	≤ 80,000	kg/hr

4.4 Wongsri (2012) New Control Structures Design Procedure

Wongsri procedure (2012) consists of eight steps of the plantwide control structure design which makes use of chemical engineering and process knowledge and heuristics. The design of plantwide control structure should be viewed *as a whole; taking into consideration of the whole plant.* The design step called plantwide level design is the decision of how to regulate the whole plant albeit a single entity as smoothly as possible. Then the designs of control loops that locally function are handled at the unit level design.

In the plantwide level control, a fixture plant is established for creating a material-balanced process plant. The establishing a fixture plant can be done by: keeping the raw materials entered to the reactor fixed, adjusting the flow of exit material streams (products, by-products, and inert) according to their accumulations, and locating the quantifiers for the rest of the components to design the control loops to regulate their inventories. For operating a plant as smoothly as possible, the disturbance effects can be diminished by designing the control loops to reject or direct the disturbances taking a whole plant into consideration. The design of the control loops at each step follows the material balance of the whole plant and the fast and efficient rejection of disturbances though out the process. In the other words, the selection of control loops is not done in unitwise manner instead they are designed by looking from perspective of a whole plant. The heat disturbance management principle is used to design the control loops for rejection the effects of any thermal disturbances that de and do not directly relate to the product quality to the environment; while the material pathway analysis is used to design control loops to direct the material disturbances.

In the unit level control, the control loops are designed at the units that are not level-, pressure-, or flow-controlled, e.g., pumps and compressors.

If the opportunities for heat integration and process modification exist, we later design the control structures of the heat integrated plant (HIP) and modified plant. The control structure of the new designs then will be compared with the previous designs. The trade-off between cost savings and control performances will be discussed.

The design procedure is carried out in eight steps as follow:

Step 1: Gather relevant plant information and control objective including constraints for control. Before initiating work on the control structure design, it is necessary to obtain all information relevant to process control. The process objective and control constraints determine the lower/upper bounds of the controlled variables as well as setpoints on the controlled variables.

Step 2: List manipulated variables (control degree of freedom, CDOF).

The manipulated variables can be obtained using the guideline given in Table 4.4 and the guideline for pairing the controlled variables with the manipulated variables is presented in Table 4.5.

Table 4.4 Degree of freedom for simple units

Unit	DOF / unit
Independent stream	1
Heater, cooler, pump, and compressor	1
Heat exchanger with a by-pass stream	1
Adiabatic plug flow reactor	0
Non-adiabatic plug flow reactor	1
Adiabatic flash separator	2
Simple distillation column	5

Table 4.5 Guideline pairing of manipulated and controlled variables

NO.	Guideline
1.	A control and manipulated variables must have strong causal relationship (high gain).
2.	The manipulated variables should not be far from the control variables (zero or minimal dead time).
3.	The time constant of the quality loops should be short and the time constant of the inventory loops should be last.
4.	The manipulated variables should not be saturated for the whole range of the disturbances.
5.	The manipulation of the manipulated variables should not have or have less effects on others variables (low gains with the remainder of the variables).

Step 3: Establish the fixture plant.

The principal idea of establishing a fixture plant is to have an entire plant fluid-filled and a material-balanced. This idea is similar to creating *hydraulic control structure* proposed by Buckley.

(3.1) Keep the materials entered combined with reentered fixed. However, if the composition of the recycle stream differs from the fresh feed significantly, each stream should be flow-controlled separately. In this settlement, the flow of the recycle cannot be used to regulate the inventory of its upstream unit, e.g., the level of the reflux drum or the column pressure.

(3.2) Adjust the flow of exit material streams (products, by-products, and inerts) according to their accumulations.

(3.3) Locate quantifiers, i.e., the indicators of the representative accumulation, for the rest of the components and design the control loops to regulate their inventories in the plant. The quantifier can be volume (mass), pressure, or flow rate.

Step 4: Handling the disturbances.

(4.1) Any thermal disturbances are divided into 2 categories. Heat Disturbance Category 1 (HDC1) is the heat disturbances that do not directly affect product qualities, such as heat disturbance in a process stream toward to a heater, a cooler, or a process-to-process heat exchanger. Heat Disturbance Category 2 (HDC2) is the heat disturbances affected the product qualities, such as heat disturbance in a process stream toward to a reactor or a separator.

(4.1.1) Direct the thermal disturbances that are not directly related to the product quality to the environment via the next and nearest exit points, usually heaters or coolers, to keep the thermal conditions of process stream fixed. The thermal condition of process stream is changed along the process plant, usually by heater, cooler, or process to process heat exchanger.

(4.1.2) Manage the thermal disturbances that related to the product quality in order to maintain the quality within its specification.

(4.2) Material disturbances.

The configuration of the control loops depend on the desired material pathways. The pathways can be obtained by analyzing the results of the material disturbance tests. The test is suggested to be done on the changing of composition, total flow, and component flow. The material disturbances can be generated at reactors and separators, besides coming with feeds and recycle streams. So, if the feeds combined with the recycle streams are fixed, the only places that change the material (total or component) flow rates are the reactors and the separators. At reactor, its inlet temperature is adjusted in order to keep a component flow rate or a composition in the reactor product stream. The decision of whether how to choose to control the component flow or the composition or not to control depends on the profit maximization, the smooth operation, or other control policies.

Since the distillation columns, usually the one-point control is common. The temperature control at upper or lower of the distillation column feed depends on the material disturbance rejection policy.

Step 5: Design the control loops for the remaining control variables and/or adding enhanced controls, i.e., cascade, feed forward controls.

Step 6: Energy management via heat exchanger networks.

If the opportunities for the process modification and/or the heat integration exist, e.g., adding process-to-process heat exchangers with the by-pass streams, it should be performed and then listed additional controlled and manipulated variables.

Step 7: Optimize economics and/or improve the control performance.

The economic optimization may be the change of the operating, or the process modification (e.g., the feed location, the sequence of separation), etc. Examples of control performance improvement are the control scheme modification at the reactor (e.g., temperature/composition sensor location for the plug flow reactor), the distillation column (e.g., using reflux-to-feed ratio control), etc. However, if the optimization is performed, the control structure design should be backtracked to the previous step as dictated.

Step 8: Validate the designed control structures by rigorous dynamic simulation, and compare the designed structure to each other.

The measures in the comparison may be costs, raw material and energy consumptions, control performances, etc. of the total plant or some selected loops.

CHAPTER V

CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION

This research follows the 8-step of Wongsri for designing the control structure of ammonia process. Plantwide controls are considered because of complex of the process such as heat integration and recycle streams. The new control structures completed by Wongsri procedure are compared with the structure established by Araújo and Skogestad (2008). The new control structures are accomplished by the following steps:

5.1 New Control Structures Design

Here, we will apply the above plantwide control structure design procedure to the ammonia production process.

Step 1: Starting with the process information given in section 4.2 and the process conditions given in (Appendix A). The purity of the ammonia product at 96.9 mol% with capacity of 621,583 tons/year is essentially requisites to meet process objectives.

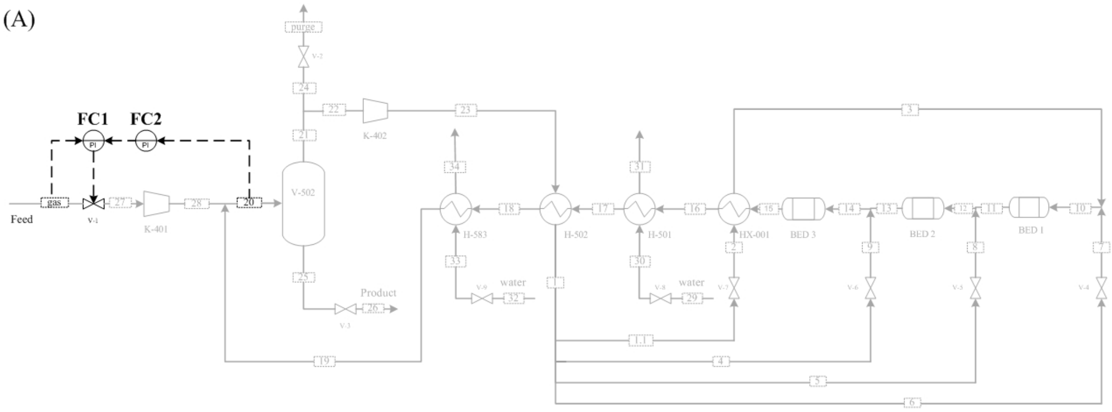
Step 2: List manipulated variables (control degree of freedom, CDOF). The CDOF can be obtained using the guideline given in Table 5.1.

Step 3: Establish fixture plant. The material entered, and in-process stream must be maintained to ensure that the plant is smoothly operated.

Table 5.1 The control degree of freedom for the ammonia production process.

Unit	**Manipulated variable**	**Quantity**	**DOF**
External feed streams	Flow rate	1	1
Splitters (purge)	Flow rate	1	1
Splitters (cold shots reactor)	Flow rate	1	3
Compressors	Power	2	2
Separator	Vapor flow out Liquid flow out	1	2
Adiabatic bed reactors	-	3	0
Heat Exchanger with by-pass	By-pass flow rate	1	1
Heat Exchangers with cooling water	Water flow rate	1	1
Total			11

Step 3.1: The objective of this step is to keep the stream entered (fresh and recycled) the plant fixed; therefore we regulate the combined feed to the separator by adjusting flow rate of the fresh gas feed (Fig.5.1A). Another scheme, if we consider the first section of the plant is the reactor section, which in general is the case, is controlling the reactor section feed (Fig.5.1B) to ensure that we have the smooth feed flow. Two resulted control loops are depicted in Fig.5.1.



