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PLANTWIDE CONTROL STRUCTURES DESIGN FOR MODIFIED ETHYL BENZENE PROCESS

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A Thesis Submitted in Partial Fulfillment of the Requirements
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In this thesis, plantwide control structure design of ethyl benzene (EB) process has been investigated. The ethyl benzene process incorporates the reaction of benzene with ethylene to form the desired EB product and the undesired di-ethyl benzene (DEB) by-product. The DEB is continuously recycled with no exit or recycled to “extinction’’ (no net DEB product produced). The optimum flowsheet is obtained from Luyben (2010). Two effective plantwide control structures are developed using Wongsri’s procedure. The main emphases of the procedure are establishing a fixture plant (material-balanced control and fixed process inputs) and disturbance management. An analysis of results shows that the design structures have better control performances compared to Luyben (2010).

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NOMENCLATURES

CS	Control Structure
CV	Controlled variable
D	Distillate flowrate (kmol/h)
DOF	Degree of freedom
F	Flowrate of the stream (kmol/h)
HENs	Heat Exchanger Networks
HIPs	Heat Integrated Processes
IAE	Integral Absolute Error
ID	Column diameter
K_C	Controller gain (dimension less)
K_U	Ultimate gain
Q	Heat load
MV	Manipulated variable
P	Proportional controller
PI	Proportional integral controller
PID	Proportional integral derivative controller
P_U	Ultimate period
R	Reflux flow
RR	Reflux flowrate to distillate flowrate ratio (R/D)
R/F	Reflux flowrate to feed flowrate ratio
τ_I	Controller integral time (min)

CHAPTER I

INTRODUCTION

1.1 Importance and reasons of research

The most industrial applications involve problems with multiple processing units that interact with each other and contain many units, such as reactors, furnaces, absorbers, heat exchangers, and distillation columns. The topic of plantwide control deals with unit to unit interactions through the choice of controlled and manipulated variables in each unit. The challenge of plantwide control is the design a control structure to counteract of disturbances before they propagate to other units.

Procedures of control design applied to industry have a many different unit operation, complicated process flowsheet containing recycle stream and energy integration. The goal of plantwide control structure design is selection of controlled and manipulated variables that quickly respond and counteract of disturbances. The minimum capital costs are considered while operating (optimum utilization of materials and energy) that is no more complicated and expensive than necessary and that, when built, can be operated easily by typical plant operators. Ultimately, the only definitive way of validating a selected plantwide control system design is by plant tests and by the operating plant’s performance. Finally, the new control structures are compared with basecase by using the plantwide control procedure of Wongsri (2012).

Ethyl benzene process is widely process used in most industry because this plant is a realistically complex chemical process. In this research, the ethyl benzene is studied on steady state, the efficiency of the designed control structure and observes the dynamic behaviors though Wongsri’s procedures. The effective operation is analyzed by using commercial process simulator and evaluated the performance of the designed structures on dynamic simulations.

1.2 Research Objectives

To design new plantwide control structures of ethyl benzene process proposed by Wongsri (2012).

1.3 Scopes of research

1. Simulation of the ethyl benzene plant is performed by using a commercial process simulator
2. Description and data of ethyl benzene process is given by Luyben (2010).
3. Present new control structure design procedure of Wongsri (2012) for plantwide control of ethyl benzene process.
4. Compare the new design control structures with the work proposed by Luyben (2010).

1.4 Expected Contributions

1. Steady state and dynamic models of ethyl benzene process is obtained by using commercial process simulator.
2. Evaluate the performance of the new designed plantwide control structures.

1.5 Research Procedures

The procedures of this research are as follows:

1. Study of general plantwide control structure theory, ethyl benzene process and concerned information.
2. Simulate of ethyl benzene process at steady state and dynamic.
3. Study about procedure design plantwide control structures of Wongsri (2012).
4. Design new control structures of ethyl benzene process as following Wongsri’s procedure.
5. Simulate the dynamic of the new design plantwide control structures to develop ethyl benzene process.
6. Assessment the dynamic performance of the design plantwide control structures.
7. Analyze the simulation results.
8. The research provides conclusions.

1.6 Research Framework

The thesis matter is classified six chapters as follow;

Chapter I: is an introduction to this research. This chapter consists of importance and reasons for research, research objectives, scopes of research, expected contributions and research procedures.

Chapter II: presents literature review related to plantwide control structures design procedures, review of previous work on the ethyl benzene process design, and control structure design.

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

Chapter IV: describes process description and the design control structure for ethyl benzene process.

Chapter V: describes the design of plantwide control structures and dynamic simulation results and compares with control structures of Luyben (2010).

Chapter IV: presents the conclusion of this research and makes the recommendation for future work.

This is follow by:

References

Appendix A: Ethyl benzene Process Stream and Equipment.

Appendix B: Parameter Tuning of Control Structures

Appendix C: IAE Results Data

CHAPTER II

LITERATURE REVIEW

2.1 Review of plantwide control structure design

Luyben (1994) presented a numerical case study of a recycle system that exhibited the "snowball" effect. The example process consisted of a continuous stirred-tank reactor followed by two distillation columns. In the simple binary first-order case of A → B, an analytical solution can be found for the recycle flowrate as a function of the fresh feed flowrate and fresh feed composition. Two other kinetic systems are studied numerically: consecutive first-order reactions A → B → C occurred in the reactor, with component B as the desired product. The volatilities of the three components were assumed to $\alpha_A > \alpha_B > \alpha_C$. Unreacted component A was recycled back to the reactor from the top of the first column. Luyben proposed the generic rule that one flowrate in a liquid recycle loop should be flow controlled. Results confirm the case study findings that snowball problems can be prevented by using a control structure that fixes the flowrate of one stream somewhere in a liquid recycle loop. In processes with one recycle, the flowrate of the reactor effluent can be set. In processes with two or more recycle streams, the flowrate of each recycle can be fixed.

Luyben (1996) presented one of the central problems in developing a steady-state process flowsheet. There is finding the number of variables that must be specified to completely define the process. This number is called the design degrees of freedom. The number of design optimization variables can be calculated by subtracting all variables that are set by specifications on production rate, product qualities, safety constraints, and environmental limitations. For complex industrial processes, there are many hundreds of variables and equations, and it is difficult to make sure that the correct variables and equations have been defined. The design of a control structure requires that the control degrees of freedom be known. It is very easy to calculate the number of variables that can be controlled because it is equal to the number of manipulated variables. These variables are different than the design optimization variables. Several progressively more complex recycle process case studies are used to show these results. The practical significance is that we do not need a model and we can avoid the error procedure of accounting for all variables and equations.

Luyben, et.al (1997) proposed the plantwide control structure design procedure by heuristics. The nine-step of this 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, component balances and economic or process optimization. They illustrated this procedure with three industrial examples: the vinyl acetate monomer process, Eastman process and hydrodealkylation (HDA) process. The procedure produced a workable plantwide control structure.

Larsson, et.al (2003) presented control structure selection for a simple plant with a liquid-phase reactor, a distillation column, and recycle of unreacted reactants. A definition of the operational objectives, constraints, and degrees of freedom is clearly specified. Active constraints should be controlled to optimize the economic performance. The selection of the suitable controlled variable for remaining unconstrained degree of freedom is main focus. The concept of self-optimizing control is used which is to search for a constant setpoint strategy with an acceptable economic loss. Both for the case with given feed rate where the energy costs should be minimized and for the case where the production rate should be maximized. A good feed variable is the reflux ratio L/F. This applied to single-loop control as well as multivariable model predictive control.

Skogestad (2004) presented a systematic procedure for control structure design for complete chemical plants. It started with defining the operational and economic objectives, and degree of freedom available to fulfill them. Other issues include inventory and production rate control, decentralized versus multivariable control, loss in performance by bottom-up design, and a definition of a the “complexity number” for the control system.

Konda, et.al (2005) presented the novel plantwide control (PWC) methodologies are becoming increasingly important as chemical processes are becoming more and more integrated with recycles for reason of safety, environmental considerations, and economics. They proposed an integrated framework of simulation and heuristics. By adopting this framework, simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The proposed framework is then successfully applied to an industrially relevant case study: the hydrodealkylation of toluene (HDA) process. An analysis of results shows that the proposed framework build synergies between the powers of both the simulation and the heuristics, thereby resulting in a practical plantwide control structure methodology that leads to a viable control system.

Suchada Suntisrikomol (2008) presented the “Fixture Point Theorem” for hydrodealkylation process (HDA) to select appropriate the set of controlled variables from a large number of candidate output. The fixture point control theorem states that the most disturbed points must be satisfactorily controlled by giving them consideration before other controlled variables. The maximum (scaled) gain is used to selecting and paring controlled variables with manipulated variables. In her study, the set of first rank of controlled variables are same as Luyben (1998). She selected three set of controlled variables (second and third rank from fixture point) and five control structures were designed and compared. In order to illustrate the dynamic behaviors of the control structures when economic disturbance load occur (such as change in methane composition in fresh feed gas and quencher outlet temperature), the performance of designed control structures were presented in IAE value and compared with reference structure. The designed structures are fast response and the most effective on compared with Araujo et al, (2006) and Luyben (1998).

Saowani Detjareansri (2009) proposed the control structures for alkylation process using new design procedure of Wongsri. The designed control structures are evaluated the dynamic performance compared with Luyben (2002) by two types of disturbances: material and thermal disturbances. She designed eight plantwide control structures. All the designed control structures have a good performance because it handle disturbances entering the process and can maintain product quality as compared by integral absolute error (IAE) and total energy use low. The Wongsri’s procedure is a useful design procedure for complex industrial process that leads to a good performance plantwide control system.

2.2 Review plantwide control structure design of ethyl benzene process

Luyben (2002) presented simplify process version of the ethyl benzene process with the process equipment and chemistry trimmed down to make the simulation easier, which it still contain the important topology of the process and illustrates the essential features of the plantwide dynamics simulation. The process consists of two liquid recycle which cause snowball effect. One of the heuristics of plantwide control is to put a flow controller somewhere in all liquid recycle loops, which prevents the snowball effect. The two liquid recycle can present both steady state and dynamic difficulties. The plantwide control structure for EB process, this system does an effective job in providing a basic regulatory control scheme. Then, he concluded that the "snowballing" of recycle streams is avoided by placing a flow controller in a location (the effluent of the second reactor) through which both recycle stream flow.

Luyben (2010) developed the economic optimum steady-state design to minimize total annual cost (capital and energy). An effective plantwide control structure is also developed. He designs and controls of an interesting multiunit process have been explored. The EB process displays several unusual features. The most unusual is the recycling to extinction of an undesirable byproduct DEB. Significant design trade-offs between reactor size and recycle flowrates exist that require detailed economic analysis to find the optimum design that balances the competing effects of the design optimization variables. A modified valve position control structure solves these problems by changing the benzene to ethylene ratio in response to changes in the DEB recycle flowrate. Very large disturbances can be effectively handled with the EB purity being maintained very close to its specification.

CHAPTER III

THEORY

Plantwide process control is very important to control a chemical plant with many interconnected unit operations. A typical chemical plant flowsheet has a mixture of multiple units connected that consist of reaction section, separation section and heat exchanger network. So plantwide process control is complex process control. We must devise the necessary logic and strategies to operate the plant safely and to achieve its design objectives. Our purpose of this chapter is to present plantwide control fundamentals.

3.1 The plantwide process control

A chemical plant may have thousands of measurements and control loops. By the term plantwide control it is not meant the tuning and behavior of each of these loops, but rather it meant the control philosophy of the overall plant with emphasis on the structural decisions. The structural decisions include the selection/placement of manipulators and measurements as well as the decomposition of the overall problem into smaller sub problems. In conclusion, plantwide control that meant control structure design for complete chemical plant.

In an industrial environment, a plant’s control strategy should be simple enough, at least conceptually, so that everyone from the operator to the plant manager can understand how it works. Our governing philosophy is it is always best to utilize the simplest control system that will achieve the desired objectives. The more complex the process, the more desirable it is to have a simple control strategy. This view differs radically from much of the current academic thinking about process control, which suggests that a complex process demands complex control. Our viewpoint is a result of many years of working on practical plant control problems, where it is important to be able to identify whether an operating problem has its source in the process or in the control system.

The design of a plantwide control strategy becomes a more important part of the overall process control design problem. The interrelation of the plantwide control strategy with the process chemistry and economics requires both control theory and also process knowledge. It has become apparent that the design of plant-wide control strategies involves not only the development and application of process control theory but also, in a more fundamental sense, the development of a methodology one uses to approach the plantwide control problem.

The need for a plantwide control perspective arises from three important features of integrated processes: the effects of material recycle, of chemical component inventories and of energy integration. However, we did not describe how we arrived at these strategies, and many of our choices may seem mysterious at this point. Why, for instance, did we choose to use fresh liquid reactant feed streams in the control of liquid inventories? What prompted us to have a reactor composition analyzer? Why were we concerned with a single direct handle to set production rate?

The subject of plantwide control deals with unit-to-unit interactions through the choice of measured and manipulated variables in each unit and the selection of a control strategy-namely, how to pair controlled and manipulated variables in individual loops, where to use multiloop controllers, where to use multivariable controllers.

The goals for an effective plantwide process control system include:

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

3.2 The main function of control system

Most industrial processes, the installed control system has main function.

- To reject disturbance

It is main function in the installation of process control system. The external disturbance is uncertain so the operator cannot monitor the changing in process. As a result, the control system must be installed to follow the process changing and manipulate the process variables to compensate for the external disturbance factors.

- To maintain stability

Every control system must guarantee first the stability. The control system is set to improve the process stability for ensure of product quality and safety to equipment of process and plant.

- To keep the highest performance of process

Besides the rejection of disturbance and maintaining stability, the control system can achieve the great profit because it losses less energy and raw materials during the operating. Furthermore the product will meet the desired specification and have production rate.

3.3 Integrated Processes

Basic feature of integrated chemical processes are the root of our need to consider the entire plant control system as follow:

1) The effect of material recycles
2) The effect of energy integration
3) The need account for chemical component inventories

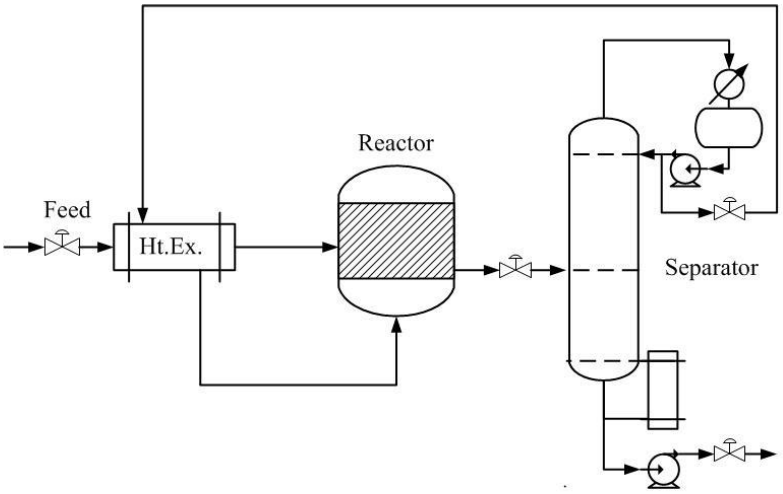


Figure 3.1 Integrated Processes Flowsheet.

From basic feature of integrated chemical processes above, if we did not have to worry, then we would not have to behave with a complex plantwide control problem. However, there are fundamental reasons why each there exists in virtually all real processes.

3.3.1 Material Recycle

Six important reasons and basic for material recycle:

1. Increase conversion: For chemical processes involving reversible reactions, conversion of reactants and products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.

2. Improve economics: In most systems it is simply cheaper to build a reactor with incomplete conversion level in one reactor or several in series. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.

3. Improve yields: In reaction systems such as $A \rightarrow B \rightarrow C$, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much of 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 of the reactants is often used so that the concentration of the other reactant is kept low. If this limiting reactant is not kept in low concentration, it could react to produce undesirable products.

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

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

3.3.2 Energy Integration

Energy integration is used for process to improve the thermodynamic efficiency, which this procedure is the fundamental reason of plantwide control. Pillar reason of this translates is reduction in utility cost. For energy-intensive processes, the savings can be quite significant.

3.3.3 Chemical Component Inventories

Species of a plant’s chemical can divided in three types: reactants, products, and inerts. A materials balance for each of these components must be satisfied. However, the real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every mole of reactants fed into the plant must be consumed via reaction or leave as a purge or impurity. Because of their value, we want to prevent loss of reactants or minimize the loss of reactants leaving from process.

This concept is an important for many chemical processes control. The point of view for the individual units, units automatically adjust their flow and composition of exit stream affect chemical component balancing is not a problem. However, when recycle streams are connected together with units. In terms of reactants, the entire system feature almost like a pure integrator in terms of reactants. If reactant is addition fed into the system without changing reactor conditions to exterminate the reactant. In the plant, this component will be create gradually because it no place to leave the system.

3.4 Plantwide Control Problems

Plantwide control problem has the cause from effects of recycle. The basic effects of recycle stream can be identified two points as follows:

3.4.1 Time constants in recycle systems

Recycle has an impact on the dynamics of the process. The overall time constant in recycle system can be much different than the sum of the time constants of individual units

3.4.2 Snowball effect

Recycle leads to the “snowball” effect. This has 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 flowrates. These disturbances can lead to even larger dynamic changes in flow, which propagate around the recycle loop.

“Snowball effect” is the high sensitivity of the recycle flowrates to small disturbances. Which snowball effect is important to note because this is not a dynamic effect but it is steady-state phenomenon. In the implications, it does have dynamic for inventory control and disturbance propagation also it has nothing to do with closed-loop stability. It is independent of the plant’s control structure. The scope of the snowball effect is very strongly dependent upon the control structure used on the contrary.

For recycle flowrates section that have the large swings are undesirable in our plant because of 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 keeps away from this effect.

3.5 Basic Concepts of Plantwide Control

3.5.1 Buckley Basics

Buckley (1964) of DuPont was the first to suggest the idea of separating the plantwide control problem. The control design procedures for the plantwide control problem are considered on two levels. The first determined the material balance control structure to handle vessel inventories for low-frequency disturbances. The second established the product quality control structure to regulate high-frequency disturbances. This procedure has been widely and effectively utilized. It has served as the conceptual framework in many subsequent ideas for developing control systems for complete plants. However, this Buckley procedure provides little guidance concerning three important aspects of a plantwide control strategy.

1. It does not explicitly discuss energy management.

2. It does not address the specific issues of recycle systems.

3. It does not deal with component balances in the context of inventory control.

By placing the priority on material balance over product quality controls, the procedure can significantly limit the flexibility in choosing the latter.

3.5.2 Stephanopoulos

Stephanopoulos (1983) clearly summarized the creativity involved in control-strategy synthesis for chemical plants. However, there is still little guidance in the literature on designing workable plantwide control systems. We present here such a systematic design procedure. Our framework in tackling a problem of this complexity is based upon heuristics that account for the unique features of plantwide control. The scope embraces continuous processes with reaction and separation sections. The procedure is based upon research by us and others, and our governing philosophy is it is always best to utilize the simplest control system that will achieve the desired objectives. Three industrial processes illustrate its application in this article. In addition, the procedure has been used successfully over several years in a number of commercial processes at DuPont.

3.5.3 Douglas doctrines

Jim Douglas (1988) 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. This implies that tight control of stream compositions exiting the process is needed.