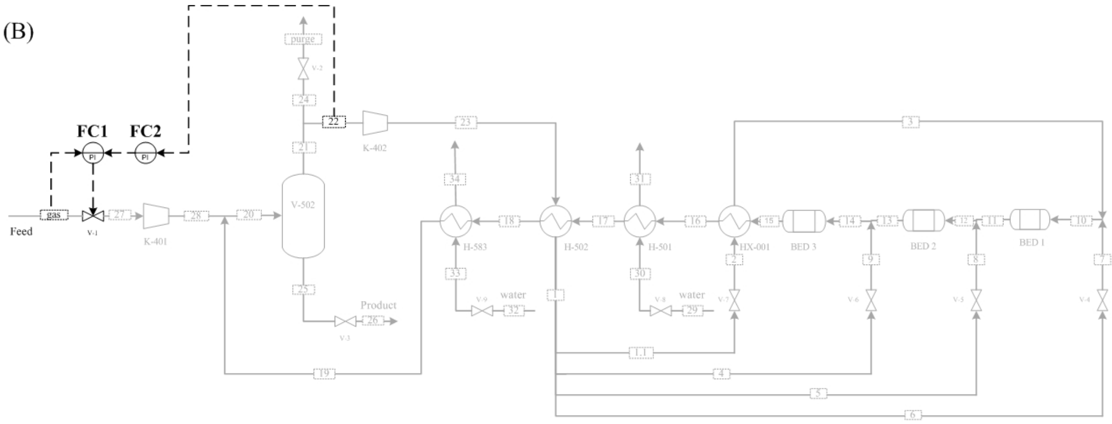


Figure 5.1 Control structure for keep the materials entered and reentered fixed.

Step 3.2: The exit material streams of the ammonia production plant are the product stream and the purge stream. The inert purge stream is flow-regulated to keep the accumulation of inerts in the system. The ammonia product flow rate is adjusted by the level of the separator. The obtained control structure is shown in Fig.5.2.

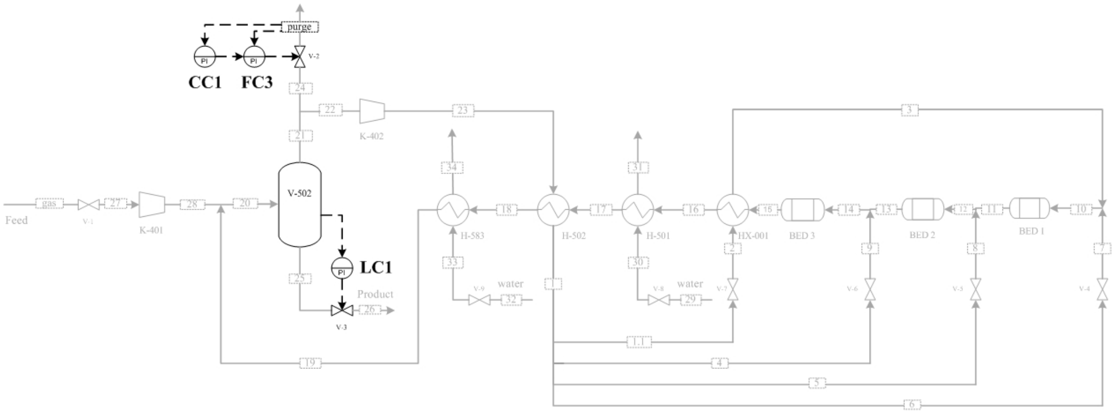


Figure 5.2 Control structure for adjust the flow of exit material streams

Step 3.3: Hydrogen and nitrogen is the rest components. We control the quantifier of their by fixed the pressure in the flash separator. The obtained control structure is shown in Fig.5.3.

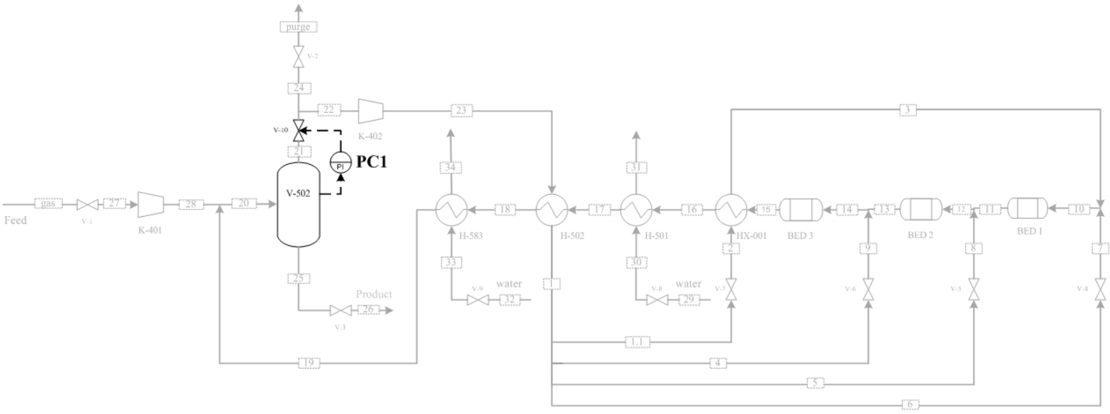


Figure 5.3 Control structure for located the quantifier of H_2 and N_2

Step 4: This step is to design the control loops to deal both thermal and material disturbances.

Step 4.1: The thermal disturbance is divided into 2 categories: Heat Disturbances of Category1 (HDC1) are handled by H-501, H-502, and H583. H-583 regulates the temperature of the separator feed. The temperature of the reactor feed is kept at the set point by manipulating the by-pass flow of H-502. The thermal disturbance generated in the reactor section is rejected via H-501. Heat Disturbances of Category 2 (HDC2) are those presented in the feed to the reactors. The three reactor feed temperatures are control by adjusting the interstage cooling streams via direct mixing. In our design we have regulated the flow rate of process streams, in order to establishing a fixture plant we must also the thermal condition of the process stream. The results control loops are shown in Fig.5.4.

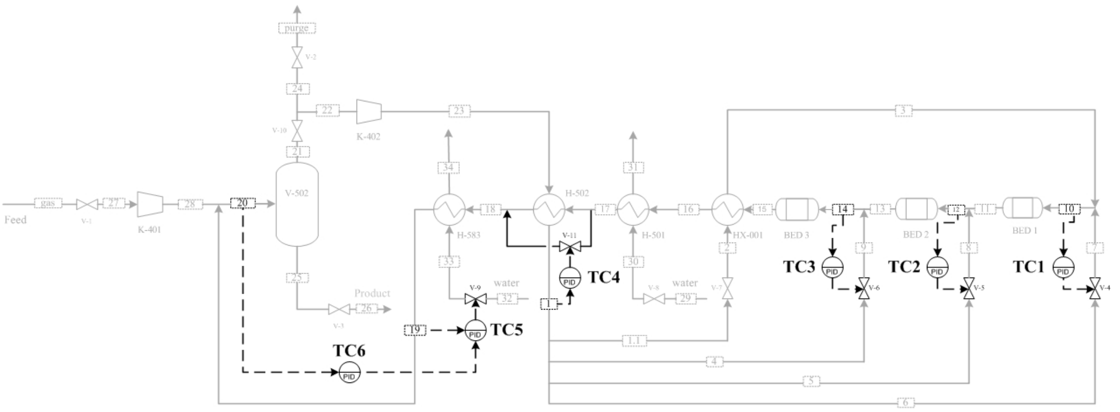


Figure 5.4 Control structure for handle the heat disturbance.

Step 4.2: The combined hydrogen and nitrogen pathway is shown in Fig.5.5. The inert pathway is presented in Fig.5.6. Finally, the ammonia product pathway is illustrated in Fig.5.7. The ammonia is controlled via TC1, TC2, TC3, and LC1. The inerts is regulated via CC1 and FC3. The reactants (hydrogen and nitrogen) are adjusted via PC1.

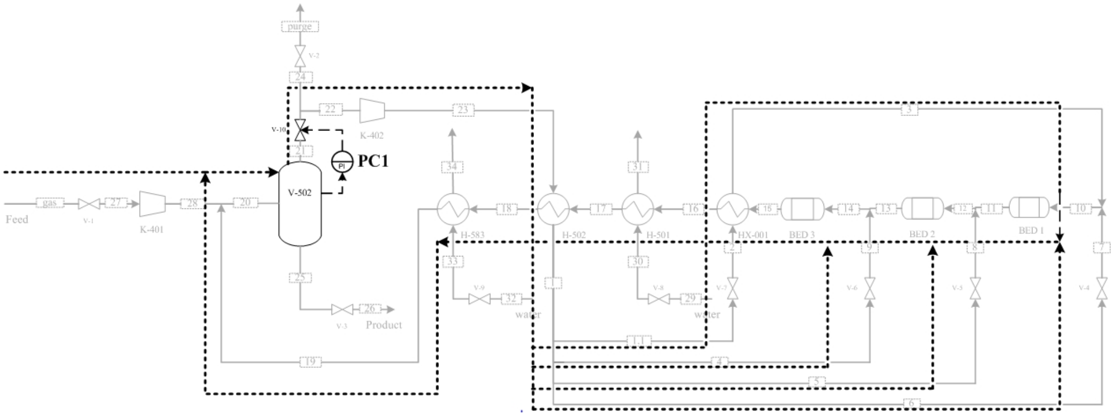


Figure 5.5 Control structure for manage the hydrogen and nitrogen pathway.

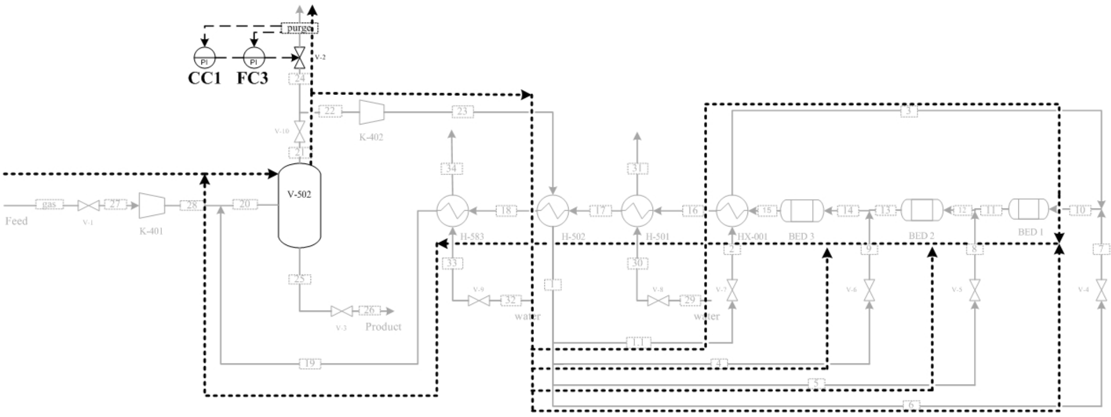


Figure 5.6 Control structure for manage the inerts pathway.