2. Maximize flowrates through gas recycle systems to improve the yield. This rests on the principle that yield is worth more than energy.

The control structure implication is that it is not attempted to regulate the gas recycle flow and the recycle flowrate is maximized. This removes one control-degree of freedom and simplifies the control problem.

3.5.4 Downs drill

Jim Downs (1992) has insightfully pointed out the importance of looking as the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. We must ensure that all components (reactants, products, and inerts) have a way to leave or be consumed within the process. Most of the reactants fed into the process must be chewed up in the reaction because we want to minimize raw material costs and maintaining high purity products. And the stoichiometry must be satisfied down to the last molecule. Chemical plants often act as pure integrators in terms of reactants due to the fact that we prevent reactants from leaving the process through composition controls.

3.5.5 Luyben laws

Luyben (1997) has proposed a result of a number of case studies of many type of system, Bill Luyben suggests the following:

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

2. For system with reaction types such as $A+B \longrightarrow$ Products, a fresh reactant feed stream cannot be flow-controlled unless there is essentially complete one-pass conversion of one of the reactants.

3. If the final product comes from a distillation column, the column feed should be:

- Liquid, if the product is in the distillate flow.
- Vapour, if the product is in the bottom flow.

By this arrangement, disturbances in the feed flowrate or the feed composition have a smaller dynamic effect on the product than otherwise.

3.5.6 Richardson rule

Bob Richardson of Union Carbide suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel, because it provides more muscle to achieve the desired control objective. 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.

3.5.7 Shinskey schemes

Greg Shinskey (1988) has proposed a number of "advanced control" structures that permit improvements in dynamic performance. These schemes are not only effective, but they are simple to implement in basic control instrumentation. Liberal use should be made of:

- Ratio control
- Cascade control
- Override control
- Valve-position (optimizing) control.

3.6 Luyben’s plantwide control design procedure

The design procedure is carried out in nine steps, which contented the two fundamental of the overall conservation of energy and mass. Additionally, the procedure accounts for nonconserved entities within a plant such as chemical components (produced and consumed) and entropy (produced). Five of the nine steps deal with plantwide control issues that would not be addressed by simply combining the control systems from all of the individual unit operations. Steps 1 establish the control objectives. Step 2 determines the available degrees of freedom. Step 3 establishes energy management within the process and ensures production of heat (entropy) is properly dissipated. In Steps 4 and 5 the business objectives are concerned production rate, product quality, and safety. Step 6 involves total mass balance control, whereas in Step 7 check component balances, ensures chemical components are accounted because of nonconserved. In Step 8 individual unit operations complete for the control systems. Finally, Step 9 uses the remaining degrees of freedom for optimization and improved dynamic controllability. This heuristic procedure will generate a workable plantwide control strategy, which is not necessarily the best solution. Because the design problem is open-ended, the procedure will not produce a unique solution.

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 criteria lead to different control structures. These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.

Step 2: Determine Control Degrees of Freedom.

Count the number of control valves available.

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

Step 3: Establish Energy Management System.

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

We use the term "energy management" to describe two functions:

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

2. If heat integration does title for economic and operational reasons. Hence we should select manipulated variables such that the dynamic relation occur between process streams, then the second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensures that the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

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.

Determine what valve will be used to set throughput. Often design constraints require that production be set at a certain point. An upstream process may establish the feed flow sent to the plant. A downstream process may require on-demand production, which fixes the product flowrate from the plant. If no constraint applies, then we select the valve that provides smooth and stable production rate transitions and rejects disturbances.

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.

These important quantities are severed for economic and operational reasons. Hence the manipulated variables should be selected with the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times a large steady-state gains. The former give small closed-loop time constants, and the latter prevents problems with the range ability of the manipulated variable (control-valve saturation). The magnitudes of various flowrates also come into consideration.

Step 6: Control Inventories (Pressures and Levels) and Fix a Flow in Every Recycle Loop.

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

Determine the valve to control each inventory variable. These variables include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. In most processes a flow controller should be present in all liquid recycle loops. This is a simple and effective way to prevent potentially large changes in recycle flows that can occur if all flows in 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 disturbances. 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.

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. 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 (Shinskey, 1988). For example, Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

Step 9: Optimize Economics or Improve Dynamic Controllability.

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

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

3.7 Wongsri's Plantwide Control Design Procedures

Luyben et al. (1997) proposed a nine step heuristics procedure to design the plantwide control structure. This procedure is widely studied and used the plantwide process control community. Although the heuristic methodologies are easier to understand and implement but they just need the basic understanding of the process along with some experience. Thereby the structural design procedure is given explicitly. The designer's process engineering insight is necessity to pair CVs and MVs. Skogestad (2004) presented the new design procedure based on mathematical analysis. First, the operational objectives and the dynamic and steady state degree of freedom are identified. Then the set of primary controlled variables are selected. They basically are the active constraints and variables that must be maintained to achieve minimal economic loss when disturbances or implement error occur. Then the production rate is set based on the optimization resulted in the previous step. The secondary controlled variables are selected and the pairing of the choose sets of MVs and CVs are done hierarchically: regulatory control, supervisory control and optimization layers. In these steps, several analysis tools are utilized, e.g. pole vector analysis, RGA, CLDG analysis, linear and nonlinear optimization. This procedure does not discuss about the precedence of control variables and how to handle the disturbances.

3.7.1 Fixture Point Theorem

Hagglund (1995) present the real-time oscillation detection by calculates the integrated absolute deviation (IAE) between successive zero crossing of controller error signal. Its motivation is automatic monitoring of control-loop performance. The concept of material and energy disturbance propagation controls lead to fixture point theorem.

The plantwide control structure design procedures are developed by Wongsri via fixture point theory. The heuristic is used to select pairs of controlled and manipulated variables and uses the dynamic simulation to obtain the main control structure.

Fixture point theorem analysis:

1. The process is considered at dynamic mode (we run the process until the process responses are at the steady state).

2. Controlled variable can be arranged to follow the most sensibility of the process variable by step changes of the manipulated variable in open loop control (change only one MV, the other should be fixed then alternate to other until complete).

3. Study the magnitude of integral absolute error (IAE) of all process variables that deviates from steady state.

4. Select controlled variable (CV) by considering CV that gave the most deviation from steady state (high value score).

3.7.2 New plantwide control structure design procedures of Wongsri (2012)

The new plantwide control design procedure extended in detail each of the eight steps, which proposed by Wongsri (2012). The new plantwide control design procedure emphasis on maintaining the plant operating conditions, i.e. establishing a fixture plant. The amount of components is accounted by regulating the material quantifiers which are locations within the plant indicating the amount of the components. The material quantifier is a more general term than the material inventory, it includes flowrate. Additionally, the entered disturbance must be forced to leave the process plant at the nearest exits to avoid disturbance propagation through the plant. The plantwide control structure design is indeed a structural decision about placing control loops though out the plant to above objectives. It is divided into two levels: plant level and unit level designs. The new design procedure is carried out in eight steps, the major steps deal with plant level design. Step 1 gathers the process plant information and the control objective of the process plant. Step 2 analyzes the available degrees of freedom, heat and material pathways, and reaction and separation sections; locates the material quantifiers. Step 3 establishes the fixture plant to ensure that all chemical components are accounted for. Step 4 ensures the heat and material disturbances are rejected to environment, compensated within, or directed to the designated pathways. Step 5 is about unit level design, i.e. design the rest of the control loops using only unit level information. Step 6 conserves the thermal energy via the heat exchanger network. This step creates the heat integrated process design alternatives (HIPs). Step 7 optimize economics and/or improve control performance. Step 8 Validate the designed control structures by rigorous dynamic simulation.

The design procedure is carried out in eight steps. Lists below are the fundamental concepts and techniques of Wongsri’s procedure:

Step 1: Gather relevant plant information and control objectives

Information and control objectives include constraints for control. Before initiating work on the control structure design, is it necessary to obtain all information relevant to process control. The process objectives and constraints will determine the lower/upper bounds on the control variables as well as set points on quality variables.

Step 2: Plant Analysis.

2.1 Control degree of freedom (CDOF). List manipulated variables (control degree of freedom, CDOF).

List all control variables:

I. An independent stream must have a control valve (1 DOF) you cannot place two control valves on a single stream.

II. A heater, cooler, pump, or compressor has one degree of freedom (to adjust heat load or duty or work load)

III. A process to process heat exchanger has one degree of freedom by adding a by-pass line.

IV. A reactor has zero or one degree of freedom depends on its type. For example, an isothermal reactor need heat input to keep its temperature constant, while an adiabatic reactor has zero degree of freedom.

V. A flash separator has two degree of freedom.

VI. A simple distillation column has five degree of freedom.

The guideline for pairing the controlled variables with the manipulated variables is presented in Table 3.1.

Table 3.1 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 longer.
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).
6	The change of the manipulated variables should not or have little effect on others variables (low gains with the remainder of the variables)

2.2 Heat pathway.

Three different "heat pathways" introduced in Luyben (1997) is also useful in plant analysis from a plantwide perspective. The first pathway is from inside the process and flows out to the environment heat generated by exothermic reactions and by degradation of mechanical work. The second pathway carries heat from utilities into the process and to the environment. The third pathway is internal to the process. The heat flow is circular and its magnitude depends upon the heating and cooling needs and the amount of heat integration implemented. The fourth pathway is introduced here. This pathway is accounted for the enthalpies entered and leaved the plant via process stream.

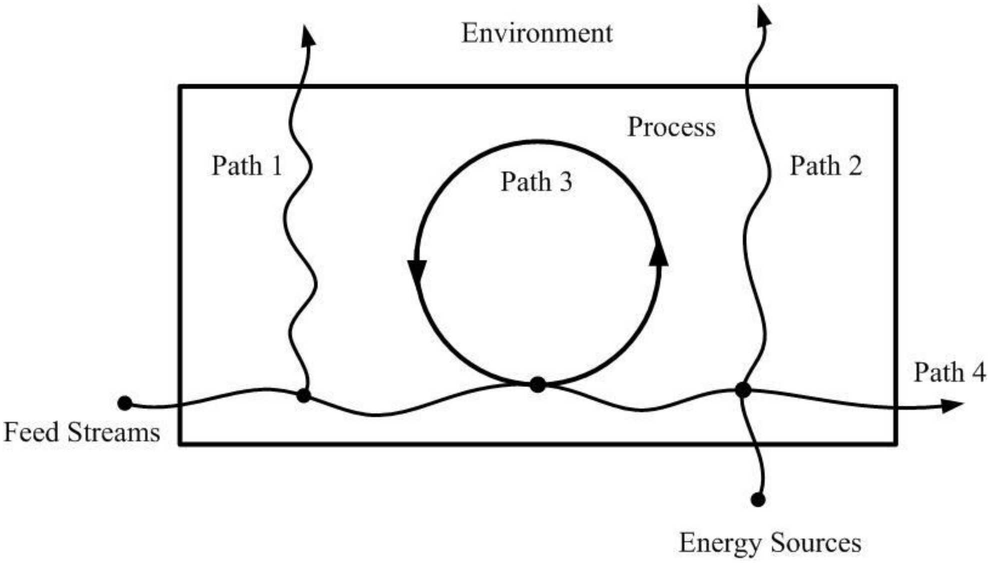


Figure 3.2 Heat pathways.

The level of heat circulated of the four pathway can be adjusted to optimize the energy used (step 7). The heat pathway is used to design control loops to reject the disturbances or to maintain the product qualities.

2.3 Material pathway.

The concept of material pathway is introduced here. The pathway is the flow path of a component from an entry point or an originated point to an exit point or an end point. The material pathway is useful for component balance and in control design as discussed in section 3 and section 4.2.

2.4 Material quantifier.

The notion of material quantifier is also introduced here. In order to regulate a component balance in a process plant, a place representing the amount of material in the plant must be identified to provide its handle. A material balance for each component must be satisfied. From the viewpoint of individual units, chemical component balancing is not a problem because exit streams from the unit 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. For example, we want to minimize the loss of reactants exiting the process since we would lose its value. This means we must ensure that most of reactant fed to the process is consumed by the reactions. If reactants increase, the reactor conditions must be adjusted to consume more reactants. In the case that increasing one reactant composition will decrease the other reactant composition with an uncertain net effect on reaction rate. If this case is not effectively handled, the process will shut down when manipulated variable constraints are encountered in the separation section. Luyben (1997) gives a more complete discussion of this phenomenon. The features of material recycle and chemical component inventories mentioned above which have profound implications for a plant's control strategy (Luyben, 1997) can be handled quite readily by making use of quantifiers. By locating a quantifier, we can regulate the quantity of a component quantified by using its handle.

It is seen that a material quantifier is not the same as a material inventory, i.e. it can be a quantity other than volume or pressure. It is used to indicate the representative amount of component(s) in the plant for the purpose of keeping a plant at a designed state.

2.5 Reaction section (where to measure the extent of reaction).

Practical aspects of industrial reactor control must be studied to obtain necessary information for reactor section control design. Since relatively little literature on chemical kinetics and reactor engineering has been written on the practical aspects of industrial reactor control

2.6 Separation section (disturbances tests to find the best place to detect the disturbances.)

The sensitivity test is suggested to be done on the changing of composition, total flow, temperature, and component flow while keeping the reboiler heat duty and reflux flow or reflux ratio constants. This sensitivity test is to spot the tray with the largest changes in temperature from the initial steady state. This is the exact situation happen right after the disturbance entering the column, when the column temperatures are controlled by manipulating the reboiler heat duty and reflux flow or reflux ratio. Hence the trays with largest changes may be good locations to control.

Step 3: Establish fixture plant.

The principal idea of establishing a fixture plant is first to have an entire plant fluid-filled and a material-balanced. This idea is similar to creating hydraulic control structure proposed by Buckley (1964). By establishing a fixture plant we mean creating a material-balanced process plant:

3.1 keep the materials entered and reentered fixed.

$$q_i(t) + q_r(t) = \text{constant} \tag{3.1}$$

This leaves the recycle streams free to adjust; one degree of freedom is added to the process. If the composition of the recycle streams differ from the fresh feed stream significantly, each stream are separately controlled:

$$q_i(t) = \text{constant} \tag{3.2}$$

$$q_r(t) = \text{constant} \tag{3.3}$$

In this settlement, the flow of recycle stream cannot be used to regulate, e.g., the level of the reflux drum.

3.2 Regulate the production rate.

3.2.1) Consume the limiting reactant. The limiting reactant should be totally consumed at the reactor for the economic reason. Determine the most appropriate manipulate variable to control this, i.e. the reactor temperature, the reactor pressure, or the reactor holdup.

3.2.2) Regulate the production rate. The product rate can be regulated through 3.2.1. If this is done and the production rate does not reach the objective or the production demand, the limiting reactant feed rate must be increased. The reaction information about the accumulation or depletion of the limiting reactant must be used to determine the control strategy. However the design constraint may limit this strategy concerning increasing the reactant feed rate.

3.3 adjust the flow of exit material streams (products, by-products, and inert) according to their accumulations.

$$q_o(t) = q_i(t) - dq/dt \tag{3.4}$$

3.4 Control the inventory of the rest of the component at their 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 flowrate.

$$q_p(t) = - dq/dt \tag{3.5}$$

$$q_p(t) = \text{constant} \tag{3.6}$$

In retrospect, the material balances are checked in this step, since the control loops generated accomplish the plantwide material balances. Therefore, it is guaranteed the plantwide inventory will be regulated.

Step 4: Disturbance Management

In this step, the disturbances are handled by configuring the control loops employing the principle of disturbances management:

4.1 Heat Disturbance Management

. The Heat disturbance is divided into 2 categories. Heat Disturbance Category 1 (HDC1) is the heat disturbance that does not directly effect on 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 disturbance that will affect 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 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 or cooler of process to process heat exchanger.

4.1.2 Manage the thermal disturbance that related to quality in order to maintain the product specification constraints.

4.2 Material Disturbances Management.

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 material disturbances can be generated at reactors and separators, besides coming with feeds and recycle streams. So if the feeds and recycle streams are fixed, the only places that alter the material (total or component) flowrates are the reactors and the separators. At reactor, its inlet temperature is adjusted in order to keep the reactor component flowrate or its composition in outlet stream. The decision of whether how to choose to control the component flow or the composition or not to control is based on the profit maximization or the smooth operation policies. The control structure we select must reject the disturbance to the desired pathways. As in the case of heat disturbance management, we direct the material disturbances to the environment via the next and nearest exit points, usually separators, to keep the material conditions of process stream fixed.

How to direct material disturbance? At a splitter (e.g. a distillation column), we must decide which paths to push extra loads or disturbances to. It is depend on how we want to manage the extra loads to keep the plant running smoothly and the quality of the products. For example, we don't want to push the extra loads to the product stream. It is always designable to reject the disturbance out of the process plant as soon as possible. Thirdly, we prefer to keep the recycle flow constant in the case that its composition differs significantly from the make-up feed. However if this is not allowed, we must trade-off between pushing the extra loads to the recycle stream and keeping it constant.

Ratio Control on Feeds, add ratio control to accommodate the variation of one of the fresh feed in the case that the two feeds must be proportional.

Single-end Control, which End? Since the distillation columns, usually the one-point control is common. To control top or bottom temperatures, depend on the material disturbance rejection policy. The control policy of a distillation column is to reject or direct disturbances to the designated pathways. For example, a recycle distillate flow must be maintained. Product purity must be maintained.

Fixing Reflux flow, Reflux Ratio or Reflux to feed, to aid in making this choice, a series of dynamic simulation runs can be made in which the effects of changes in composition, temperature, total flow and component flow of distillation column feed.

Single-end or dual-end control, if there are two locations with large changes in the temperature profiles when the sensitivity test is performed (see Step 2.6), so it may be possible to use dual-temperature control if this structure is required.

Step 5: Design the rest of the control loops.

5.1 Design the control loops for the remaining control variables, i.e. the rest of the inventories.

5.2 Adding enhanced controls, i.e. cascade, feed forward controls.

Step 6: Energy management via heat exchanger networks.

If potential heat exchanger networks or alternative heat integrated processes (HIPs) exist, list additional control variables and manipulated variables.

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

For example, the controls scheme/structure of the reactor (e.g. temperature/composition sensor location), the control scheme of the distillation column (e.g. reflux to feed ratio control), the optimal operating temperatures of the reactors, the recycle flowrates, the sequence of separation, etc. If the opportunity of optimization exists, we might backtrack to the previous step as dictated.

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.

CHAPTER IV

ETHYL BENZENE PROCESS

4.1 Introduction

Ethyl benzene (EB) is an aromatic hydrocarbon. It is an important commodity chemical. Much of its production is used to make styrene. Most commercial ethyl benzene (EB) is produced from benzene (liquid phase) and ethylene (vapor phase). The ethyl benzene process consists of several unit operation, two reactors in series (Both the reactors operate at high pressure to maintain liquid in the reactor at high temperatures required for reasonable reaction rates), two distillation columns and two liquid recycle streams. In the ethyl benzene process, fresh feed ethylene (pure) and benzene are mixed with recycled benzene (99.89% benzene and 0.001% ethyl benzene) fed to the first of two CSTR reactor. Thus it provides a nice example of a multiunit complex process that is typical of many chemical plants found in industry.

4.2 Reaction Mechanism and Kinetics

First reaction, the production of EB takes place via the direct addition reaction between ethylene and benzene

$$C_2H_4 \quad + \quad C_6H_6 \longrightarrow C_8H_{10} \tag{4.1}$$

Ethylene + Benzene ⟶ Ethyl benzene

A second reaction, the reaction between ethyl benzene and ethylene to produce di-ethylbenzene (DEB) which there is undesirable reaction also takes place. We can present second reaction as follow:

$$C_8H_{10} \quad + \quad C_2H_4 \longrightarrow C_{10}H_{14} \tag{4.2}$$

Ethyl benzene + Ethylene ⟶ Di-ethylbenzene

A third reaction, the DEB reacts with benzene to form EB. We can present third reaction as follow:

$$C_{10}H_{14} \quad + \quad C_6H_6 \longrightarrow 2C_8H_{10} \tag{4.3}$$

Di-ethylbenzene + Benzene ⟶ 2Ethylbenzene

This reaction makes it possible to recycle the DEB back to the second reactor where an excess of benzene exists and drives the reaction to the right to produce EB. Thus there is essentially no DEB leaving the system despite the fact that a large amount is produced in the first reactor and passes through the two distillation columns.

Table 4.1 shows the reactions kinetic, which including activation energy and intrinsic rate constant. Kinetic parameters have been adjusted to give reasonable rates of generation of the two components of interest (EB and DEB) in the reactors. Where R is reaction rate in kmol/(s-m^3) (consistent with commercial process simulation requirements), k is intrinsic rate constant, E is reaction activation energy in cal/mol, temperature units are Kelvin and concentration units are molarity (kmol/m^3).

Table 4.1 Ethyl Benzene Reaction Kinetics

	R1	**R2**	**R3**
k	1.528×10^6	2.778×10^7	1,000
E (cal/mol)	17,000	20,000	15,000
Concentration terms (kmol/m^3)	$C_E C_B$	$C_E C_{EB}$	$C_B C_{DEB}$

4.3 Ethyl benzene process description

Component physical property data for the ethyl benzene process are described from Luyben (2010) in a fair amount of detail.

Reaction section: There consist of two CSTR reactors in series. Both reactors size are containing 200 m^3 with half full liquid (5.03 m. in diameter, 10.01 m. in length). The operate temperature of the first reactor is set at 434 K and high pressure 20 atm. The temperature of the saturated steam is 414 K, which achieved by feeding boiler feed water (BFW) to the jacket/coil cooling system. The heat of the exothermic reaction is removed (cooling) by generating stream in this reactor. The heat transfer rate is 10.3 MW. Before exporting steady state simulation file into dynamics simulation, option dynamic heat-transfer configurations in the CSTR reactor model is completed. The Constant temperature heat-transfer option is suitable and this option is selected for the ethyl benzene reactor. In dynamics simulation, the temperature is manipulated by changing the setpoint of a steam pressure controller with boiling feed water.

Fresh feed ethylene and benzene are each 630.6 kmol/h with recycle benzene stream fed to the first reactor. Total benzene stream is 1,600 kmol/h. Total benzene stream is fresh feed benzene plus recycle stream from the distillate of the first column (969.4 kmol/h). The effluent from the first reactor is fed into the second reactor along with recycle stream of di-ethylbenzene from the bottom of the second column at a molar flowrate 282.2 kmol/h. The di-ethylbenzene in the first reactor is generated from reaction between ethyl benzene with ethylene. The essential of the di-ethylbenzene generated is converted to ethyl benzene. So the di-ethylbenzene is recycled back to extinction, which reaction occurring in the second reactor (adiabatic reactor).

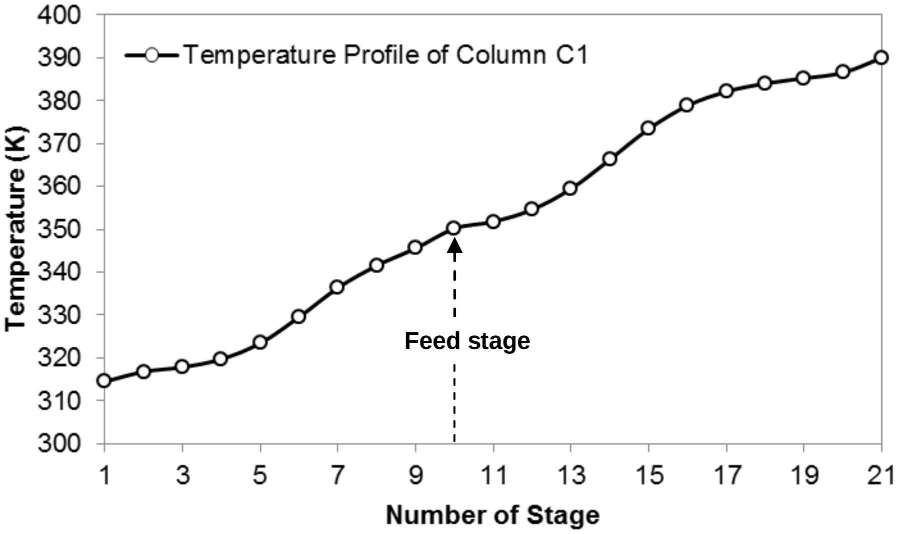
Column C1: The effluent from the second reactor is fed into the first distillation column C1. The first distillation column has 21 trays and is fed on stage 10. Reflux ratio is 0.774. The column operates under medium vacuum with a condenser pressure of 0.3 atm. The diameter of column is 4.80 m. The reflux drum temperature is 314 K which heat duty of the condenser used is 15.6 MW. Heat duty of the reboiler is 8.13 MW and the base temperature is 390 K. The design specification is to kept benzene from dropping out the bottom and affecting the purity of the ethyl benzene product leaving in the distillate of column C2. Since the specified ethyl benzene purity is 99.9 mol%, a very small benzene composition in the bottoms (0.03 mol %) is required. Benzene is the main component in the liquid recycle loop, which removed in the distillates stream and recycled back to mix with the fresh benzene makeup feed. Figure 4.1a and 4.1b gives temperature and composition profiles in Column C1, respectively.

Column C2: The bottom of the first column is fed to a second distillation column that produces ethyl benzene distillate and di-ethylbenzene bottoms. The column has 25 trays and is fed on stage 15. The column operates under low vacuum with a condenser pressure of 0.3 atm. The diameter of column is 5.78 m. The reflux drum temperature is 338 K which heat duty of the condenser used is 11.7 MW. Heat duty of the reboiler is 10.2 MW and the base temperature is 403 K. The separation required of this column is the removal of EB from DEB. The distillate of column is high purity of EB (99.9 %mol). The bottom of column is mostly DEB which is recycled back to reaction section in the second reactor. The design specification is to attain high-purity ethyl benzene in the distillate and minimize the loss of ethyl benzene in the bottoms. The bottoms composition is set at 0.05 mol% ethyl benzene. The distillate composition is 99.9 mol% ethylbenzene using the low 0.661RR. The temperature and liquid composition profiles of column C2 are displayed in Fig. 4.1c and 4.1d, respectively.

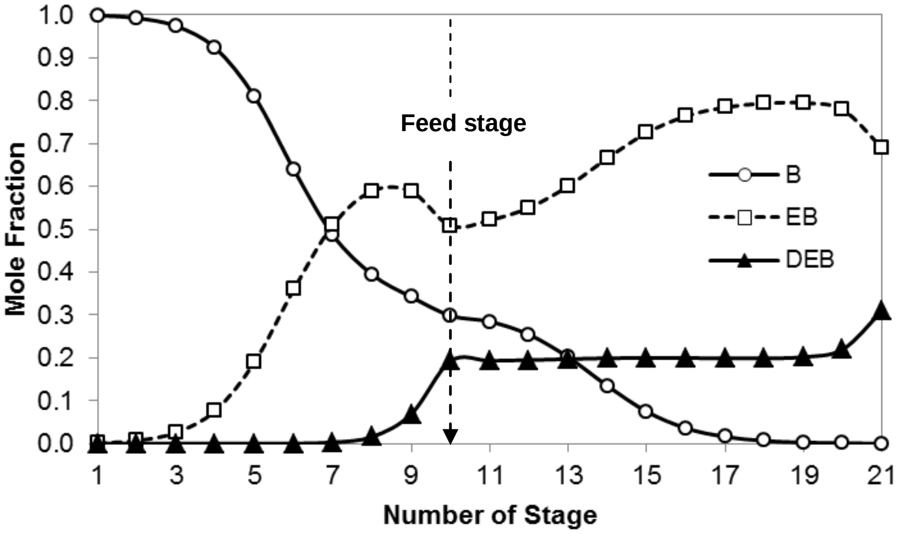
4.4 Steady state modeling

The steady state model of the ethyl benzene process is using the flowsheet and equipment design information from Luyben (2010). It is highly important to select the most suitable fluid package for realistic simulation. The success of any steady-state simulation model largely depends on the selection of a suitable thermodynamic package. In this study, improved Choa-Seader equation of state is selected for property estimation. The normal boiling points of components are 353K, 409K and 457K for benzene, ethyl benzene and di-ethylbenzene, respectively.

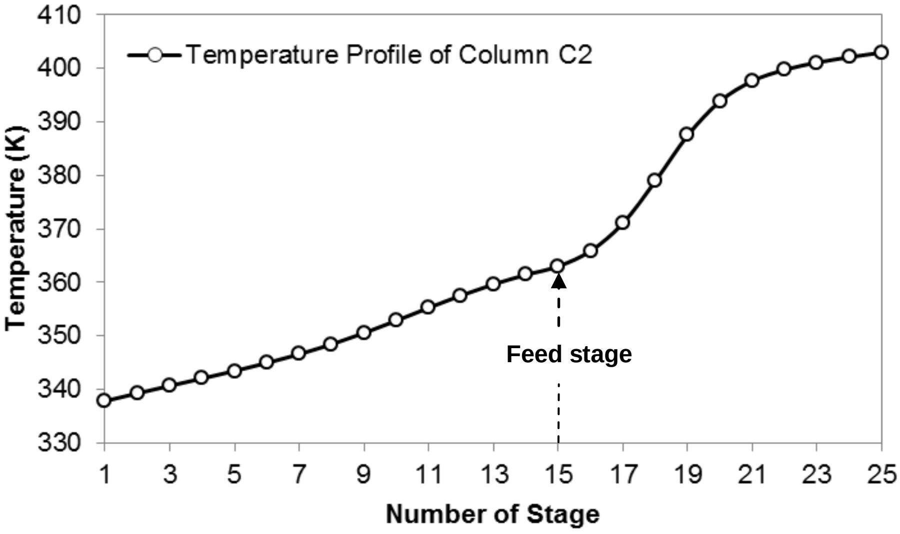
Both columns are simulated using the distillation column module. In steady state, the specification of inlet stream, pressure profiles, number of trays and feed tray need for model. Besides, two additional variables should be additionally specified for column. These could be duties, reflux rate, reflux ratio, boilup, distillation to feed, bottoms to feed ratio, etc. For the ethyl benzene process, reflux ratio and distillation rate is specified at column C1, bottom rate and reflux ratio is specified at column C2. Figure 4.2 presents the steady state flowsheet of ethyl benzene process described in Luyben by using commercial process simulator.


Temperature Profile of Column C1
Temperature (K)
400
390
380
370
360
350
340
330
320
310
300
Feed stage
1
3
5
7
9
11
13
15
17
19
21
Number of Stage

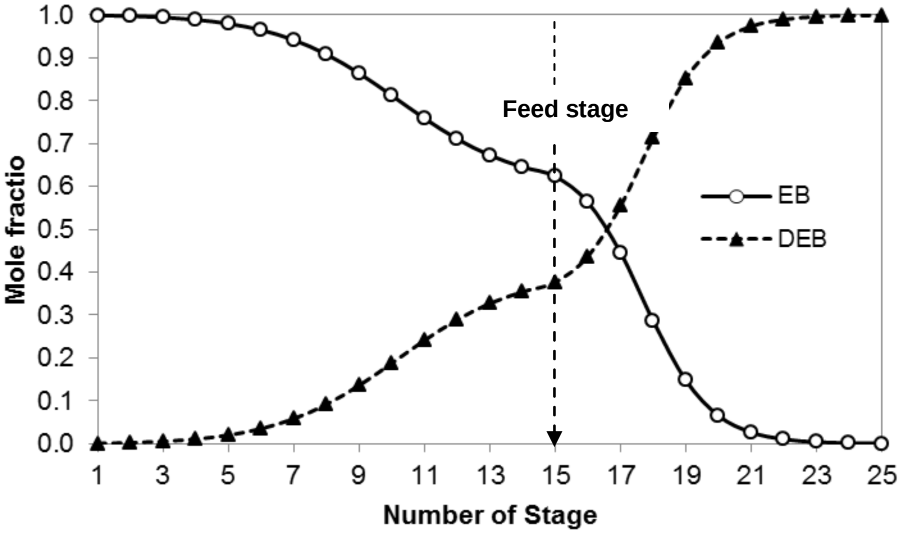
(a)


Mole Fraction
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Feed stage
B
EB
DEB
1
3
5
7
9
11
13
15
17
19
21
Number of Stage

(b)



(c)



(d)

Figure 4.1 Temperature and composition profiles

(a) Temperature profile of Column C1

(b) Composition profiles of Column C1

(c) Temperature profile of Column C2

(d) Composition profiles of Column C2

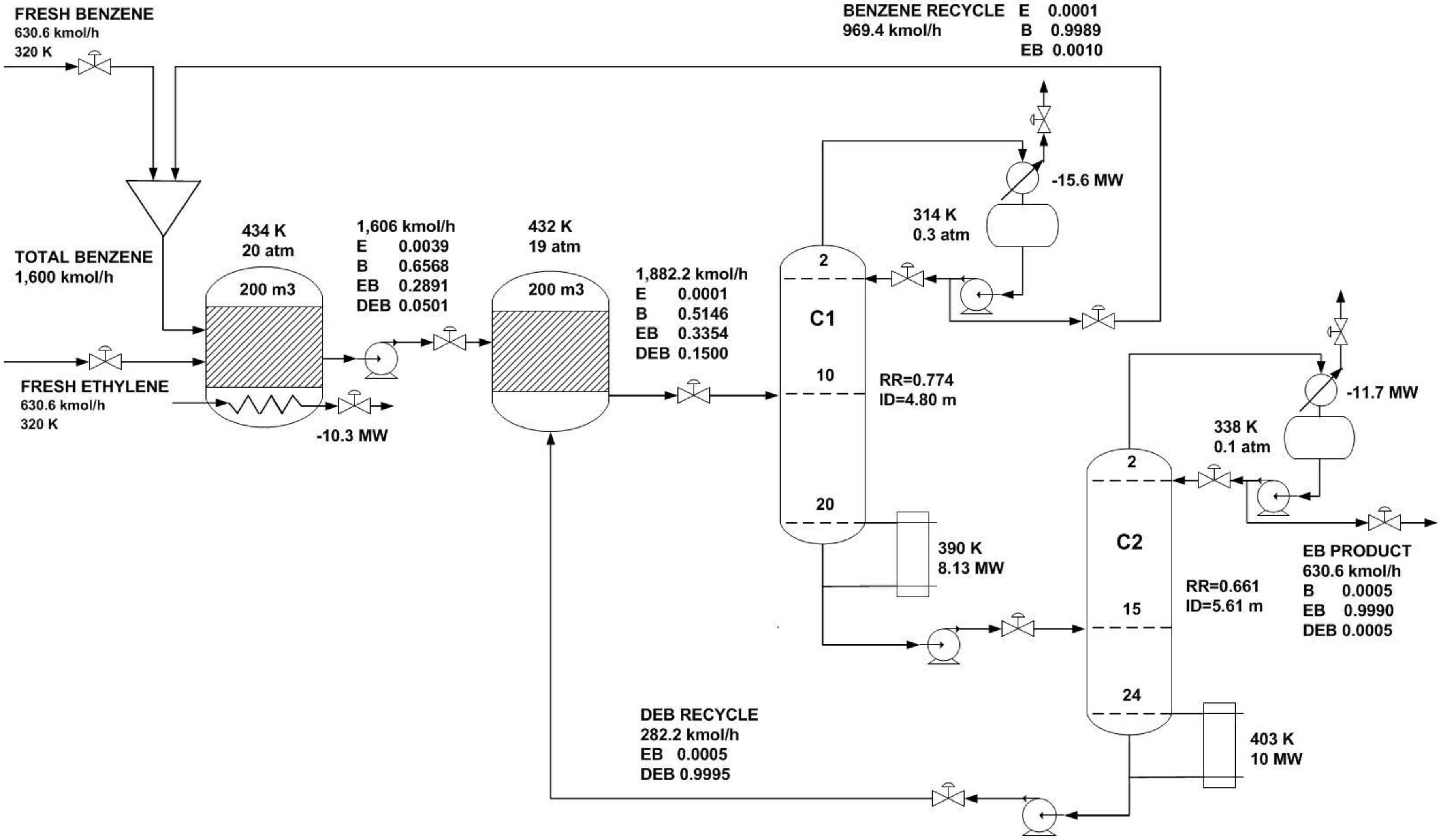


Figure 4.2 Ethyl benzene process flowsheet (Luyben, 2010).

Table 4.2 Basic of Economics and Equipment Sizing

For optimizing the design of a distillation column is to determine values of the design optimization variables that minimize the total annual cost. The design optimization variables include pressure, total number of trays, and feed tray location. The cost estimations for the equipment are based on information from Douglas (1988) and Turton (2008).

Column diameter: Aspen tray sizing using double-pass trays

Column length: NT trays with 2 ft. spacing plus 20% extra length

Column vessel (diameter and length in meters):

Capital cost = $17{,}640(D)^{1.066}(L)^{0.802}$

Condensers (area in m^2):

Heat-transfer coefficient = 0.852 kW/K-m^2

Differential temperature = Reflux drum Temperature - 310 K

Capital cost = $7{,}296(A)^{0.65}$

Reboilers (area in m^2):

Heat-transfer coefficient = 0.568 kW/K-m^2

Differential temperature = Steam temperature - Base temperature

Capital cost = $7{,}296(A)^{0.65}$

Reactor (diameter and length in meters):

Half full of liquid

Aspect ratio = 1

Capital cost = $17{,}640(D)^{1.066}(L)^{0.803}$

Energy cost:

LP steam (433 K) = \$7.78/GJ

MP steam (457 K) = \$8.22/GJ

HP steam (537 K) = \$9.83/GJ

Value of steam generated in reactor:

LP steam (410 K) = \$6.00/GJ

$$\text{TAC} = \frac{\text{Capital cost}}{\text{Payback period}} + \text{Energy cost}$$

Payback period = 3 years

CHAPTER V

CONTROL STRUCTURES DESIGN

5.1 Introduction

The issues of plantwide control structure design for the ethyl benzene process are described base on the new design procedure given by Wongsri (2012). The major eight steps for plantwide control structure design are discussed in detail each step. The plantwide control design procedure presented here is developed after many years of work and research in the field of process control and process design. Plantwide control structure design procedure of Wongsri (2012) satisfies the two fundamental chemical engineering principles of the overall conservation of energy and mass. Lists below are the fundamental concepts and techniques of Wongsri's procedure.

5.2 Control Structure Design Procedures Applied to the Ethyl Benzene Process.

In this section, control structure design procedure is applied to the ethyl benzene process. Plantwide control system is developed and tested for the innovated flowsheet. Wongsri's procedure is used for design, which illustrated in previous section. The design of a plantwide control system consists of eight major steps as follows:

Step 1: Gather plant information and control objectives.