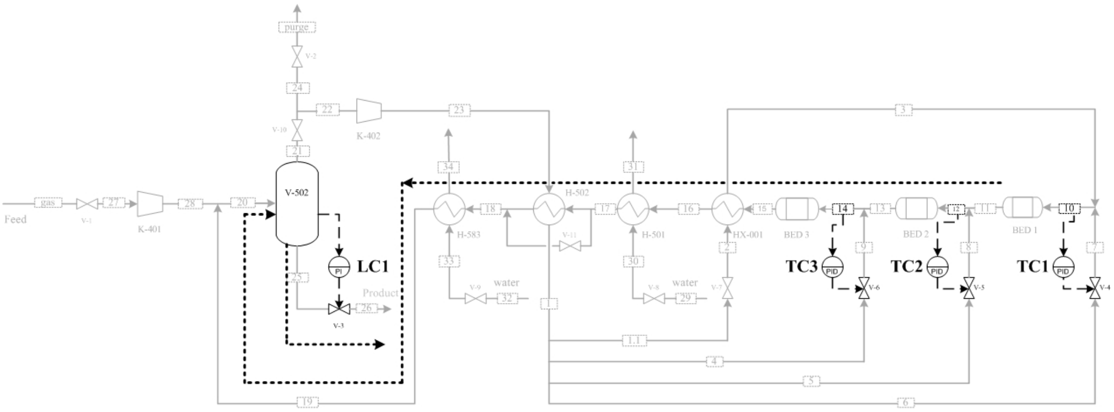


Figure 5.7 Control structure for manage the ammonia product pathway.

Step 5: Design the control loops for the remaining control variables and/or adding enhanced controls, i.e. cascade, feed forward controls.

There is no controlled variable left. This step is skipped.

Step 6: There are two process-to-process heat exchangers HX-001 and H-502. The nominal heat loads of these two heat exchangers are 2.252×10^7 kcal/h and 6.986×10^7 kcal/h.

Table 5.2 Thermal data of the ammonia production process.

Units	**m (kg/hr)**	**C_p (kJ/kg-˚C)**	**mCp (kJ/hr-˚C)**	**Temp (˚C)**
Stream 2	243,588	3.512	855,481	231.7
Stream 15	483,310	3.638	1,758,281	412.4
Stream 16	483,310	3.574	1,727,350	358.7
Stream 17	483,310	3.504	1,693,518	296.9
Stream 18	483,310	3.351	1,619,572	120.1
Stream 23	483,310	3.775	1,824,495	67.6
Stream 30	80,000	4.050	324,000	15.1
Stream 33	700,000	4.050	2,835,000	15.1

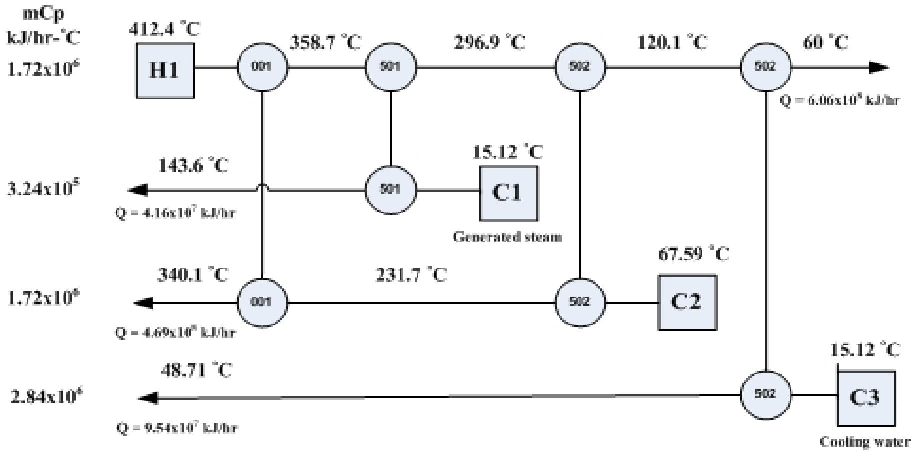


Figure 5.8 Grid diagram of the heat exchanger network

Step 7**:** Optimize economics and improve control performance**.**

To control the performance of the process, the PID controllers are employed to control all quality loops, which are TC1, TC2, TC3, TC4, TC5, and TC6

All control structures are established in Figure 5.9-5.11, control structure presented by Araújo and Skogestad (2008) (Base case), control structure 1-2 (CS1-2).

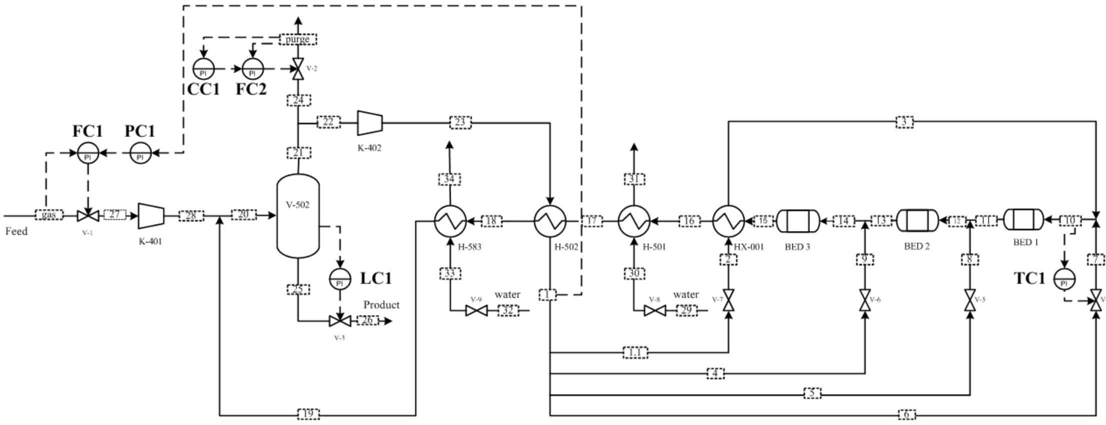


Figure 5.9 Control structure of base case.

Table 5.3 Control structure list of base case

Equipment	**Control**	**Controlled variable**	**Manipulated variable**	**Type**	**Action**
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse
Reactors	PC_1	Inlet Pressure	Set point of FC_1	PI	Reverse
Separator	LC_1	Liquid level	Liquid flow out	P	Reverse
Purge	FC_2	Flow rate	Purge flow rate	PI	Reverse
	CC_1	Methane composition	Set point of FC_2	PI	Direct
Reactor1 (R_1)	TC_1	Inlet temperature	By-pass flow rate	PI	Direct

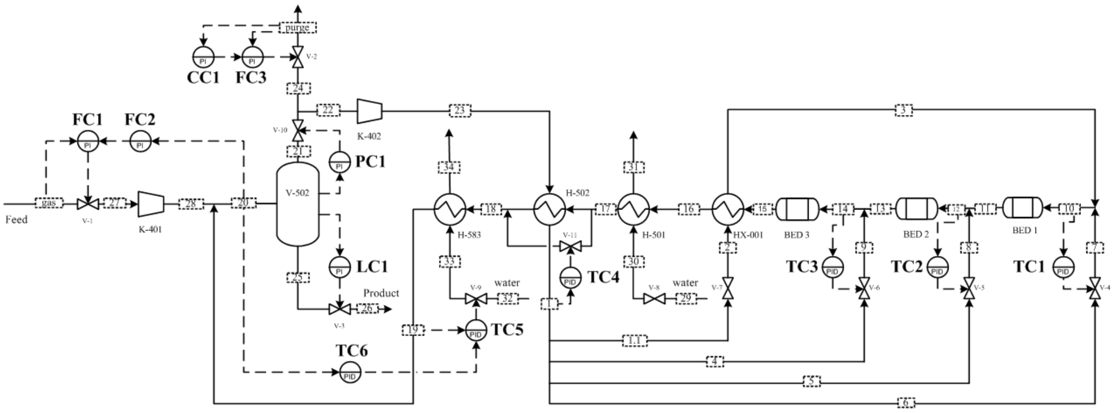


Figure 5.10 Control structure of CS1.

Table 5.4 Control structures list of CS1

Equipment	Control	Controlled variables	Manipulated variables	Type	Action
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse
Feed gas	FC_2	Total flow rate	Set point of FC_1	PI	Reverse
Separator	PC_1	Column pressure	Vapor flow out	PI	Reverse
	LC_1	Liquid level	Liquid flow out	PI	Reverse
Purge	FC_3	Flow rate	Purge flow rate	PI	Reverse
	CC_1	Methane composition	Set point of FC_3	PI	Direct
Reactor1	TC_1	Inlet temperature	By-pass flow rate	PID	Direct
Reactor2	TC_2	Inlet temperature	Flow rate of cooling stream	PID	Direct
Reactor3	TC_3	Inlet temperature	Flow rate of cooling stream	PID	Direct
Heat exchanger 502	TC_4	Outlet temperature	By-pass flow rate	PID	Direct
Heat exchanger 583	TC_5	Outlet temperature	Water flow rate	PID	Direct
	TC_6	Inlet temperature of separator	Set point of TC_5	PID	Direct

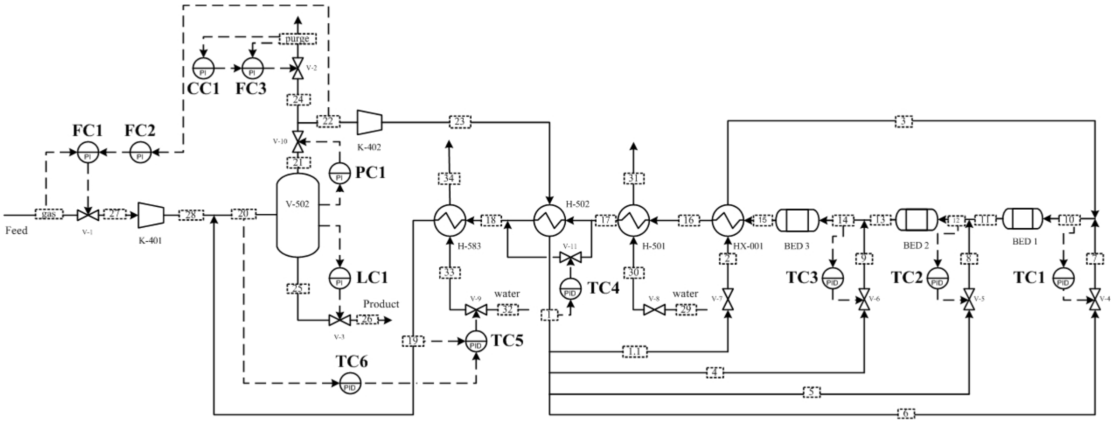


Figure 5.11 Control structure of CS2.

Table 5.5 Control structures list of CS2

Equipment	**Control**	**Controlled variables**	**Manipulated variables**	**Type**	**Action**
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse
Reactor	FC_2	Flow rate	Set point of FC_1	PI	Reverse
Separator	PC_1	Column pressure	Vapor flow out	PI	Reverse
	LC_1	Liquid level	Liquid flow out	PI	Reverse
Purge	FC_3	Flow rate	Purge flow rate	PI	Reverse
	CC_1	Methane composition	Set point of FC_3	PI	Direct
Reactor1	TC_1	Inlet temperature	By-pass flow rate	PID	Direct
Reactor2	TC_2	Inlet temperature	Flow rate of cooling stream	PID	Direct
Reactor3	TC_3	Inlet temperature	Flow rate of cooling stream	PID	Direct
Heat exchanger 502	TC_4	Outlet temperature	By-pass flow rate	PID	Direct
Heat exchanger 583	TC_5	Outlet temperature	Water flow rate	PID	Direct
	TC_6	Inlet temperature of separator	Set point of TC_5	PID	Direct

Step 8: Validate the designed control structures by rigorous dynamic simulation. The measures can be costs, raw material and energy consumptions, control performances of the total plant or some selected loops, etc.

This step, the disturbances; which are gas feed, temperature feed and methane composition in feed are tested to the ammonia process (Base case, CS1 and CS2). The data of disturbances are shown in Table 5.6 and the responses of the entire process are presented as a graph plotted versus operates time in Table 5.7–5.9.

Note that: the disturbances are applied 1 hr after the beginning of each simulation run.

Table 5.6 Disturbances to the effect of dynamic simulations for base case and design control structures.

No.	**Description**	**Nominal**	**Disturbance**
Dyn1	Gas feed rate F_{gas} (kg/hr)	84,108	± 5%[a]
Dyn2	Temperature in the gas feed (˚C)	17	± 5 C
Dyn3	Mole fraction of CH_4 in the gas feed	0.0033	± 1%[b]

[a] Gas feed rate disturbance considered as measurement error.

[b] Mole fraction of H_2 in the gas feed is reduced by the same amount.

Table 5.7 Dynamic responses with Gas feed changed.

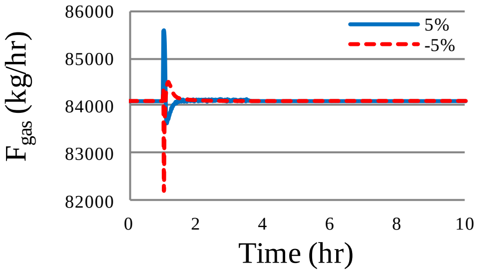
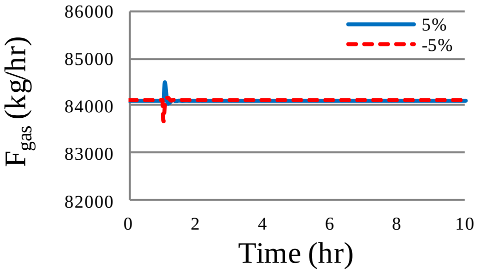
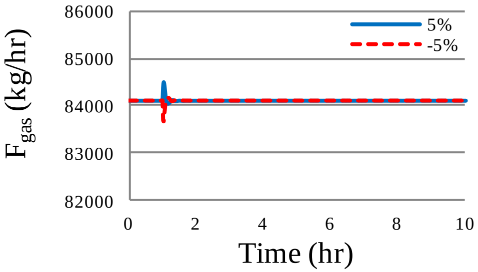
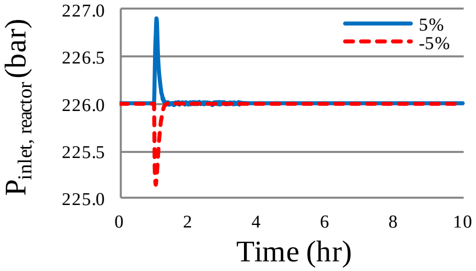
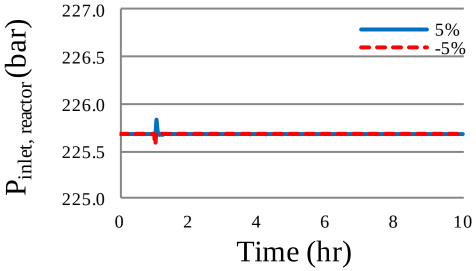
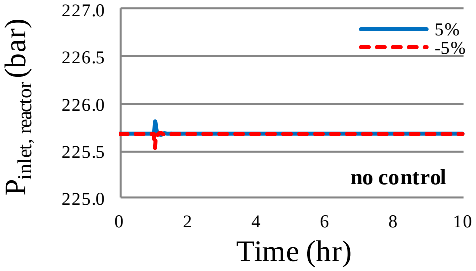
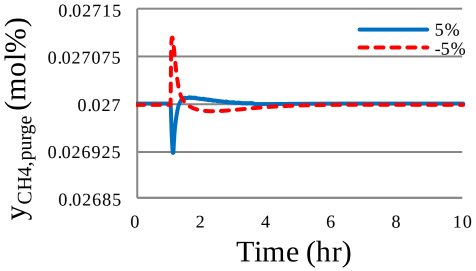
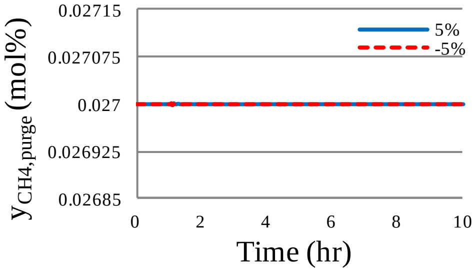
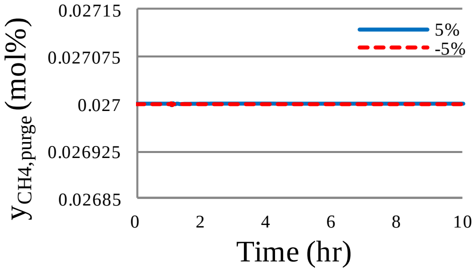
	Base Case	**CS1**	**CS2**
a.			
b.			
c.			

Table 5.7 Dynamic responses with Gas feed changed. (Continue)

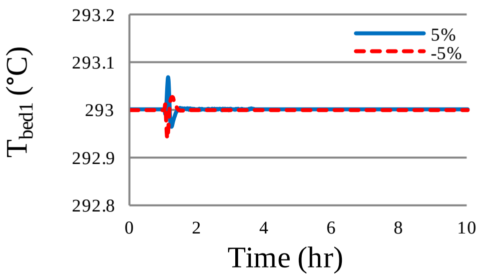
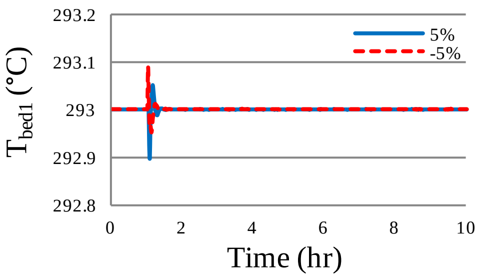
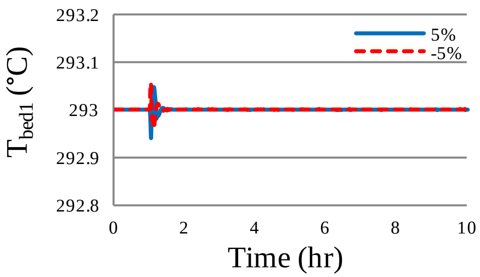
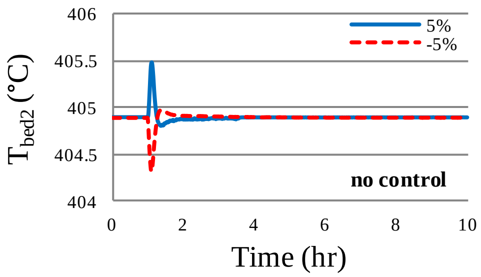
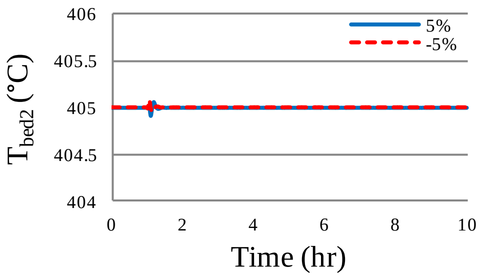
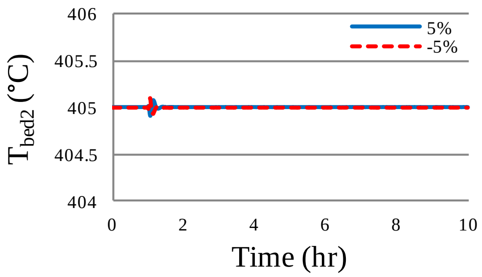
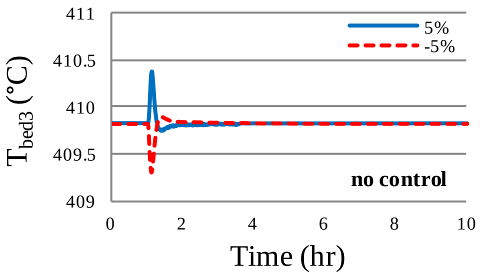
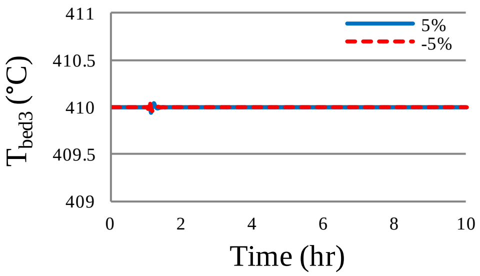
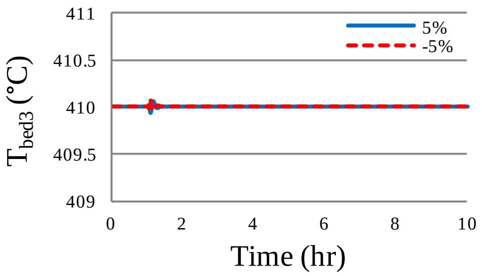
	Base Case	CS1	CS2
d.			
e.			
f.			