In this step, two categories of plant information must be provided are

1. Plantwide control objectives.
2. Process constraints.

The plantwide objective includes product quality and plant production rates. Normally, the plantwide control objectives depend on customer requirements, expected sales and operating costs. In part of the process constraints, stabilizations of the process are considered. Identify process constraints that must be satisfied, which include safety requirements, environmental constraints and operating conditions. For the ethyl benzene process, the objectives are the same as those listed in table 5.1.

Plantwide objectives for the ethylbenzene process as follows:

1. Product quality: The product should contain approximately 99.9% mol of ethyl benzene product.

2. Production capacity: production rate about 630.6 kmol/h of ethyl benzene.

Table 5.1: Constraints for the ethyl benzene process

Constraints		**Unit**
Reactor pressure	≤ 20	atm
Reactor temperature	≤ 434	K
Bottom column C2 temperature	≤ 403	K

From lists of all process constraints, the ratio of total benzene to ethylene has to be at least 2.537 at the inlet. This to avoiding coking that takes place at higher temperatures. Also, a large excess of benzene must be recovered and recycled to reduce activation energy of the undesirable reaction (the secondary reaction), which it’s larger than that of the desirable reaction. The outlet temperature of reactor R1 should be around 434 K to minimize the side reactions and to avoid coking (Constraints on reactor temperature and pressure assigned by materials limits). The pressure operating of reactor should not exceed 20 atm (constraint required to meet materials limits). The temperature of di-ethylbenzene recycle stream should not exceed 403 K to avoid kinetic consider for adiabatically operation of reactor R2.

Step 2: Plant Analysis.

2.1 Control degree of freedom (CDOF). List manipulated variables (control degree of freedom, CDOF).

The CDOF can be obtained using the guideline given in Table 5.2. The number of control degrees of freedom equal to the number of manipulated variables. Recall that a control degree of freedom is allocated each time a manipulated variable is utilized in a control loop, except in cascade control or in other applications where a set point is manipulated instead of a control valve. The steady-state and dynamic CDOF need to be identified. For the ethyl benzene process, as mentioned earlier, the CDOF is determined to be 20.

Table 5.2: Steady-State Degrees of Freedom for the Ethyl Benzene Process

Unit	Manipulated variable	Quantity	DOF
Independent streams	Flowrate	2	2
Pump	Work	5	5
Reactor with coolant	Heat flow and level	3	3
Distillation columns	Distillate flowrate, Bottom flowrate, Reflux flowrate Heat reboiler input Heat condenser remove	2	10
Total degrees of freedom			20

2.2 Heat pathways.

From the plantwide overall image, four different "heat pathways" are introduced in the process. The first pathway is heat of exothermic reactions and discharge of mechanical work (e.g., pump, pressure drop and friction). The second pathway, heat is send from the utilities into the process, when the process uses excess heat (or energy), it would be carried to the environment.

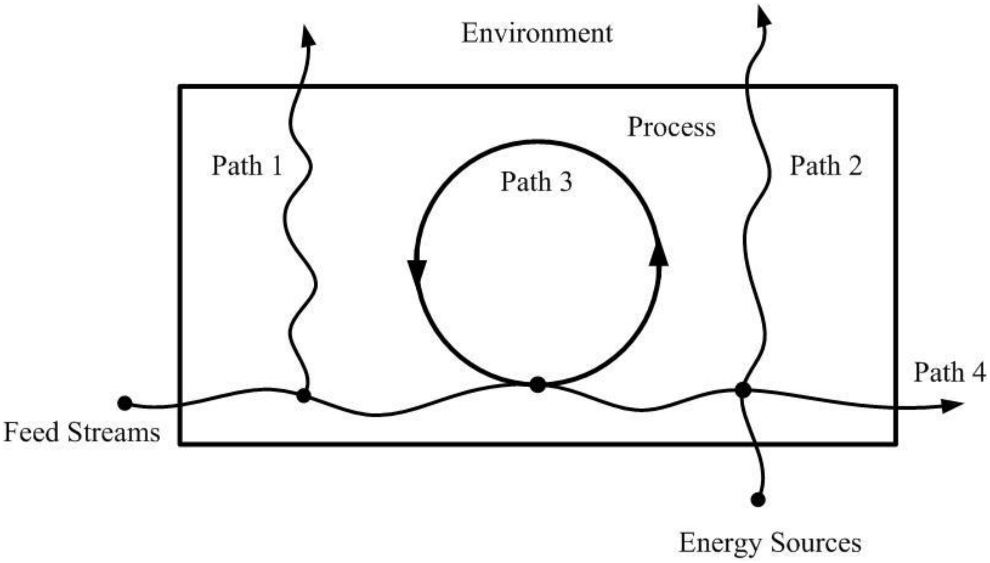


Figure 5.1 heat pathway of ethyl benzene process

The third pathway is internal heat to the process. Heat would circulate within the process and between unit operations such as recycle stream. The desired magnitude of energy depends upon the heating and cooling and the amount of heat integration implemented. Whenever the process requires heat, the heat has to be supplied from the utilities. The same amount of heat must be rejected to the environment, nearest exit point in the process or the utilities. The forth pathway is from feed stream and departed to the exit stream.

2.3 Material pathways and 2.4 Material quantifiers.

Ethylene and benzene are raw materials fed to the process, which affects to reaction and ethyl benzene product quality. The first, ethylene and benzene fed into the first reactor along with benzene recycle stream. Ethylene is converted to ethyl benzene by react with benzene, which not reacted ethylene leaves in the first reactor and fed into the second reactor to completely react. The quantifier of ethylene is feed flowrate. Unconverted benzene from the first and second reactor is also fed into the first column that produces a distillate that is mostly benzene, which benzene is recycled to the first reactor along with the fresh feed benzene again. The total benzene can be presented benzene quantifier well.

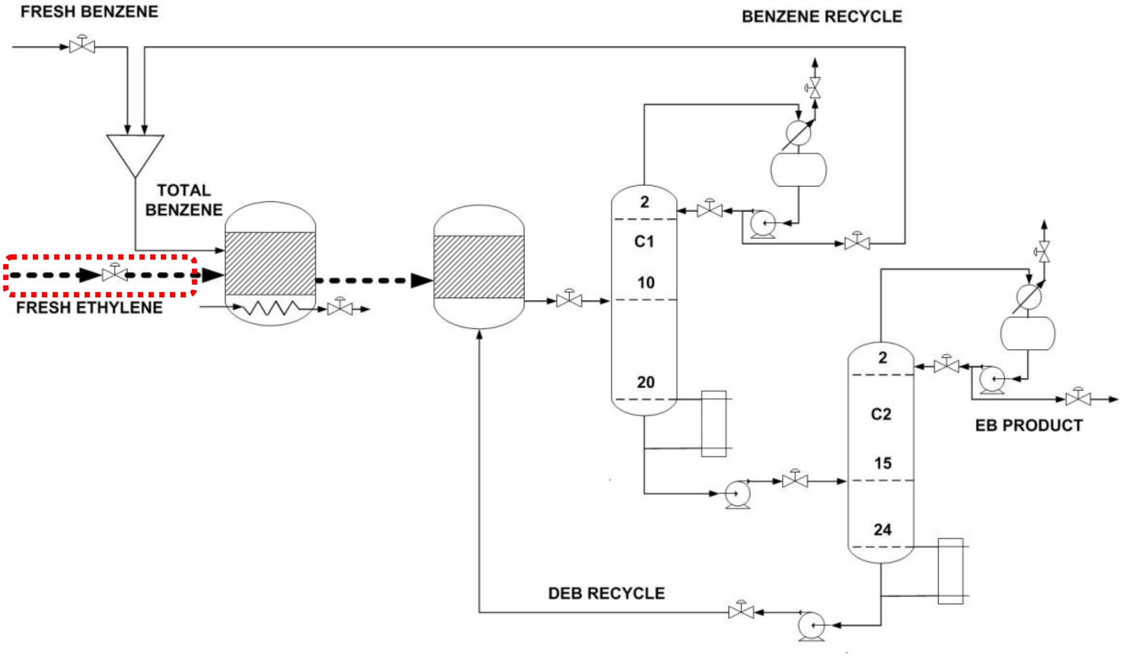


Figure 5.2 Ethylene pathway and quantifier

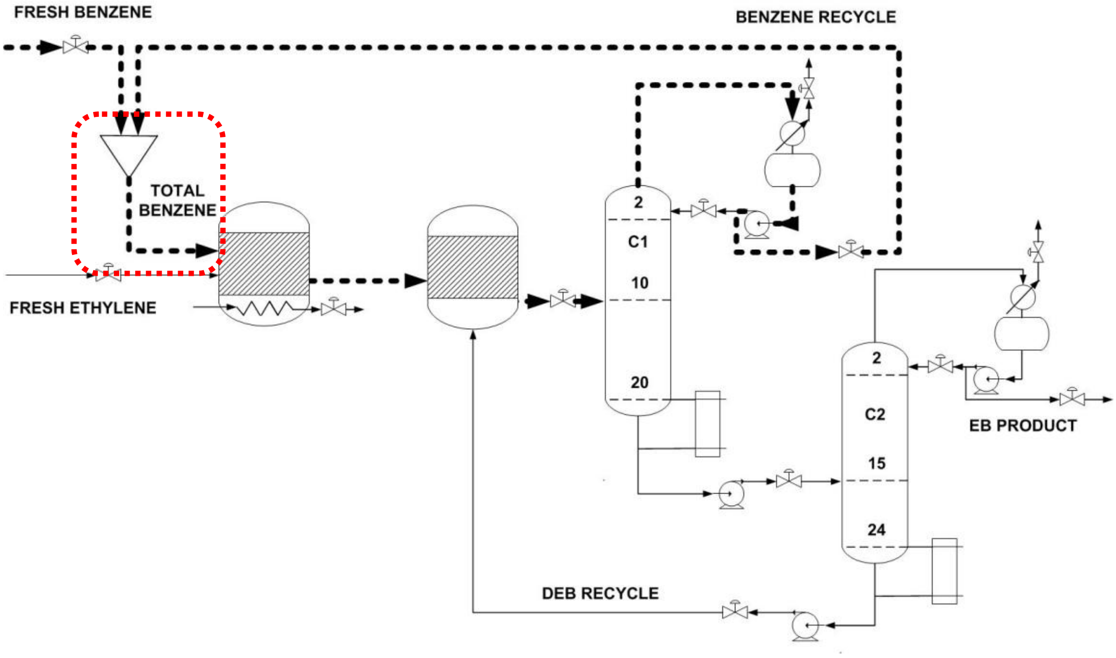


Figure 5.3 Benzene pathway and quantifier

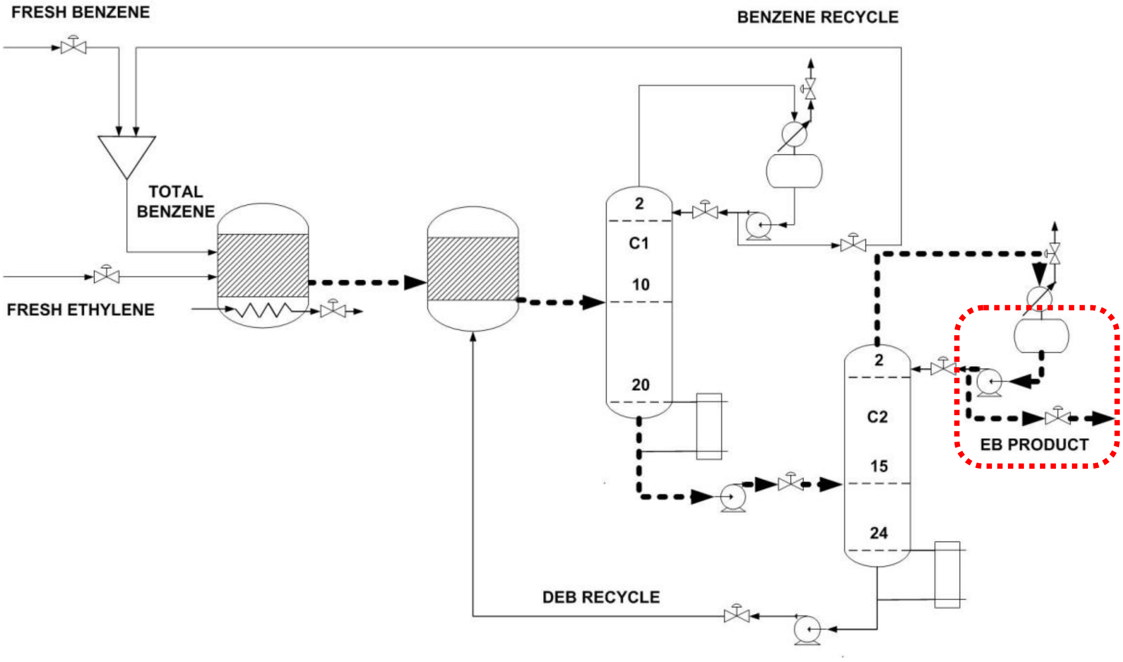


Figure 5.4 Ethyl benzene pathway and quantifier

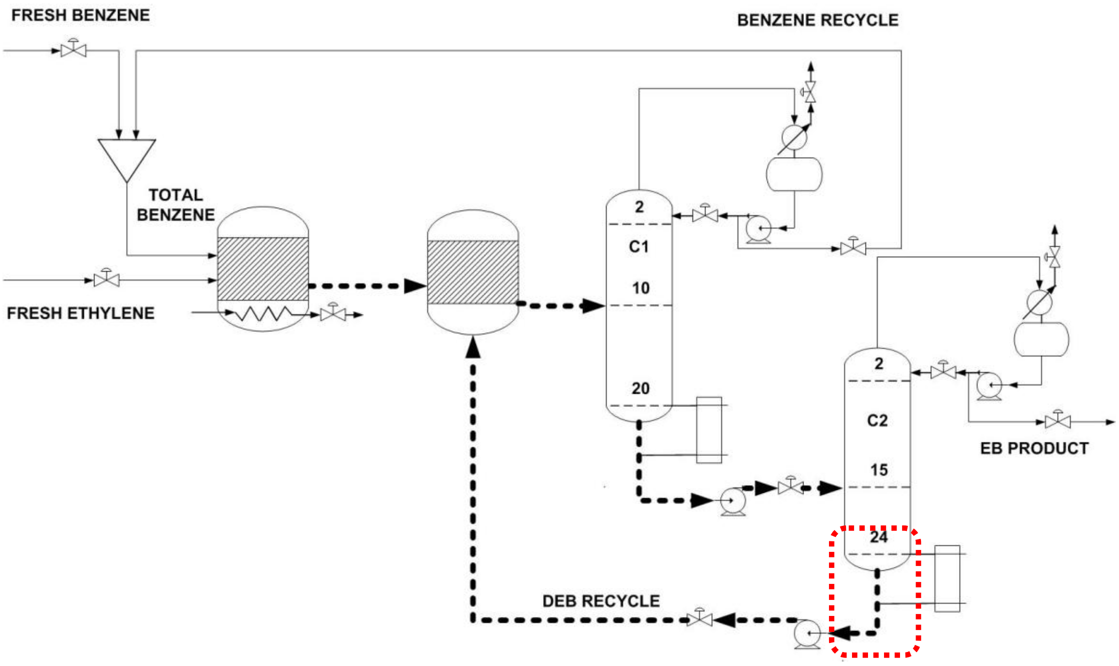


Figure 5.5 Di-ethylbenzene pathway and quantifier

Ethyl benzene product and di-ethylbenzene, they are generated in the first and second reactor and send to column C2 to separate. The effluent from the first reactor is a mixture of benzene, ethyl benzene and di-ethylbenzene. They are fed into the second reactor along with a recycle stream of di-ethylbenzene. After that, the ethyl benzene and di-ethylbenzene components are fed to first distillation column and send to the second distillation column. Both components are produced an ethyl benzene distillate and a di-ethylbenzene bottom, which di-ethylbenzene is recycled back to extinction. The ethyl benzene quantifier is the exit stream at the reflux drum of column C2. The quantifier of di-ethylbenzene is bottom level of column C2.

2.5 Reaction section

- Reactor R1 operated with cooling
- Reactor R2 operated at adiabatic condition
- Heat of exothermic reactions:

ΔHrxn 1 = -71.159 kJ/mol

ΔHrxn 2 = -83.716 kJ/mol

ΔHrxn 3 = -62.787 kJ/mol

2.6 Separation section

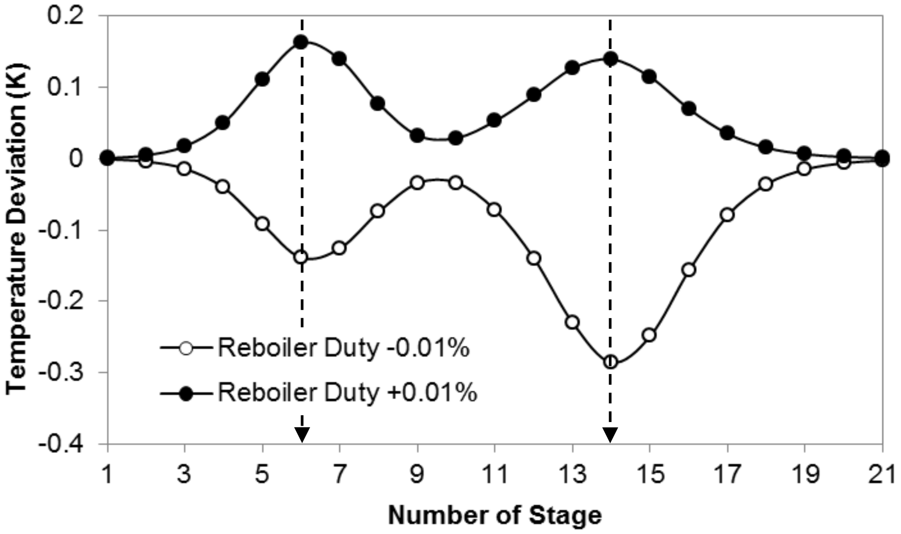
Selection for temperature control tray location.

Several methods for selecting the best tray have been proposed. The methods for selecting temperature control tray location are “open-loop sensitivity analysis” and “effect of disturbances”. Sensitivity analyses are performed on the two distillation columns. The procedure for selecting which tray to temperature control is to look at the steady state temperature profile in the column. The stages in the column are considered where there are large changes of temperature from tray to tray, which is the most disturbed or sensitive point. Note that the tray number is counted from top (condenser is 1) to bottom stage.

Column C1

Open loop sensitivity, the reflux ratio (RR) and reboiler heat input to the distillation column (QR) are fixed. Recall the two manipulated variables. Very small increases/decreases from the steady-state values of two manipulated variables are used. Fig.5.6 displays the results of an open-loop sensitivity analysis on temperature deviations with ±0.01% changes in reboiler duty and reflux ratio of the distillation column C1, respectively.

In order to determine the temperature control location, Open-loop sensitivity analysis would be performed to determine the best temperature control location. The temperature control location would be selected at a particular stage with high sensitivity to the manipulated variable. When one manipulated variable is disturbed, other manipulated variable is held at original basecase value. For the first distillation column of the ethyl benzene process, an increase in QR leads to an increase in the tray temperatures, and a decreases QR leads to a decrease in the tray temperatures of the first distillation column. RR, an increase in RR leads to a decrease in the tray temperatures, and a decreases RR leads to an increase in the tray. The temperature control locations for the column C1 are selected at 6th stage and 14th stage. These selections also agree well with another guideline to select the tray where the sharpest temperature break occurred. Therefore, stage 6 can be controlled by using either reflux or heat input, while stage 14 can be controlled by only heat input.