Table 5.7 Dynamic responses with Gas feed changed. (Continue)

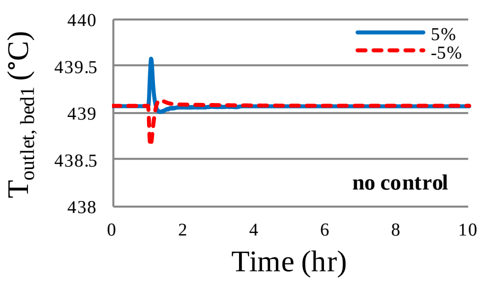
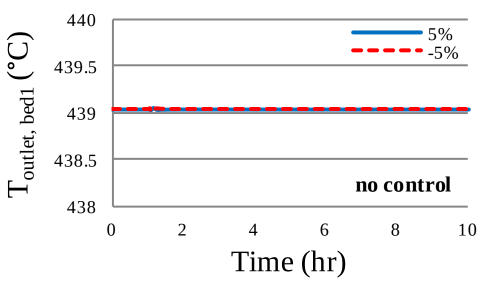
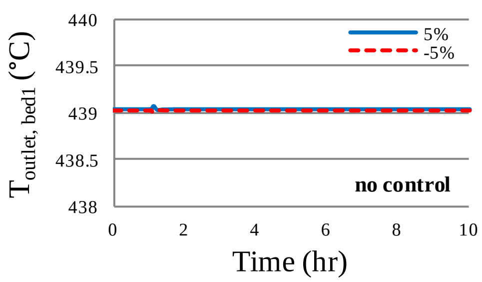
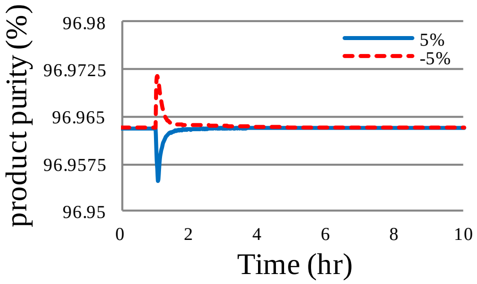
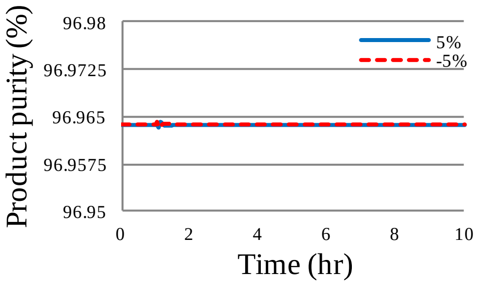
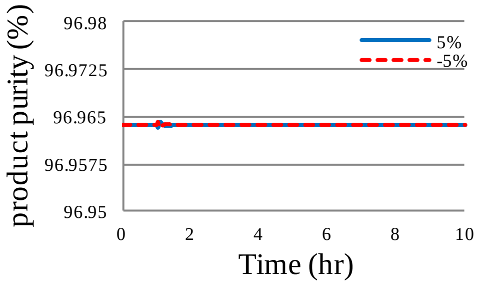
	Base Case	CS1	CS2
g.			
h.			

Table 5.8 Dynamic responses with Temperature feed changed.

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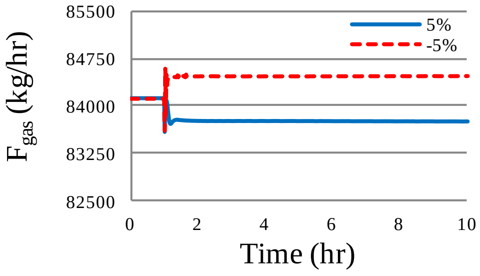
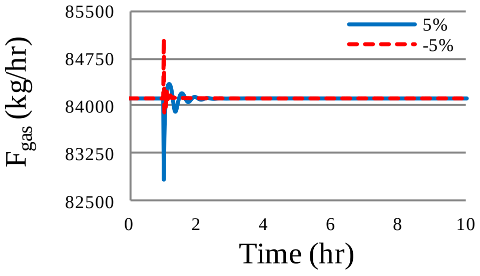
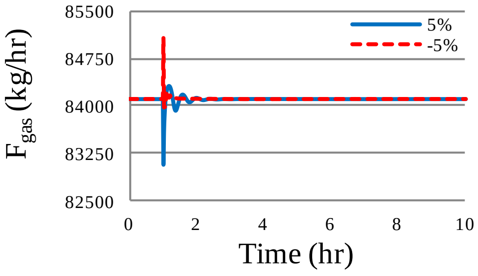
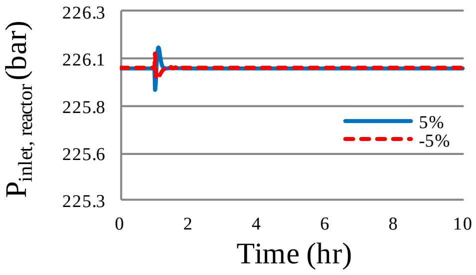
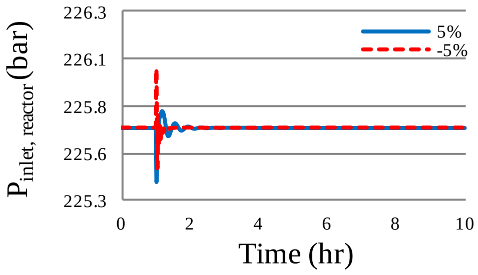
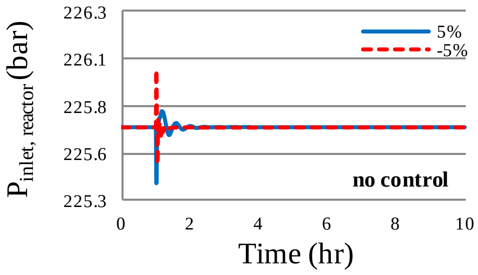
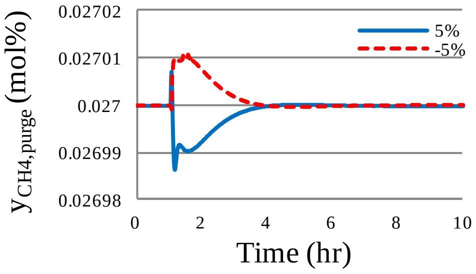
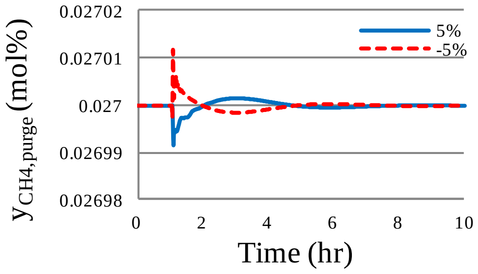
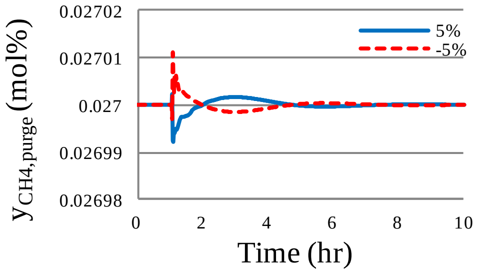
a.			
b.			
c.			

Table 5.8 Dynamic responses with Temperature feed changed.(Continue)

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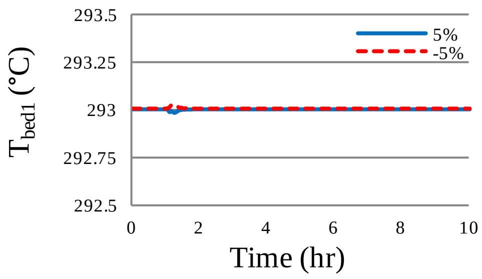
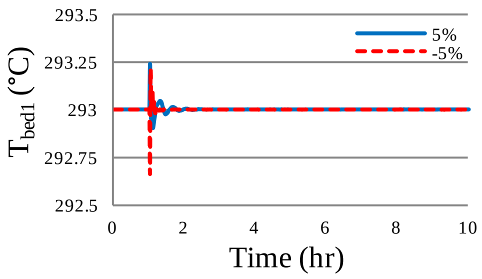
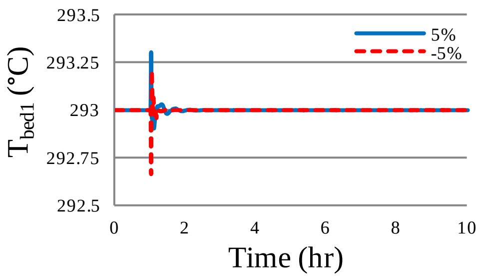
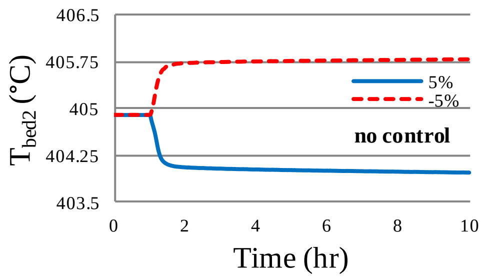
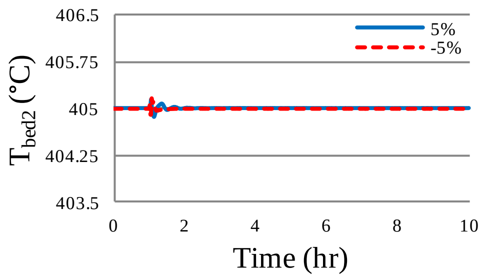
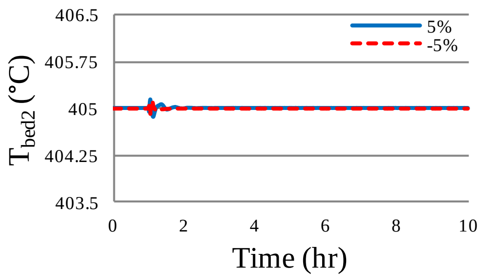
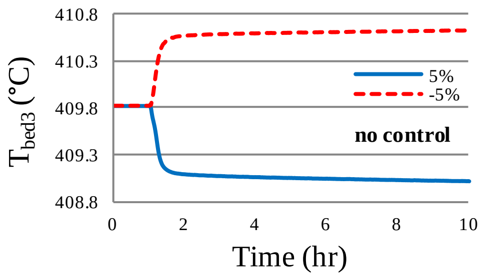
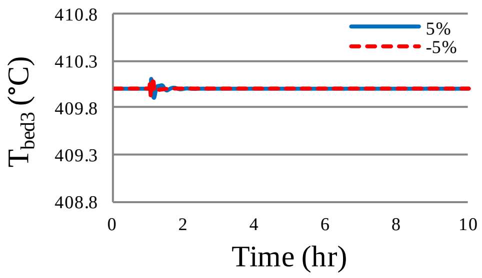
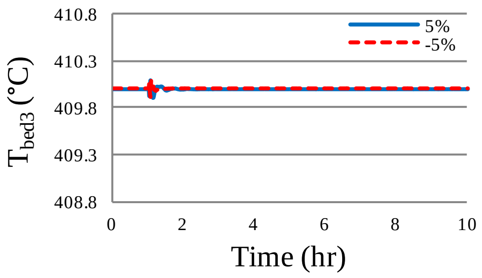
d.			
e.			
f.			

Table 5.8 Dynamic responses with Temperature feed changed. (Continue)

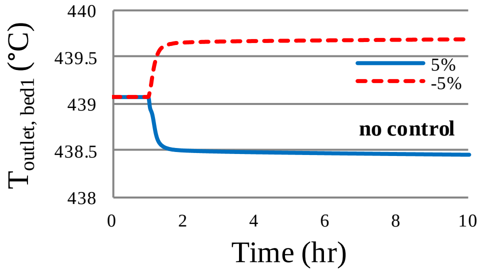
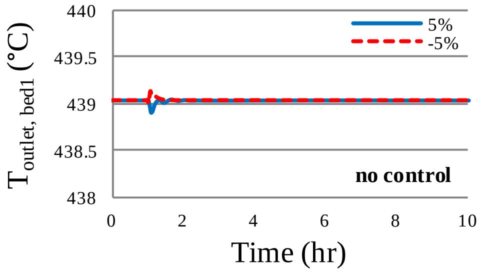
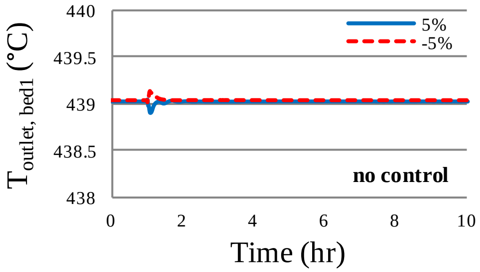
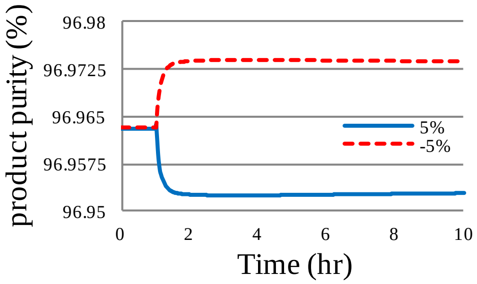
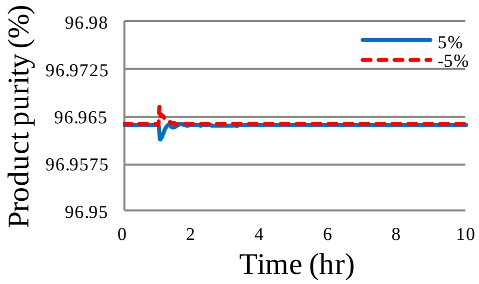
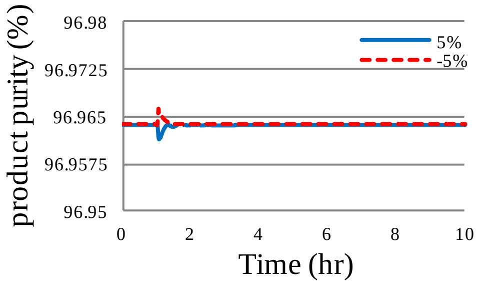
	Base Case	**CS1**	**CS2**
g.			
h.			

Table 5.9 Dynamic responses with methane composition in feed changed.

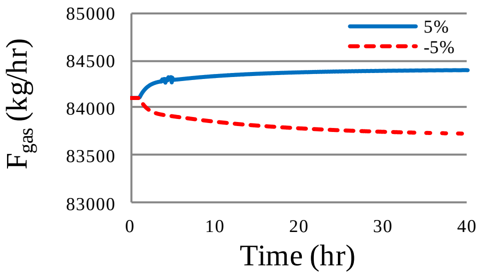
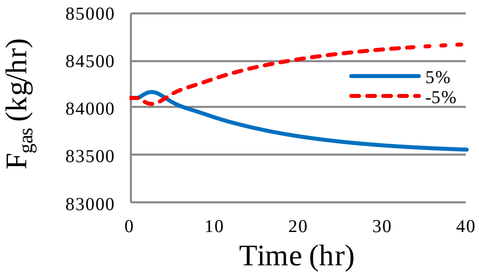
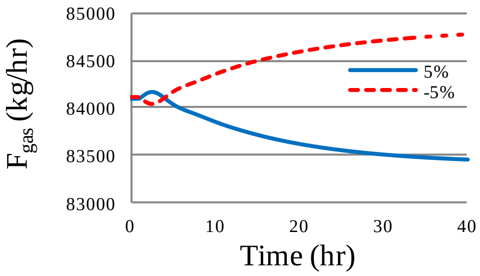
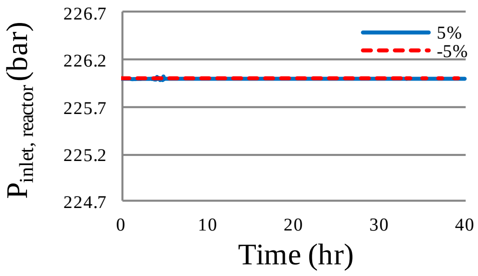
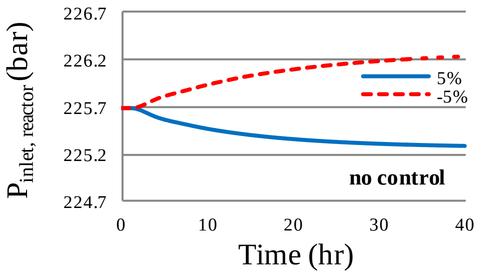
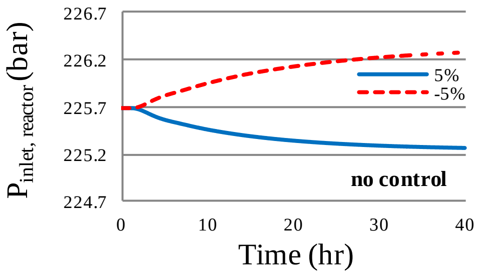
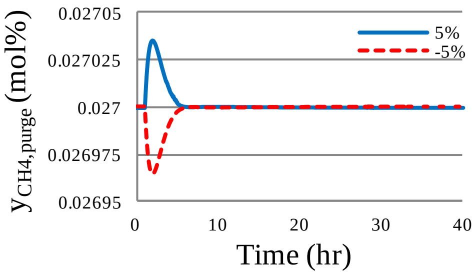
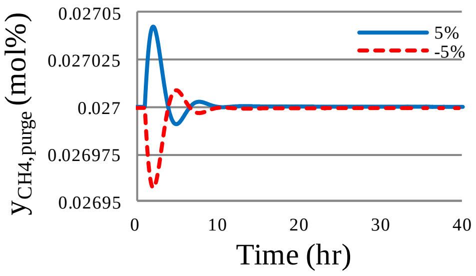
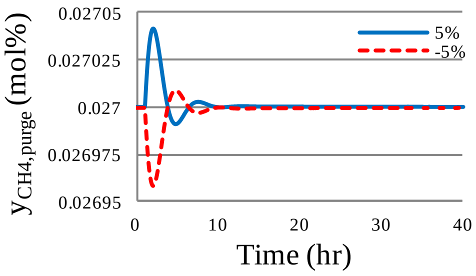
	Base Case	**CS1**	**CS2**
a.			
b.			
c.			

Table 5.9 Dynamic responses with methane composition in feed changed. (Continue)