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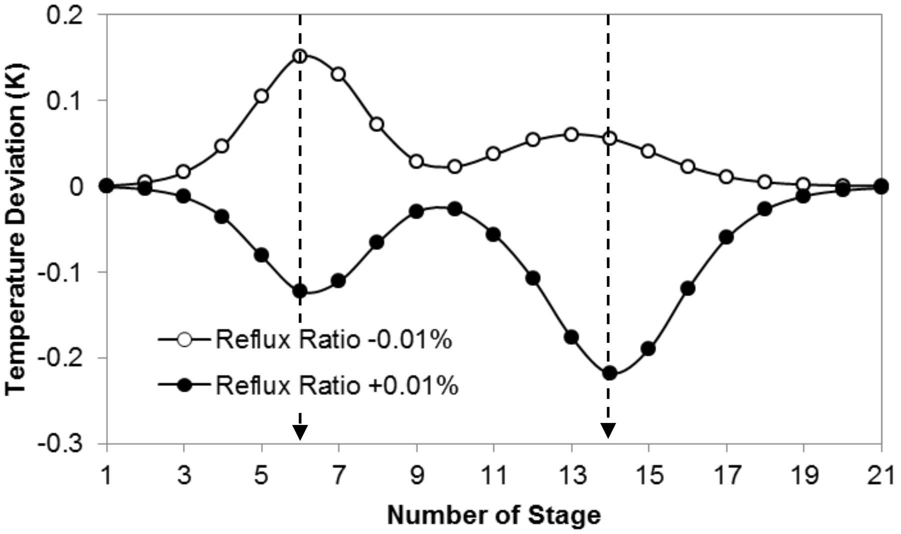


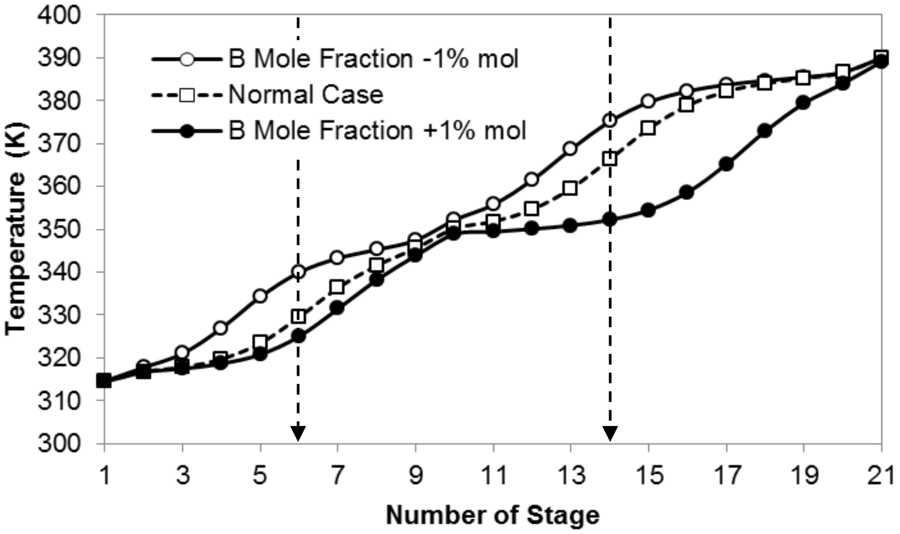
(b)

Figure 5.6 open loop sensitivity analyses between stage temperature and manipulated variables in the column C1

(a) Reboiler duty

(b) Reflux ratio

Fig. 5.7 shows the different temperature profiles of the column C1 for various feed disturbances on steady state analysis. From the steady state simulation model, it is observed that ± 1% benzene mole fraction variation in feed stream, ± 10% variation in feed flowrate, ± 10% benzene component in feed flowrate and ± 10K feed temperature in feed stream. The temperature control location would be selected at a particular stage with the most disturbed point.



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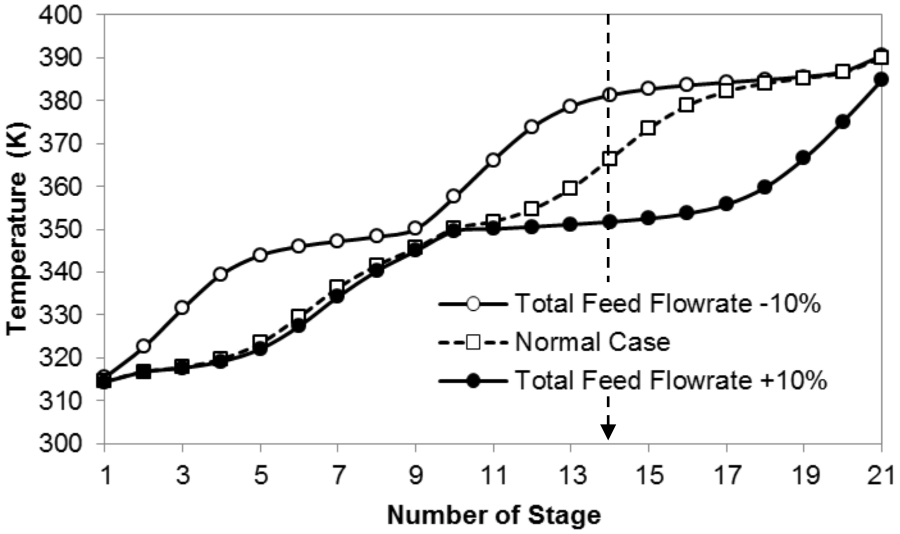

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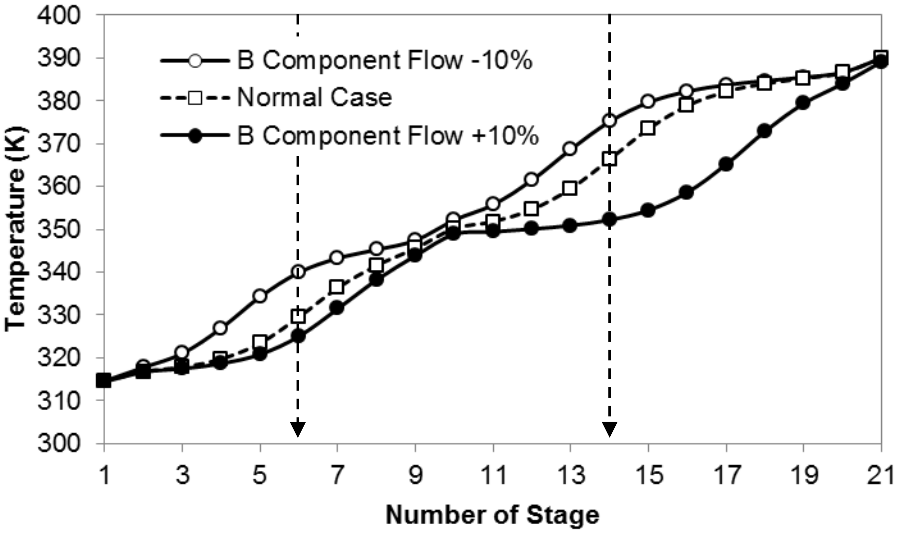

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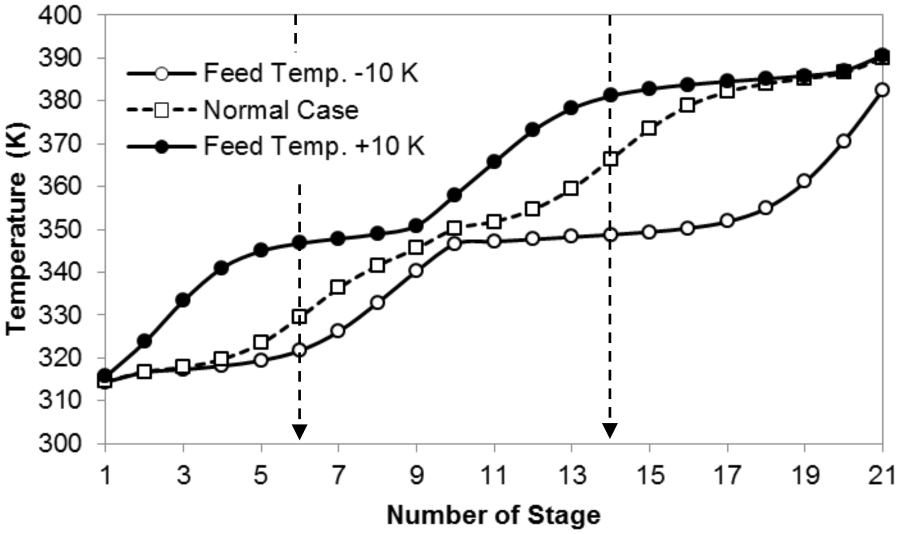


(d)

Figure 5.7 Effect of disturbances on the steady state temperature profiles of the column C1

(a) Ethyl benzene mole fraction
(b) Total feed flowrate
(c) Ethyl benzene component flow
(d) Feed temperature

Temperature profile at nominal operating condition of B mole fraction changes is shown in Fig. 5.7a. The temperature profile can be found at the top and near bottom sections (stages 6 and 14), which nominal operating condition is located within the feasible region. It indicates that the set point change of B mole fraction.

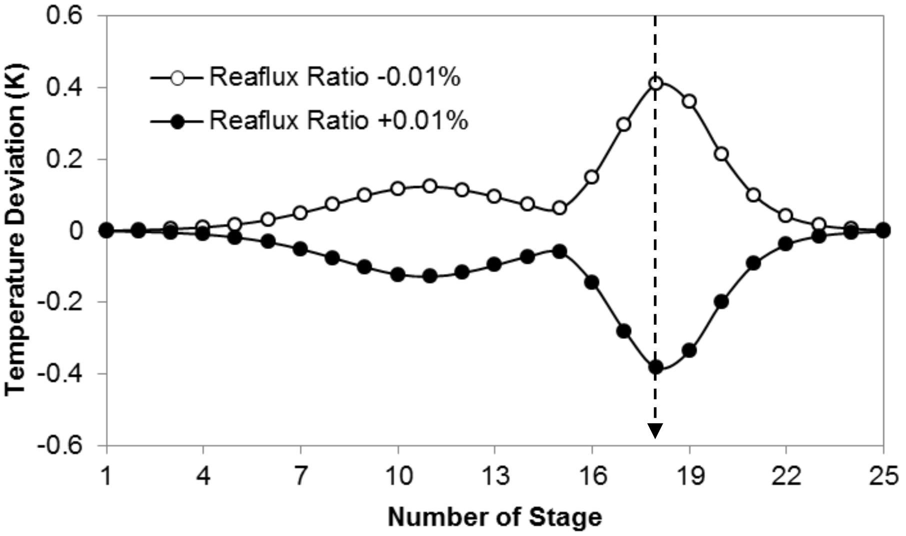
Fig. 5.7b shows the set point change of the loop using the temperature of stage 14 as the controlled variable is necessary for required compositions when there are total feed flows changes. Similar to B mole fraction test, it is proposed to reset the set point of the loop by control temperature loops with bottom temperature as the controlled variable and the set point of the inner temperature control loop as the manipulated variable.

From the steady-state analysis shown in Figs. 5.7c and 5.7d, the different feasible regions can be found for various B component flow and feed temperature. Stage temperatures 6 and/or 14 are the controlled variable needs not to be changed, when B component flow is changed from nominal values ±10%. Similar, stage temperatures needs not to be changed, when feed temperature is changed from 432 K to 422 K and 442 K

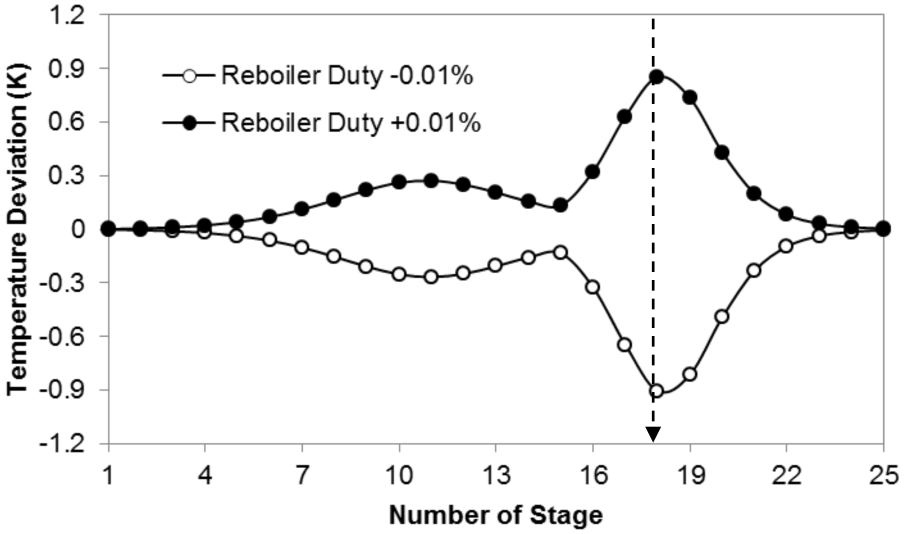
Therefore, these two stages temperature are used as the candidates of the controlled variable in the temperature control loop. It is noticed that the temperature control locations for this column is the same from a similar open-loop sensitivity analysis as shown in Figure 5.5. The temperature control locations have same two breaks, one point near the bottom stage (stage 14) and one point near the top stage (stage 6). So, two temperature controllers or dual temperature control can be used in column C1, which might be effective than one point temperature control. If two point temperatures control are selected, the TC12 controller manipulates the reboiler heat input to control the stage 14 temperature. The TC11 controller manipulates the reflux flowrate to control the stage 6 temperature. This is verified by the dynamic simulation given later in this paper.

Column C2

Fig. 5.8 showns results of open loop sensitivity analyses between stage temperature and manipulated variables in the column C2. Temperature deviations from nominal values for changes in these manipulated variables (reflux ratio and reboiler duty) of the second distillation column. Temperatures of high sensitivity with manipulated variables can be found at near bottom sections (18th stage).



(a)

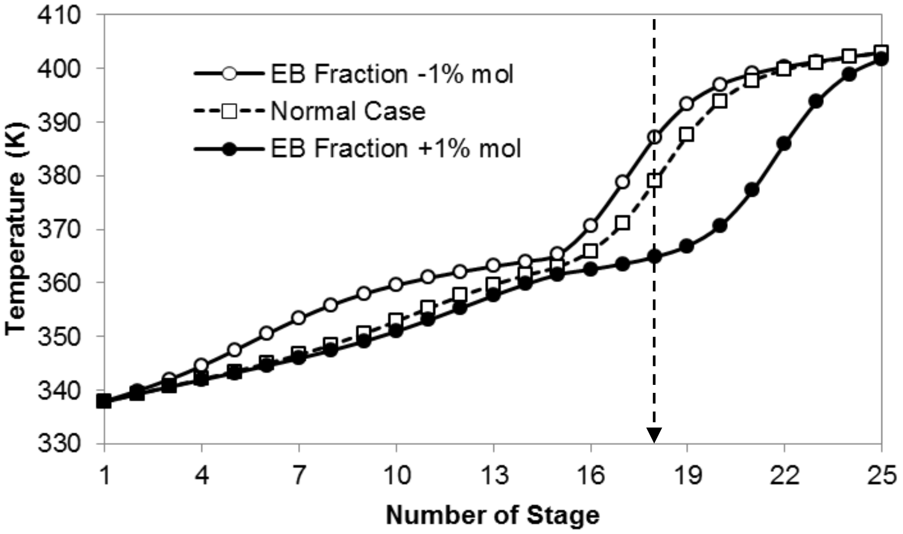


(b)

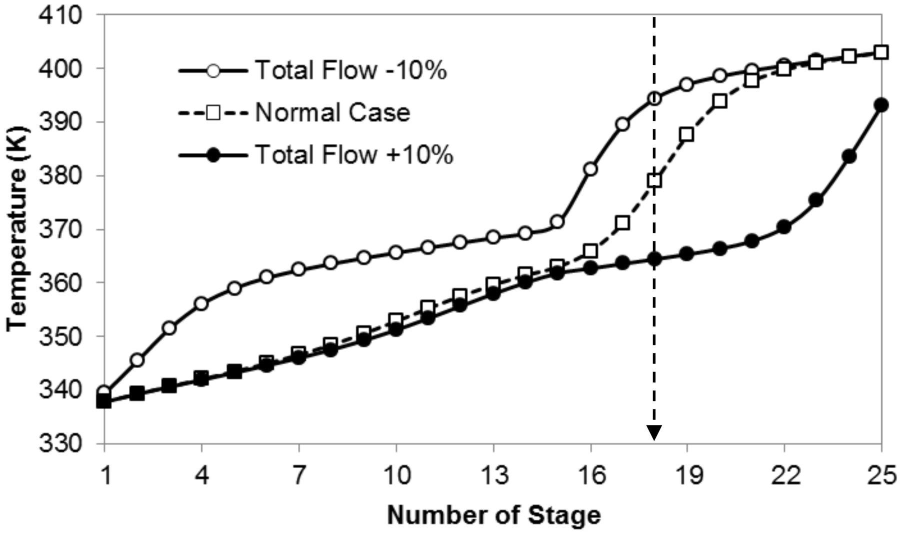
Figure 5.8 open loop sensitivity analyses between stage temperature and manipulated variables in the column C2

(a) Reboiler duty
(b) Reflux ratio

Fig. 5.9 gives the different temperature profiles of the system for ± 10% various total feed flowrates, ± 1% various EB mole fraction, ± 10% various EB component and ± 10K various feed temperatures. The temperature control location would be selected at a particular stage with the most disturbed point.



(a)



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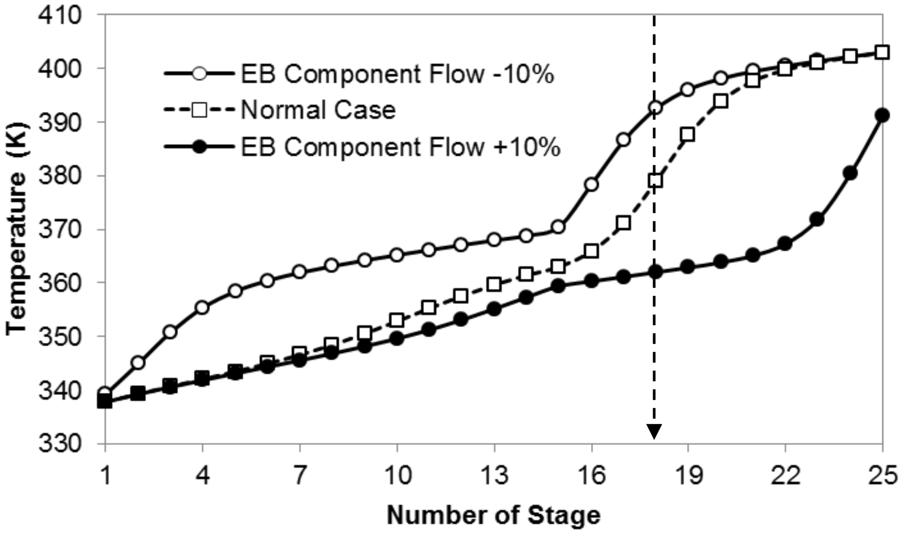

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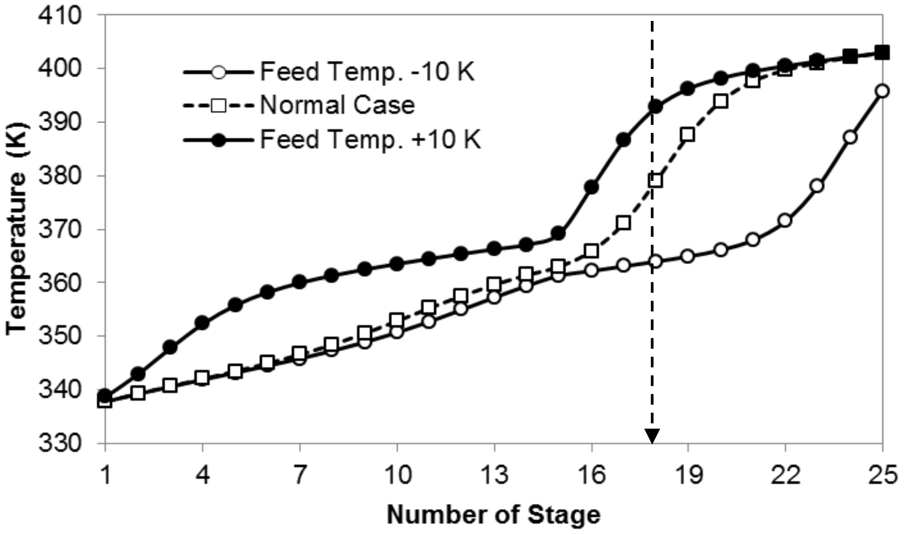


(d)

Figure 5.9 Effect of disturbances on the steady state temperature profiles of the column C1

(a) Ethyl benzene mole fraction
(b) Total feed flowrate
(c) Ethyl benzene component flow
(d) Feed temperature

Fig. 5.9a shows that there is little affect for the changes of EB mole fraction on the desired temperature profiles at top stage of the system. Larger variations in the desired temperature profiles are observed when setpoint changes or disturbances. The controlled temperatures are located at stage 18 from the method.

Fig. 5.9b to 5.9d shows how the temperature profile is affected by changes in these three parameters for total feed flowrates, EB component flowrates and feed temperature by the same amounts, ±10%, ±10% and ±10K, respectively. The results, the temperature control stage would be selected at a particular stage with high sensitivity and also with near-linear behavior. For the column C2, the temperature break in the lower part of the column moves toward the bottom of the column. The temperature (location shown with a perpendicular line in the bottom plot) at the 18th stage is chosen as the control stage.

Step 3: Establish fixture plant.

The principal idea of establishing a fixture plant is to first have entire plant fluid-filled and material-balanced. This idea is similar to creating “hydraulic” control structure proposed by Buckley (1964). This step in Wongsri’s plantwide control structure design procedure is classified into 4 topics.

3.1 Keep the raw materials entered and re-entered fixed

The objective of this step is to keep the entered and reentered stream fixed. The flowrate of stream fed to the process must be controlled by adjusting their flowrate. Figure 5.10 shown the points are controlled which includes pure ethylene and benzene. There are fixed to maintain the flowrate to be stable.

- The flowrate of the fresh feed ethylene stream is controlled by manipulating fresh feed flowrate to keep the flowrate and placed the controller FC.
- The flowrates of the total benzene stream is flow controlled by manipulating fresh feed benzene to keep the total flow at its desired set point (controller FC). This total flow is the sum of the fresh feed benzene plus the distillate D1 from column C1. However, because the total flowrate is fixed, the flowrate of the fresh benzene feed would be reduced by the FC flow controller**.** There is a flow controller in the recycle loop to prevent the snowball effect.

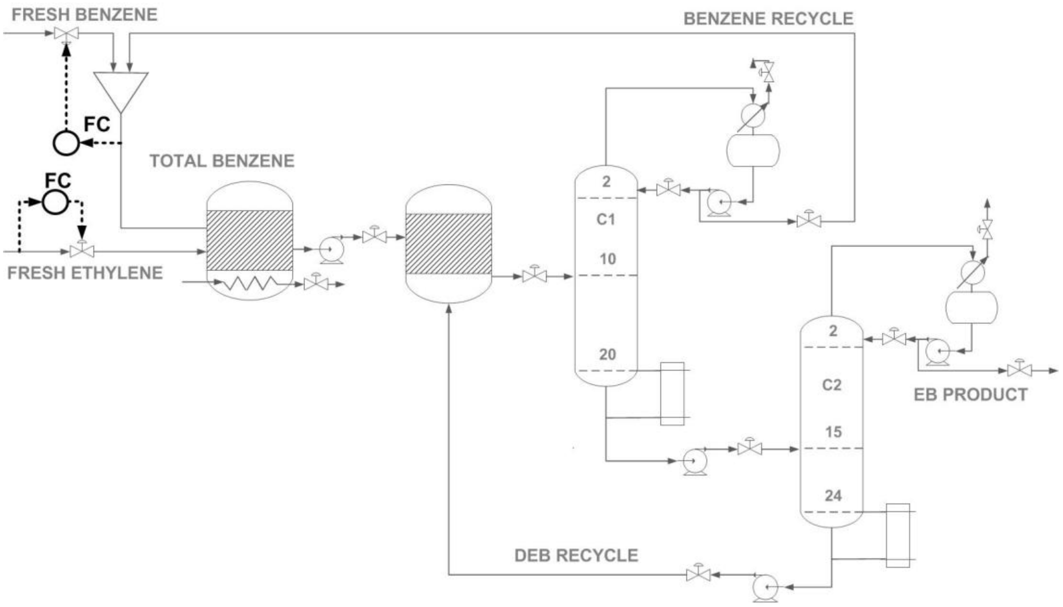


Figure 5.10 Flowsheet of ethyl benzene process to keep the raw materials entered and re-entered fixed

3.2 Regulate the production rate.

3.2.1 Consume the limiting reactant.

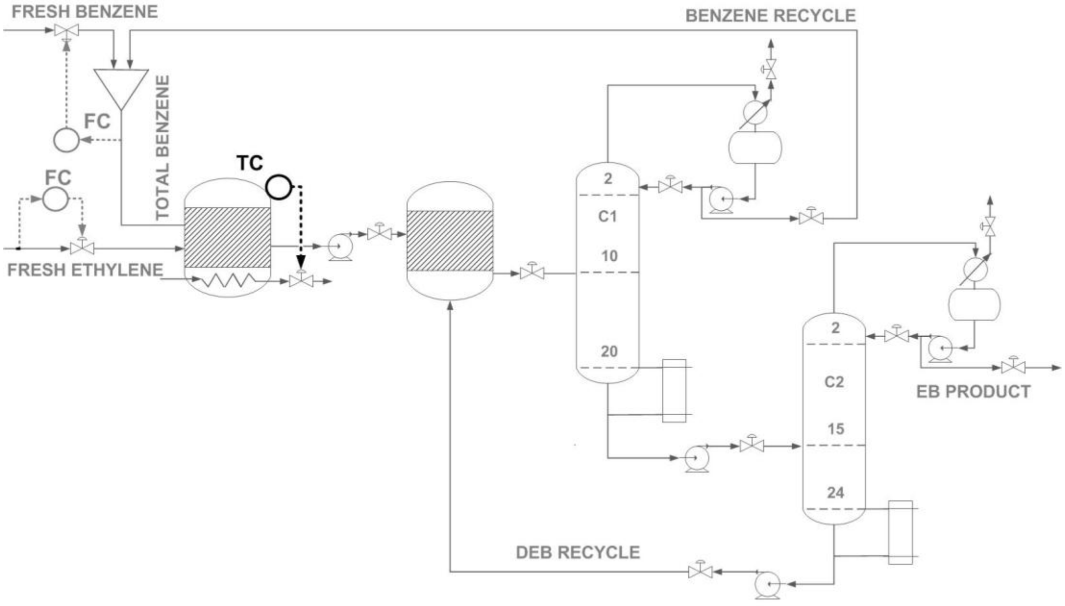


Figure 5.11 Flowsheet of ethyl benzene process for consume the limiting reactant by reactor temperature controller.

The limiting reactant should be totally consumed at the reactor for the economic reason. The first choice is maintain the temperature in reactor by manipulating cooling. The second choice is control composition of limiting reactant at outlet of reactor R2, which shown in Figure 5.11 and 5.12, respectively.

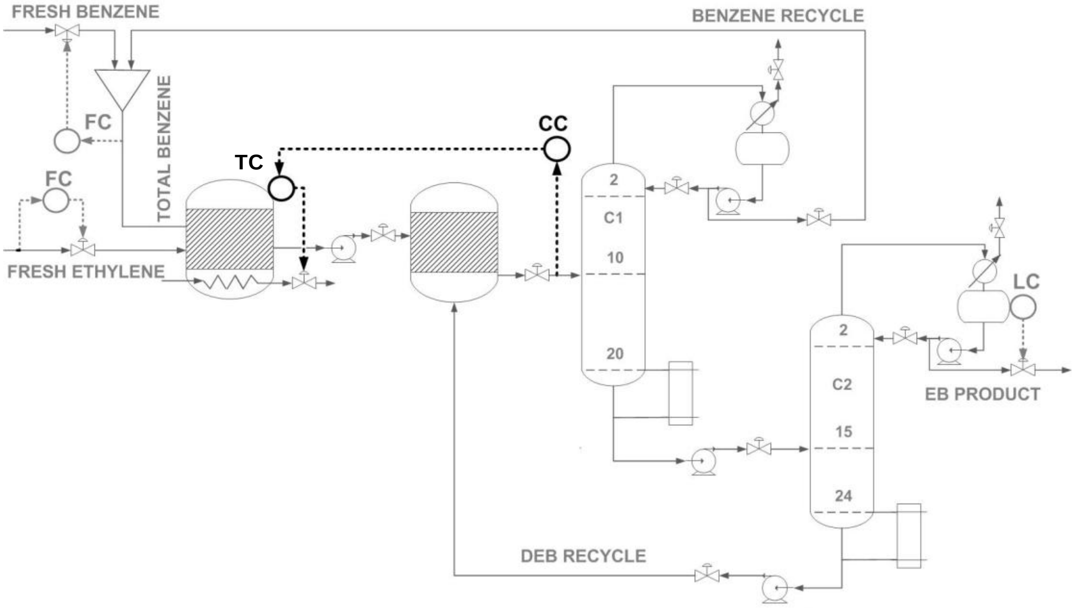


Figure 5.12 Flowsheet of ethyl benzene process for consume the limiting reactant by composition controller

3.2.2 Regulate the production rate.

For this step, the limiting reactant fresh feed flowrate is used to set the production rate.

3.3 Adjust the flow of exit material streams according to their accumulation (products, by-products and inert)

The chemical processes are classified into three types: products, by-products and inert. Figure 5.13 shows the exit material stream of the ethyl benzene product. This component conducts out of the process through the distillate of ethyl benzene column with 99.9 mol%. It’s adjusted according to its accumulation via the reflux drum level control of C2 (controller LC).

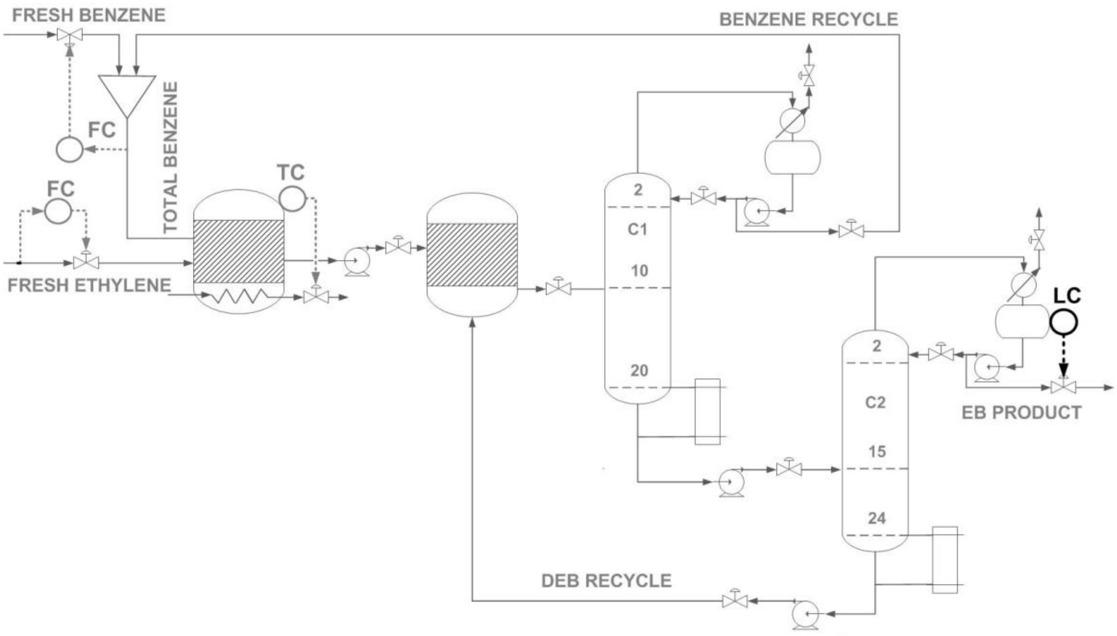


Figure 5.13 Flowsheet of ethylbenzene process for adjust the flow of exit material streams according to their accumulation

3.4 Control the inventory of the rest of the component at their quantifiers

The quantifier of components can be implies as a quantity or amount of the specified component such as level is liquid quantifier, etc. For the ethyl benzene process have 4 components: ethylene, benzene, di-ethylbenzene by product and ethyl benzene product. Quantifiers of each component are different location. Ethylene, benzene and ethyl benzene are identified in previous steps. The rest of the component is di-ethylbenzene, which the quantifier is decided to be the base level of column C2. The control loop is placed to regulate its inventory via the level controller LC, which shown in Figure 5.14.

Table 5.3: Locate the quantifiers of the components

Components	Quantifiers
Ethylene (C_2H_2)	Ethylene feed stream
Benzene (C_6H_6)	Total Benzene stream
Ethyl benzene (C_8H_{10})	Reflux drum of column C1
Di-ethylbenzene ($C_{10}H_{14}$)	Base of column C2

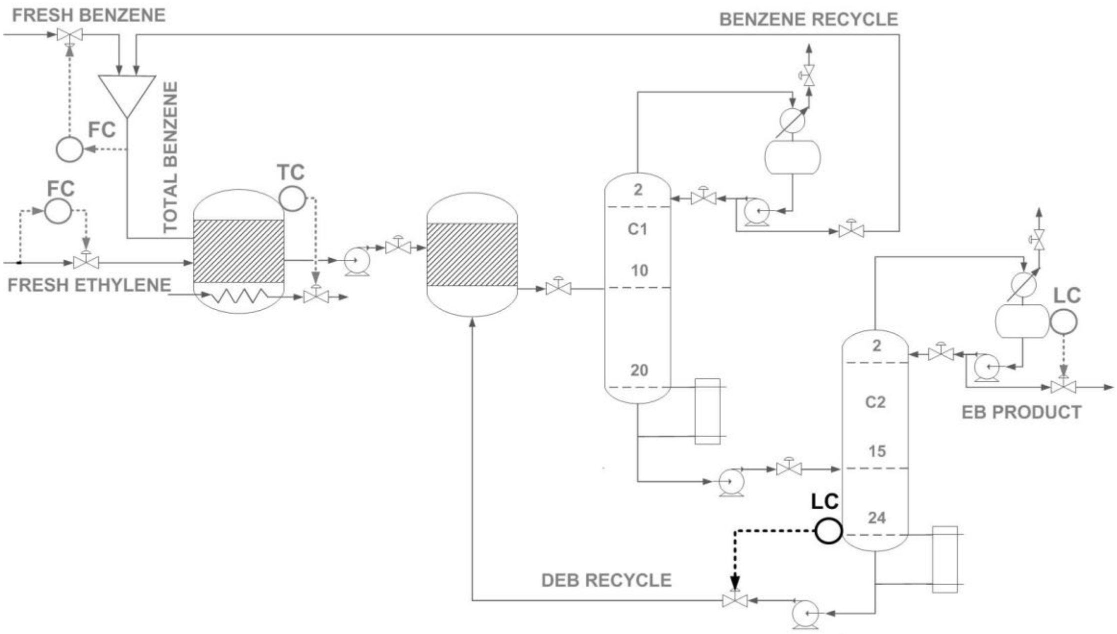


Figure 5.14 Flowsheet of ethylbenzene process for locate the rest quantifier components.

The choices of manipulated variables that can be used to control reflux drum level includes reflux flowrate and distillate flowrate. Reflux drum level is controlled by using reflux flowrate may be ineffective. Finally, the level control in the reflux drum should be controlled by manipulating distillate flowrate and the level control in the column base should be controlled by manipulating bottoms flowrate. This control scheme would be used for a column with a liquid distillate product and with a low to moderate reflux ratio (less than 4), which the column C1 and column C2 have reflux ratios of 0.774 and 0.661, respectively.

Step 4: Handling the disturbances

In this step, the quality control loops are configured by employing the notion of all disturbances management. The type and magnitude of disturbances affects to a reaction and separation section. The design of the control loops to manage with both thermal (Step 4.1) and material (Step 4.2) disturbances, which the heat disturbances are classified into 2 types. An analysis of disturbances encountered in the ethylbenzene process follows:

4.1 Heat Disturbance Management

4.1.1 Direct the heat disturbances that are not directly related to quality. HDC1 is omitted. Since there is no have thermal manage point.

4.1.2 Manage the heat disturbance that related to quality in order to maintain the product constraints.

The heat disturbances affect to product qualities and smoothly operate of process. In this section, the approach for manage thermal disturbances are explained. Our concern is to dissipate the heat disturbances away from the process. This requires that can be achieved through analyzing heat pathway, which control loops for this step are designed to reject heat disturbances. Normally, heat disturbances are transferred to environment via the nearest downstream heater or cooler. For ethyl benzene processes, the heat disturbances can be directly managed to the unit utilities, which are reactor R1, column C1 and C2.

The heat disturbance starts from the reactor inlet and goes through the first and the second reactor. This step can be completed by controlling the temperature of each unit. When the heat disturbances enter the first reactor with heat from exothermic reaction generated in reactor, it is dissipated away from the process by sent to duty before reaches in separation section. If the thermal disturbances escape to columns, the disturbances would be eliminated to utility in the distillation columns and removed from the process. Lists of the control loops for handles the heat disturbances as follows:

HDC2: The heat disturbances enter the reactor managed by the PI temperature controller to regulate the reactor temperatures by changing the setpoint of a steam pressure. If the thermal disturbances creeps to the distillation columns, it would be removed by the two PI temperature controllers, which located at the bottom stage (temperature control location is analyzed in step 2.6) of C1 and C2 by adjusting their duties. Figure 5.15 gives control loops are obtained by inspecting heat part ways, which shown its exit points.