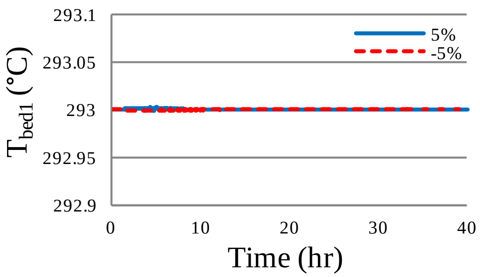
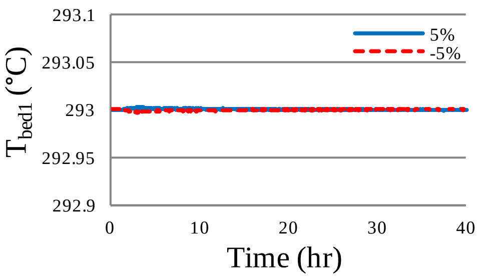
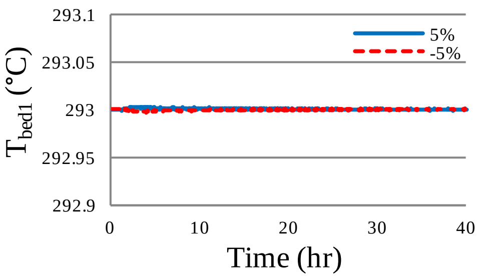
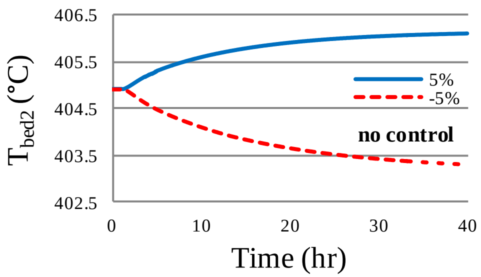
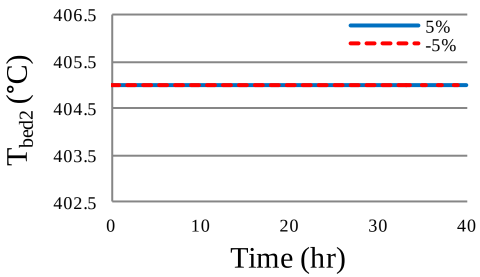
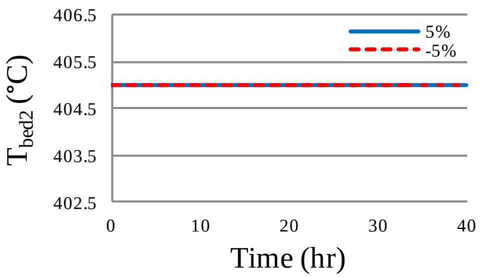
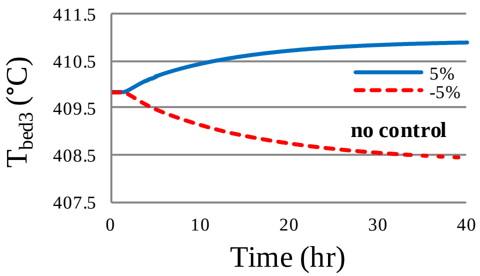
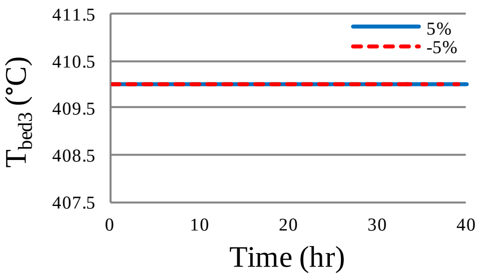
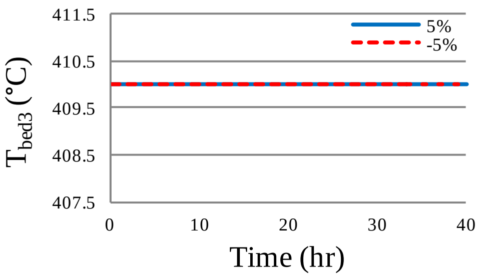
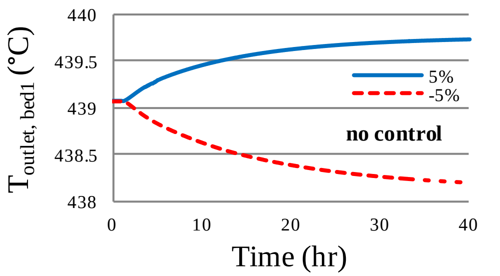
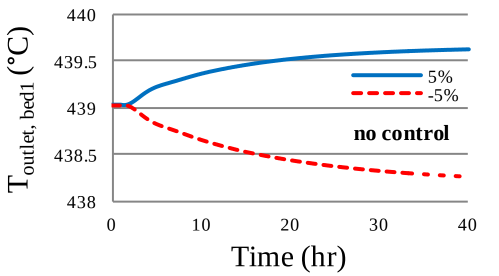
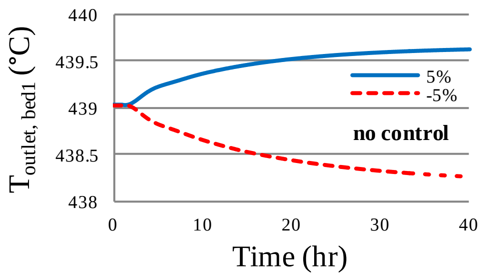
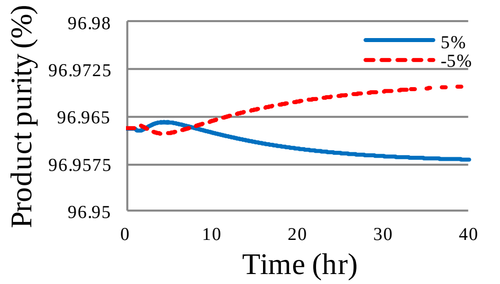
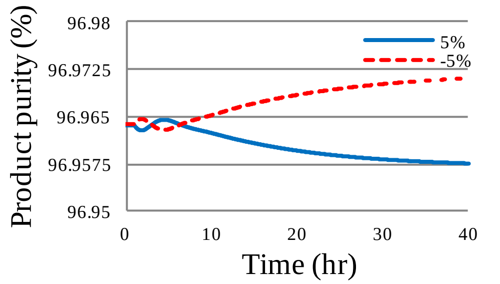
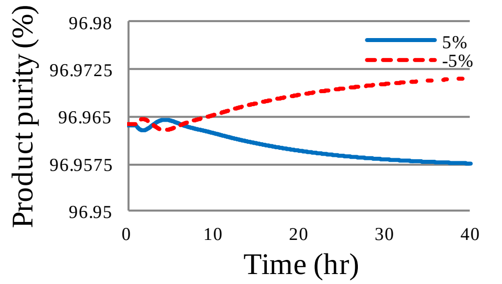
	Base Case	CS1	CS2
d.			
e.			
f.			

Table 5.9 Dynamic responses with methane composition in feed changed. (Continue)

	Base Case	**CS1**	**CS2**
g.			
h.			

5.2 Integral Absolute Error analyses (IAE)

The IAE is used for evaluating the control performance of the process when the disturbances are tested. The values of IAE are analyzed from the safety loops, which are temperature, pressure and composition. In the conclusion, the best control structure is the control structure has the minimum value of IAE. From the data given can be summarized that the control structure 2 (CS 2) has the smallest IAE value with gas and temperature feed changed. In the part of the methane composition in feed changed, the base structure (Base case) is the best control structure.

Table 5.10-5.12 shows the IAE value of each control structures which has been disturbed by several type of disturbances.

Table 5.10 IAE of safety control loop with gas feed changed.

Control structure	Composition	Temperature	Sum IAE
Base case	0.1315	0.0116	0.1431
CS1	0.0009	0.0097	0.0106
CS2	0.0013	0.0082	0.0095

Table 5.11 IAE of safety control loop with temperature feed changed.

Control structure	Composition	Temperature	Sum IAE
Base case	0.0643	0.0062	0.0705
CS1	0.0247	0.0239	0.0486
CS2	0.0245	0.0227	0.0472

Table 5.12 IAE of safety control loop with CH_4 composition in feed changed.

Control structure	Composition	Temperature	Sum IAE
Base case	0.1295	0.0023	0.1318
CS1	0.1442	0.0103	0.1545
CS2	0.1382	0.0083	0.1465

5.3 Utilities Cost

There are two types of the utilities in the process, Cooling water and Electrical power. The cooling power is used to cool the stream that outlet from reaction section and the electrical power is used to increase the pressure of feed stream and recycle stream. The cost of the both utilities are 0.03 $ per 1,000 gallon for cooling water and 0.04 $ per kWh for electrical power.

The electrical power of Base case, CS1 and CS2 is fixed (K-401 = 25,000 kW and K-402 = 3,500 kW), the cost of the electrical utilities are 9,986,400 $/year.

Table 5.13 Utilities cost when gas feed changed.

Control structure	**Cooling water (Gallon/year)**			**Utilities cost ($/year)**
	+5%	**-5%**	**Average**	
Base case	3,422,383,527	3,422,383,527	3,422,383,527	102,671.51
CS1	3,422,530,911	3,422,507,621	3,422,519,266	102675.58
CS2	3,422,552,027	3,422,510,157	3,422,531,092	102675.93

Table 5.14 Utilities cost when temperature feed changed.

Control structure	**Cooling water (Gallon/year)**			**Utilities cost ($/year)**
	+5 ˚C	**-5 ˚C**	**Average**	
Base case	3,422,383,527	3,422,383,527	3,422,383,527	102,671.51
CS1	3,468,168,098	3,377,919,654	3,423,043,876	102,691.32
CS2	3,468,180,994	3,377,929,793	3,423,055,393	102,691.66

Table 5.15 Utilities cost when methane composition in feed changed.

Control structure	**Cooling water (Gallon/year)**			**Utilities cost ($/year)**
	+1%	**-1%**	**Average**	
Base case	3,422,383,527	3,422,383,527	3,422,383,527	102,671.51
CS1	3,403,001,210	3,444,410,449	3,423,705,830	102,711.17
CS2	3,401,038,414	3,446,658,719	3,423,848,566	102,715.46

From the utilities cost table shows that for the disturbances tested, which are gas feed changed, temperature feed changed, and methane composition in feed changed, the smallest utilities cost belongs to Base case control structure followed by control structure 1 (CS1) and control structure 2 (CS2).

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The plantwide control structure design procedure of Wongsri is used to design the control structure of the ammonia process (CS1 and CS2). In the design steps, the procedure of Wongsri is simple and clearly which suitable for the novice designers.

The performance of each structure is evaluated by the IAE value. The control structure 2 (CS2) is the best control structure for the gas feed and temperature feed changed. In the part of the methane composition in feed changed, the base control structure (base case) can get the best deal.

The utilities cost of each structure is calculated from the cooling water and the electrical power. The base control structure (Base case) is smallest utilities in comparison with base case, CS1 and CS2.

6.2 Recommendation

The simulation data is referred from the work of Araújo and Skogestad (2008). In the part of simulation, the simulator program is used in this work (HYSYS dynamic simulator) that differs with Araújo and Skogestad forasmuch they used the Aspen Plus^{TM} dynamic simulator. Therefore, the data is used to simulated have a small different due to the model different in the two simulators.