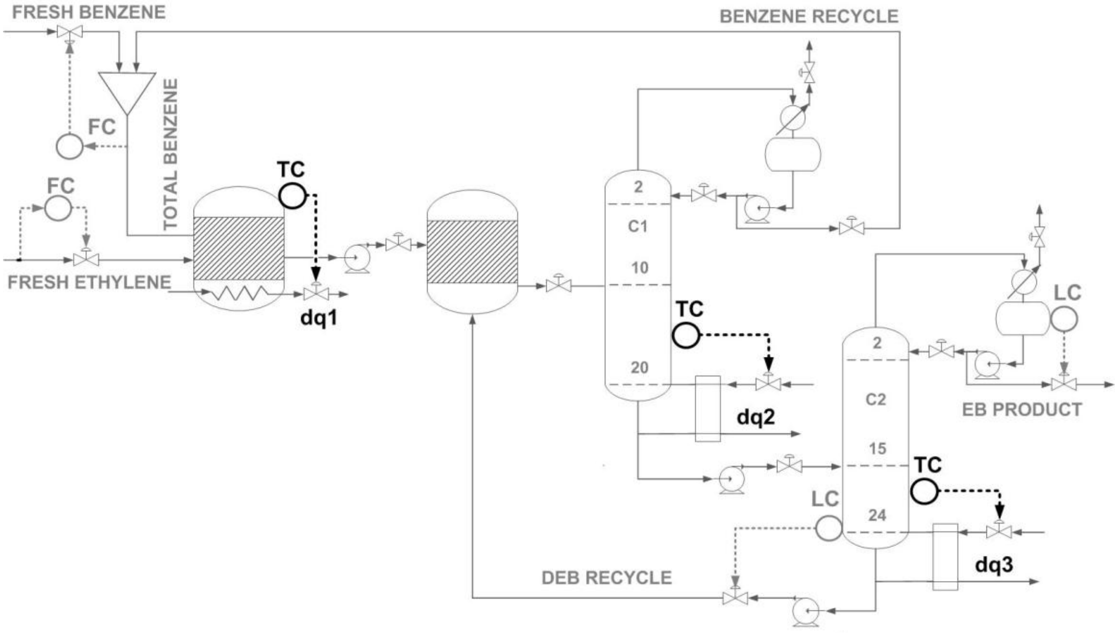


Figure 5.15 Flowsheet of ethylbenzene process for handle the heat disturbances.

4.2 Material disturbances

The frame of the control loops depend on the desired material pathways by analyzing the material disturbance tests on changes of composition, total flow, component flow and temperature. The material path ways demonstrated to manage each material according to their path ways. The material pathways of any material presented in Figure 5.2-5.5. This step is to identify and manage the material pathways of each component. Four components need to be analyzed by including ethylene, benzene, ethyl benzene and di-ethylbenzene.

Stoichiometry balances are maintained via ratio control by manipulating the fresh feed of reactant or the ratio of the fresh feeds. Ratio the limiting reactant fresh feed to the total stream of the excess reactant. This implies the composition of limiting reactant in reactor is maintained as production rate varies. Fig. 5.16 shows the ratio control configurations on feed stream. The fresh feed ethylene flowrate is as set a ratio of the total benzene stream, which is fresh feed plus the recycle stream from the distillate flowrate of the first column.

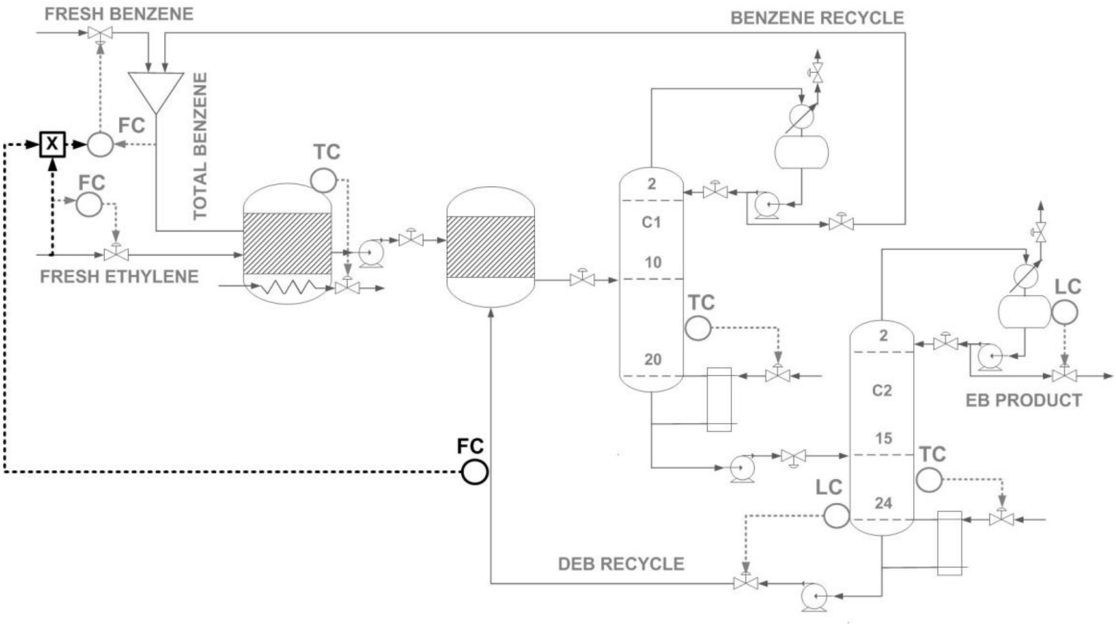
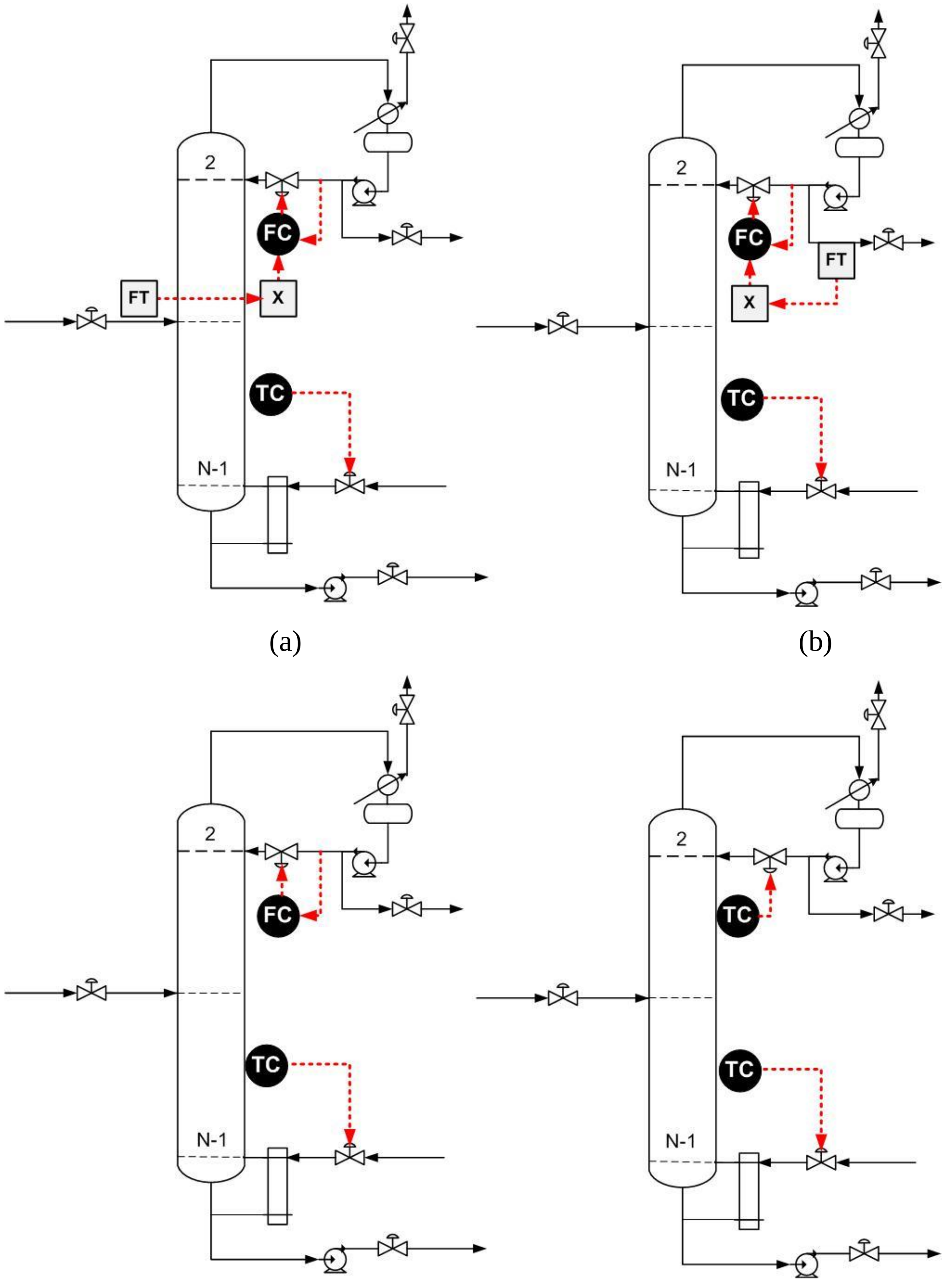


Figure 5.16 Flowsheet of ethylbenzene process for handle the material disturbances in reaction section

In this process have one recycle stream is DEB recycle, which the plantwide control problem becomes much more complex. This recycle stream leads to snowball effect if no effective control. A small change in throughput or various disturbances can lead to even larger changes in flows and propagate though whole process. The large swings in recycle streams and all process variables are undesired because their magnitude can over load the capacity of the reaction and separation section. Therefore, a way to prevent the snowball effect is liquid recycle stream should be flow cascade controlled to control a di-ethylbenzene flowrate by manipulating the ratio value on feed. In order to maintain the proper ratio of reactant streams before entering the first reactor, the fresh feed ethylene is set as a ratio of the total benzene stream. The fresh feed benzene is manipulated to maintain the flowrate of di-ethylbenzene when flowrate of di-ethylbenzene changes. From the third reaction, it is reaction of DEB with benzene to form EB. Ratio of feed must be increased to react between benzene and DEB, flowrate magnitude of DEB would decrease cause no snowball effect.



(a) (b)

(c) (d)

Figure 5.17 The control structure for handle disturbances in separation section.

a) Fixed Reflux to Feed Ratio (R/F) Control Structure

b) Fixed Reflux Ratio (RR) Control Structure

c) Fixed Reflux Rate Control Structure

d) Dual Temperature Control Structure

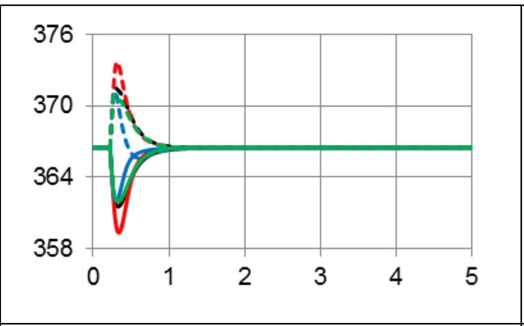
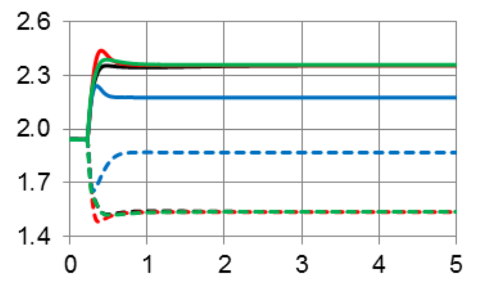
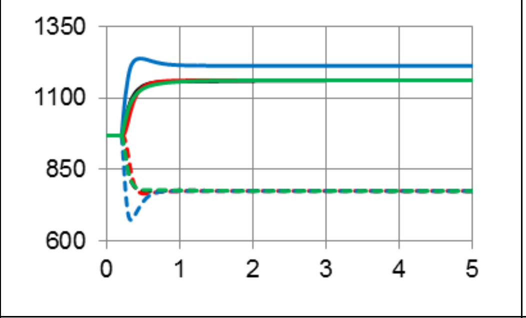
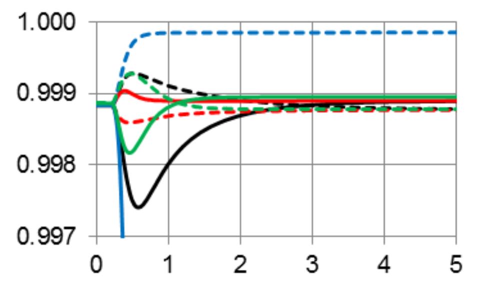
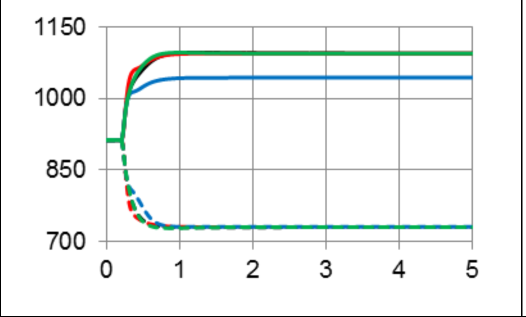
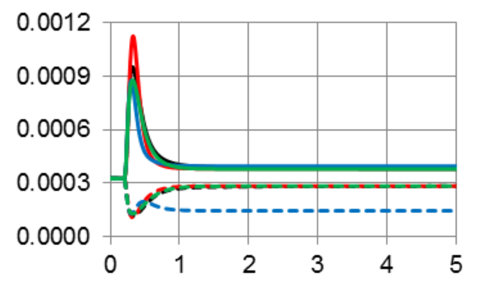
Therefore, the separation section should be analyzed as same as reaction section. The separation section are tested and analyzed in dynamic simulation. The control structures are tested such as reflux to feed ratio, reflux ratio and fixed reflux rate (if the temperature at the top can be found, should be tested dual temperature control structure). All control structures analyzed from this step are shown as following Figure 5.17.

In two columns, the effectiveness of using single-end temperature control is explored by using dynamic simulation. The required changes in fixed reflux flow, reflux ratio and reflux-to-feed ratio (and dual temperature) are considered. Changes in the light component feed compositions, total feed flowrates and light component feed flowrates to the column are tested, with the distillate and bottoms compositions held at their specified values. If either of these showed little change with variations in the disturbances, a single-end structure may be effective. The location of the tray whose temperature is controlled is selected by finding the location in the temperature profile in each column where there is a large change in the temperature from tray to tray. In all cases, there is a significant change in the temperature profile at the bottom part near stage 14 (column C1) and stage 18 (column C2), which analyzes though step.2.6.

4.2.1 Column C1.

The light key component is benzene, and the heavy key component is ethyl benzene. The disturbances test part includes total feed flowrate, light compositions and light component flowrates. All control structures are illustrated in Figure 5.17, which shown the improvement in handling disturbances achieved when single-end (the reflux ratio, reflux to feed ratio and fixed reflux flowrate) and dual-end control structures is used in column C1. Initially, the material pathway has been discussed and managed by placing controller. R/F is used in the first column to handle disturbances and maintain composition at desired value for basecase. The results shown, single-end control may not be effective. Finally, Dual temperature control for the first distillation column is considered as it is relatively more optimal than the single end control and also offers better control. The dynamic simulation results presented in Table 5.4-5.6 demonstrate the effectiveness of each control structures to handle disturbances and maintain purity very close to their specifications.

Table 5.4 the dynamic responses for total feed disturbances of column C1.

T_14 (K)		**QR (Mcal/s)**	
D1 (kmol/hr)		**xD1 (B)**	
B1 (kmol/hr)		**xB1 (B)**	
	Time (hr)		**Time (hr)**

― +20% Feed flowrate, fixed RR

― +20% Feed flowrate, fixed R/F

― +20% Feed flowrate, fixed reflux flow

― +20% Feed flowrate, Dual temperature

- - - -20% Feed flowrate, fixed RR

- - - -20% Feed flowrate, fixed R/F

- - - -20% Feed flowrate, fixed reflux flow

- - - -20% Feed flowrate, Dual temperature

Table 5.5 the dynamic responses for component flowrate disturbances of column C1.