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APPENDICES

APPENDIX A

STREAM TABLE

Table A.1 Stream table for the nominally optimal operating point for the ammonia production process

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Vapor fraction	1	1	1	1	1	1	1	1	1	1	1	1
Temperature (°C)	231.7	231.7	340.1	231.7	231.7	231.7	231.7	231.8	231.8	306.5	418.9	389.3
Pressure (bar)	206	205	204	206	206	206	204	203	202	204	203	203
Molar flow (kmole/hr)	5.207e4	2.625e4	2.625e4	6613	7238	1.198e4	1.198e4	7238	6613	3.822e4	3.556e4	4.279e4
Mass flow (kg/hr)	4.782e5	2.410e5	2.410e5	6.074e4	6.648e4	1.100e5	1.100e5	6.648e4	6.074e4	3.510e5	3.510e5	4.175e5
Heat flow (KW)	-7.882e4	-3.972e4	-1.360e4	-1.001e4	-1.096e4	-4.268e4	-4.268e4	-1.096e4	-1.001e4	-3.173e4	-3.173e4	-4.268e4
Mole fraction												
Hydrogen	0.6303	0.6303	0.6303	0.6303	0.6303	0.6303	0.6303	0.6303	0.6303	0.6303	0.5651	0.5761
Nitrogen	0.1052	0.1052	0.1052	0.1052	0.1052	0.1052	0.1052	0.1052	0.1052	0.1052	0.0756	0.0806
Methane	0.0288	0.0288	0.0288	0.0288	0.0288	0.0288	0.0288	0.0288	0.0288	0.0288	0.0309	0.0305
Argon	0.0214	0.0214	0.0214	0.0214	0.0214	0.0214	0.0214	0.0214	0.0214	0.0214	0.0230	0.0227
Ammonia	0.2413	0.2413	0.2413	0.2413	0.2413	0.2413	0.2413	0.2413	0.2413	0.2413	0.3054	0.2900
Water	0	0	0	0	0	0	0	0	0	0	0	0

Stream	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Vapor fraction	1	1	1	1	1	1	0.8414	0.9256	1	1	1	1
Temperature (°C)	415	391.9	412.4	358.3	296.9	120.1	60	64.01	63.88	63.88	70.63	63.88
Pressure (bar)	202	202	201	200	199	197	196	196	195	195	208	195
Molar flow (kmole/hr)	4.207e4	4.868e4	4.803e4	4.803e4	4.803e4	4.803e4	4.803e4	5.625e4	5.208e4	5.207e4	5.207e4	4.714
Mass flow (kg/hr)	4.175e5	4.783e5	4.783e5	4.783e5	4.783e5	4.783e5	4.783e5	5.493e5	4.783e5	4.782e5	4.782e5	43.29
Heat flow (KW)	-4.268e4	-5.269e4	-5.269e4	-7.882e4	-1.079e5	-1.890e5	-2.533e5	-2.343e5	-1.630e5	-1.630e5	-1.598e5	-14.75
Mole fraction												
Hydrogen	0.5603	0.5698	0.5570	0.5570	0.5570	0.5570	0.5570	0.5846	0.6303	0.6303	0.6303	0.6303
Nitrogen	0.0734	0.0777	0.0719	0.0719	0.0719	0.0719	0.0719	0.0977	0.1052	0.1052	0.1052	0.1052
Methane	0.0311	0.0308	0.0312	0.0312	0.0312	0.0312	0.0312	0.0271	0.0288	0.0288	0.0288	0.0288
Argon	0.0231	0.0299	0.0232	0.0232	0.0232	0.0232	0.0232	0.0203	0.0214	0.0214	0.0214	0.0214
Ammonia	0.3122	0.2989	0.3166	0.3166	0.3166	0.3166	0.3166	0.2703	0.2143	0.2143	0.2143	0.2143
Water	0	0	0	0	0	0	0	0	0	0	0	0

Stream	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	**34**	**Feed**	**Purge**
Vapor fraction	0	0.0006	1	1	0	0	0.3642	0	0	0	1	1
Temperature (°C)	63.88	63.91	17	308.2	15	15.12	143.5	15	15.12	96.76	17	63.65
Pressure (bar)	195	190	23.1	196	10	5	4	10	5	4	24.1	190
Molar flow (kmole/hr)	4172	4172	8223	8223	4441	4441	4441	3.886e4	3.886e4	3.886e4	8223	4.714
Mass flow (kg/hr)	7.096e4	7.096e4	7.100e4	7.100e4	8.000e4	8.000e4	8.000e4	7.000e5	7.000e5	7.000e5	7.100e4	43.29
Heat flow (KW)	-7.138e4	-7.138e4	-1092	1.896e4	-3.522e5	-3.522e5	-3.230e5	-3.082e6	-3.082e6	-3.017e6	-1092	-14.75
Mole fraction												
Hydrogen	0.0135	0.0135	0.7453	0.7453	0	0	0	0	0	0	0.7453	0.6303
Nitrogen	0.0046	0.0046	0.2484	0.2484	0	0	0	0	0	0	0.2484	0.1052
Methane	0.0065	0.0065	0.0033	0.0033	0	0	0	0	0	0	0.0033	0.0288
Argon	0.0059	0.0059	0.0030	0.0030	0	0	0	0	0	0	0.0030	0.0214
Ammonia	0.9696	0.9696	0	0	0	0	0	0	0	0	0	0.2143
Water	0	0	0	0	1	1	1	1	1	1	0	0

APPENDIX B

TUNING PARAMETERS

Table B.1 Type of controllers and tuning parameters of base case

Equipment	**Controller**	**Controlled variable(CV)**	**Manipulated Variable (MV)**	**Type**	**Action**	**Nominal value**	**PV range**	**Tuning Parameters**		
								K_c	τ_i	τ_D
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse	84,108 (kg/hr)	0 - 1.4×10^5	6.75	0.39	-
Reactors	PC_1	Inlet Pressure	Set point of FC_1	PI	Reverse	226 (bar)	113 - 339	5.55	4.99	-
Separator	LC_1	Liquid level	Liquid flow out	P	Reverse	50%	0 - 100	2	-	-
Purge	FC_2	Flow rate	Purge flow rate	PI	Reverse	346 (kg/hr)	0 - 600	0.5	0.3	-
	CC_1	Methane composition	Set point of FC_2	PI	Direct	0.027	0.0135 - 0.0405	93.4	72.9	-
Reactor 1	TC_1	Inlet temperature	By-pass flow rate	PID	Direct	293 (˚C)	261 - 361	8.05	1.60	

Table B.2 Type of controllers and tuning parameters of CS1

Equipment	**Controller**	**Controlled variable (CV)**	**Manipulated Variable (MV)**	**Type**	**Action**	**Nominal value**	**PV range**	**Tuning Parameters**		
								K_C	τ_i	τ_D
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse	84,10 (kg/hr)	0 - $1.7\text{x}10^5$	0.5	0.3	-
Feed gas	FC_2	Total flow rate	Set point of FC_1	PI	Reverse	536,903 (kg/hr)	0 - $1.08\text{x}10^6$	2.61	0.631	-
Separator	PC_1	Column pressure	Vapor flow out	PI	Reverse	215.64 (bar)	107.82 - 323.46	22.2	0.872	-
	LC_1	Liquid level	Liquid flow out	PI	Reverse	50 %	0 - 100	8.33	0.916	-
Purge	FC_3	Flow rate	Purge flow rate	PI	Reverse	339.9 (kg/hr)	0 - 1000	0.239	$7.24\text{x}10^{-2}$	-
	CC_1	Methane composition	Set point of FC_3	PI	Direct	0.027	0.0135 - 0.0405	30.1	30.9	-
Reactor 1	TC_1	Inlet temperature	By-pass flow rate	PID	Direct	293 (˚C)	261 - 361	6.70	1.92	0.426
Reactor 2	TC_2	Inlet temperature	Flow rate of cooling stream	PID	Direct	405 (˚C)	350 - 450	1.21	2.87	0.638
Reactor 3	TC_3	Inlet temperature	Flow rate of cooling stream	PID	Direct	410 (˚C)	360 - 460	2.50	2.34	0.520
H-502	TC_4	Outlet temperature	By-pass flow rate	PID	Direct	235.5 (˚C)	185.5-285.5	11.1	1.77	0.393
H-583	TC_5	Outlet temperature	Water flow rate	PID	Direct	47.84 (˚C)	0 - 100	2.82	3.18	0.706
	TC_6	Inlet temperature of separator	Set point of TC_5	PID	Direct	57.4 (˚C)	7 - 107	1.10	5.67	1.260

Table B.3 Type of controllers and tuning parameters of CS2

Equipment	Controller	Controlled variable(CV)	Manipulated Variable (MV)	Type	Action	Nominal value	PV range	Tuning Parameters		
								K_c	τ_i	τ_D
Feed gas	FC_1	Flow rate	Feed flow rate	PI	Reverse	8,4104 (kg/hr)	0 - 1.7×10^5	0.5	0.3	-
Reactor	FC_2	Flow rate	Set point of FC_1	PI	Reverse	452,799 (kg/hr)	0 - 9.06×10^6	2.68	0.731	-
Separator	PC_1	Column pressure	Vapor flow out	PI	Reverse	215.64 (bar)	107.82 - 323.46	21.0	0.922	-
	LC_1	Liquid level	Liquid flow out	PI	Reverse	50 %	0 - 100	7.91	0.982	-
Purge	FC_3	Flow rate	Purge flow rate	PI	Reverse	339.9 (kg/hr)	0 - 1000	0.238	5.4×10^{-2}	-
	CC_1	Methane composition	Set point of FC_3	PI	Direct	0.027	0.0135 - 0.0405	30.8	30.1	-
Reactor 1	TC_1	Inlet temperature	By-pass flow rate	PID	Direct	293 (˚C)	261 - 361	6.97	1.58	0.351
Reactor 2	TC_2	Inlet temperature	Flow rate of cooling stream	PID	Direct	405 (˚C)	350 - 450	1.22	2.84	0.630
Reactor 3	TC_3	Inlet temperature	Flow rate of cooling stream	PID	Direct	410 (˚C)	360 - 460	2.5	2.34	0.52
H-502	TC_4	Outlet temperature	By-pass flow rate	PID	Direct	235.5 (˚C)	185.5-285.5	11.2	1.74	0.386
H-583	TC_5	Outlet temperature	Water flow rate	PID	Direct	47.84 (˚C)	0 - 100	3.0	3.06	0.681
	TC_6	Inlet temperature of separator	Set point of TC_5	PID	Direct	57.4 (˚C)	7 - 107	1.30	5.18	1.150

VITAE

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