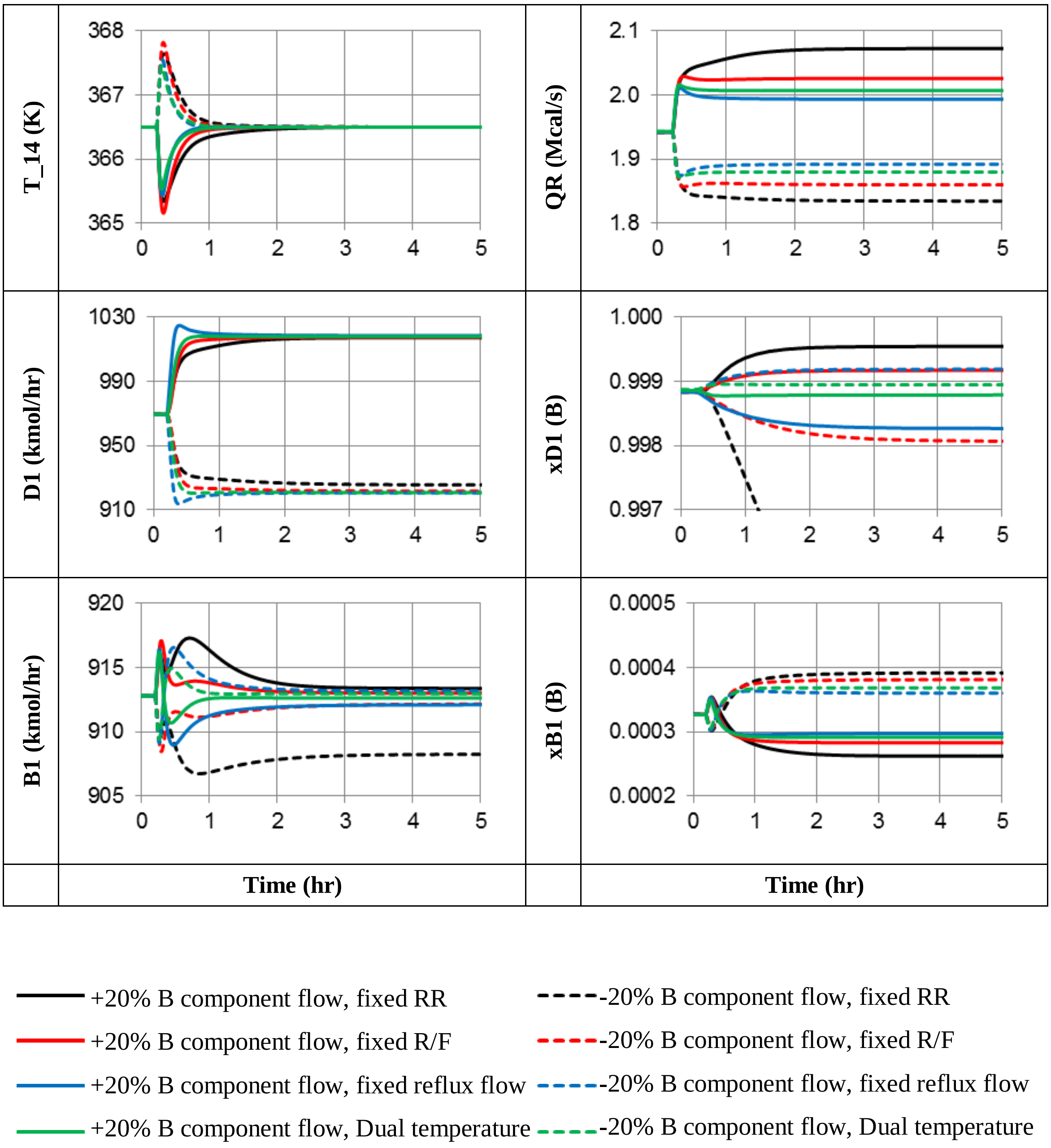
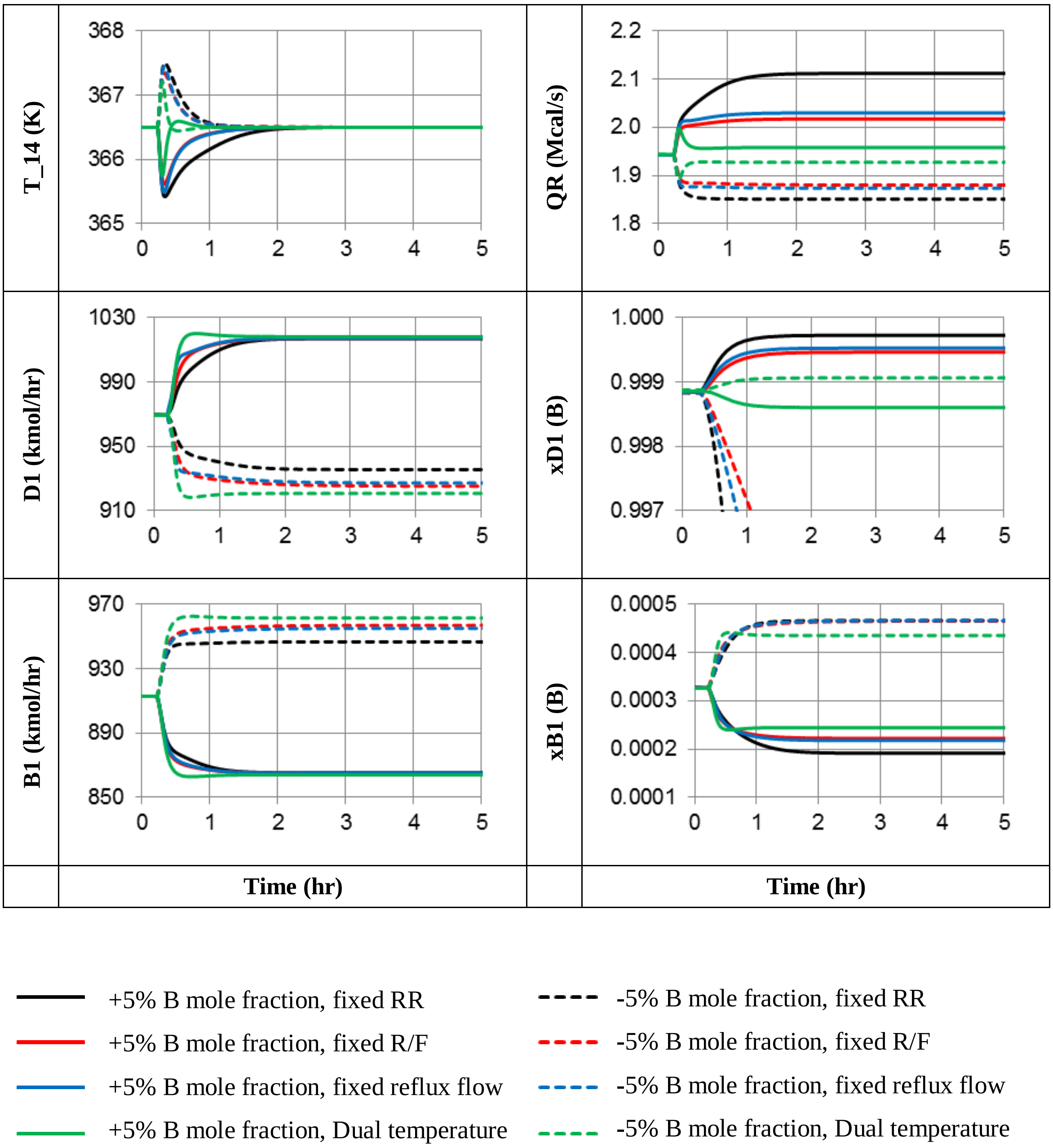


Table 5.6 the dynamic responses for composition disturbances of column C1.



Dual-end control, the purity of the benzene is held very close to its desired value because the ethyl benzene impurity does not go overhead in column C1. The stage 6 temperature controller adjusts the reflux flowrate to achieve this objective. The dual temperature control structure speeds up the dynamics simulation of the process because it prevents ethyl benzene impurity from going overhead in column C1 and affecting a little bit to the downstream column C2.

4.2.2 Column C2.

The light key component is ethyl benzene, and the heavy key component is di-ethyl benzene. The disturbances test part as same as column C1. All control structures are given in Figure 5.17, which shown the improvement in handling disturbances achieved. Single-end (the reflux ratio, reflux to feed ratio and fixed reflux flowrate) control structures only are used in column C2. The dynamic simulation results presented in Table 5.7-5.9 demonstrate the effectiveness of each control structures to handle disturbances and maintain purity very close to their specifications.

Table 5.7 the dynamic responses for total feed disturbances of column C2.

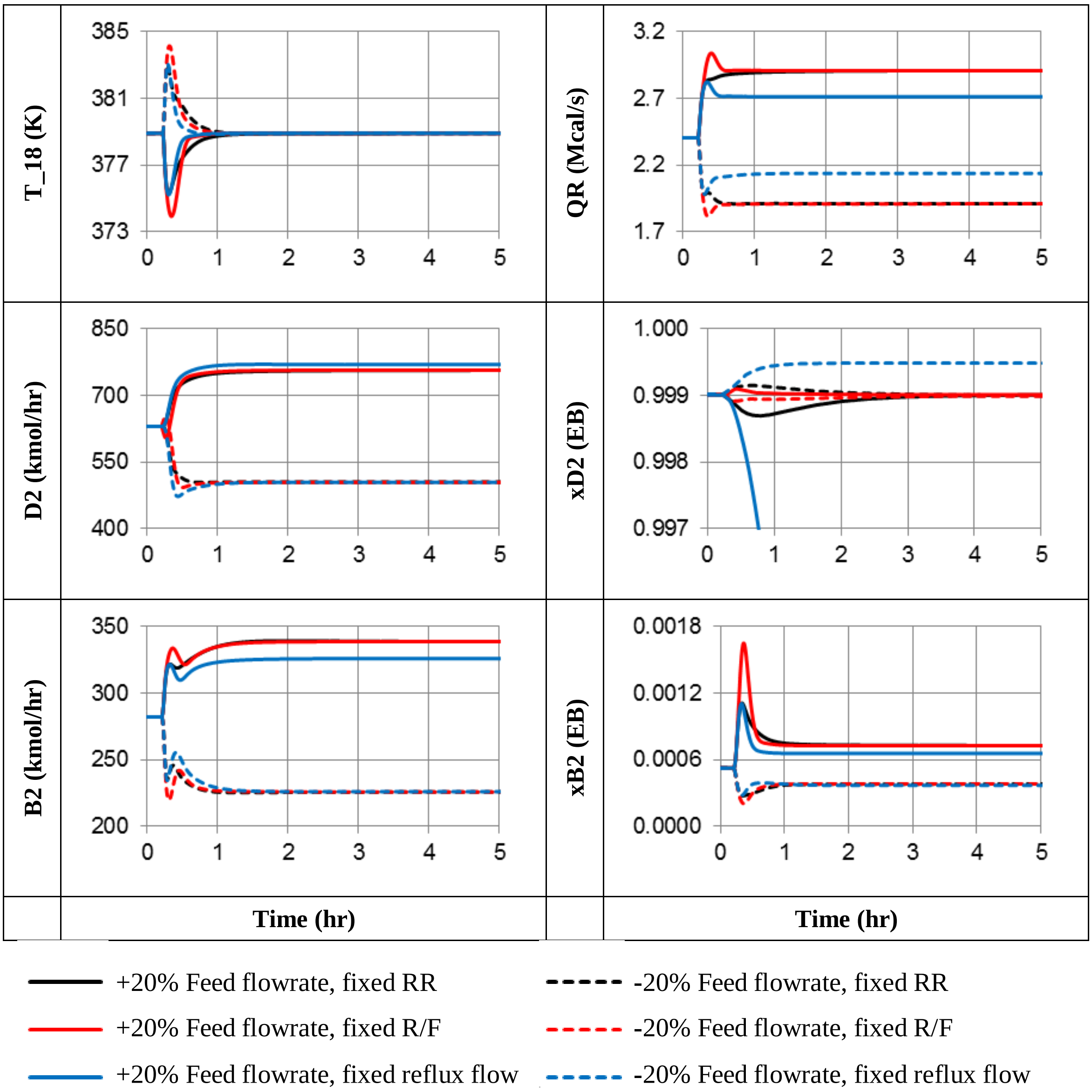
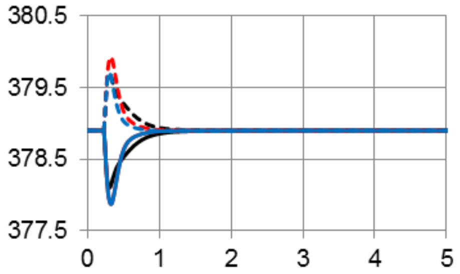
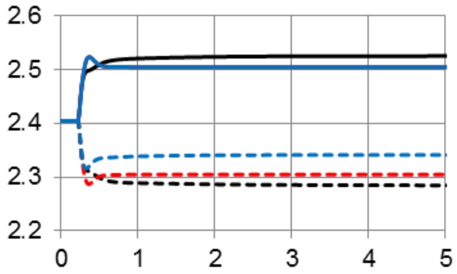
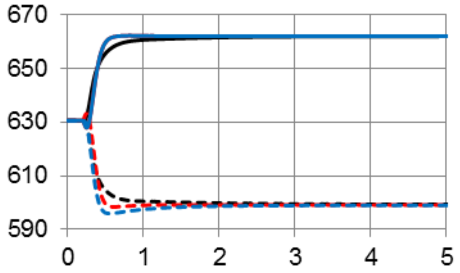
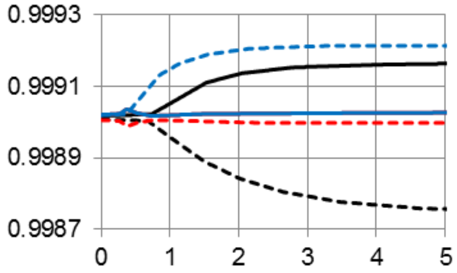
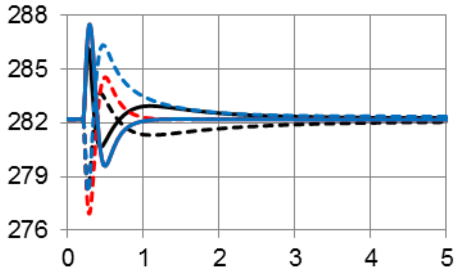
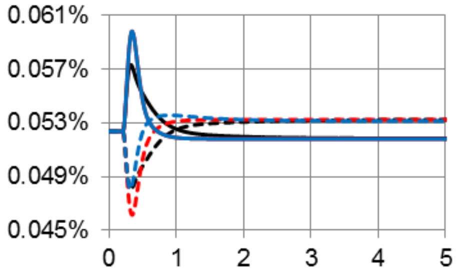


Table 5.8 the dynamic responses for component flow disturbances of column C2.

T_18 (K)		**QR (Mcal/s)**	
D2 (kmol/hr)		**xD2 (EB)**	
B2 (kmol/hr)		**xB2 (EB)**	
	Time (hr)		**Time (hr)**

— +20% EB component flow, fixed RR

- - - -20% EB component flow, fixed RR

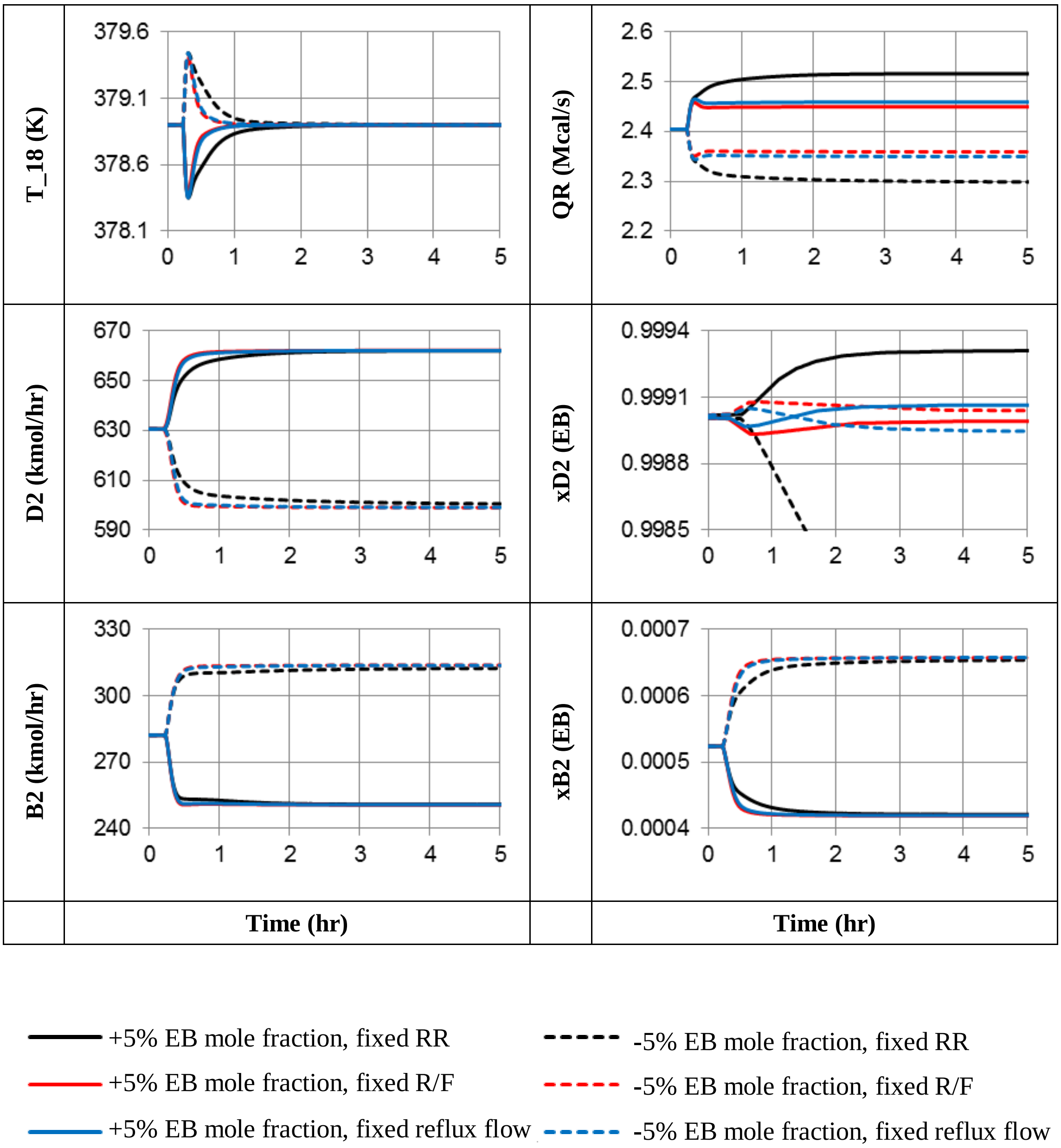
— +20% EB component flow, fixed R/F

- - - -20% EB component flow, fixed R/F

— +20% EB component flow, fixed reflux flow

- - - -20% EB component flow, fixed reflux flow

Table 5.9 the dynamic responses for composition disturbances of column C2.



The results shown single-end control may be effective. The R/F control is used in this column. The purity of the ethyl benzene is kept very close to their specifications because the di-ethyl benzene impurity does not go overhead in column C2. The reflux flowrate controller at top stage received flowrate signal from feed stream and send to adjusting the reflux flowrate to achieve this objective. The R/F control structure speeds up the dynamics simulation of the process.

Step 5: Design the control loops for the rest of the control variables or adding enhanced controls.

In this step, all unit operations are analyzed and control loops are placed wherever necessary. For example, for the

This step is design to the control loops for safety and control inventories. We can assign control loops within individual units. The rest control loops are designed and added to the process, which includes pressure and level controls. Quantifiers of each component are different location. A controller must be presented in all liquid accumulates. Four liquid levels need to be controlled: two reactors reflux drum and base of column C1. Two pressure control loops: column C1 and C2. The various loops shown in Figure 5.18 are listed below with their controlled and manipulated variables.

- Each reactor: liquid levels (LC) are controlled to maintain the quantifiers of the components by manipulating the liquid streams leaving the reactor.

- Base level (LC) and reflux drum level (LC) are controlled with bottoms and distillates flow of column C1, respectively.

- Pressure control loops: Two pressures controller (PC) must are installed in the columns. In both columns, pressure control can be achieved by manipulating condenser heat removal.

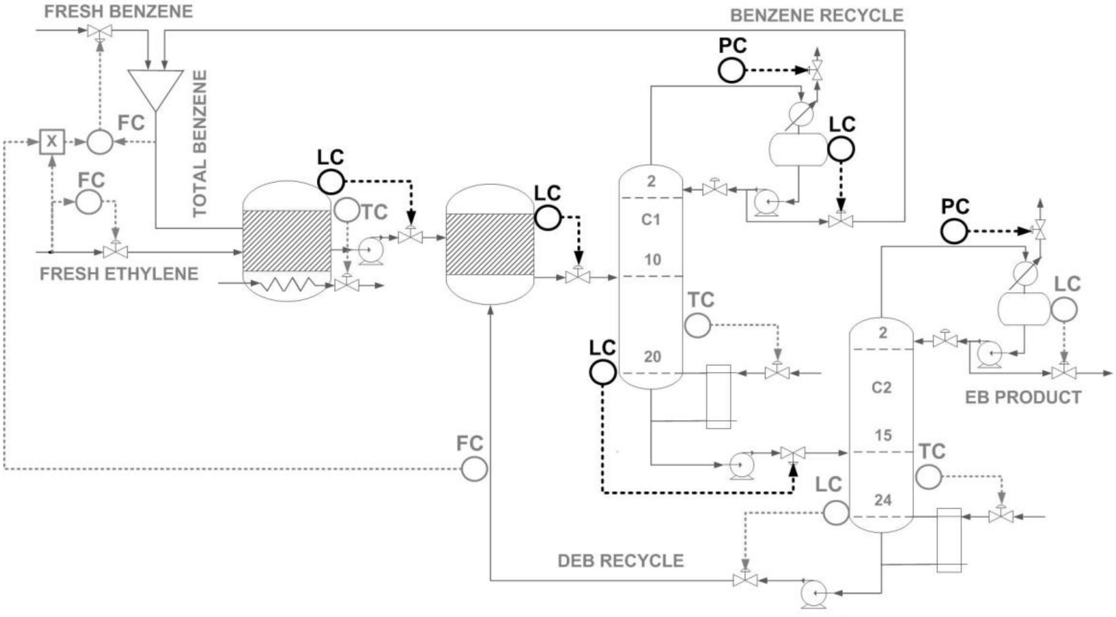


Figure 5.18 Flowsheet of ethylbenzene process for the rest of the control variables

Step 6: Energy management via heat exchanger networks.

There is no alternative heat integrated processes available in the ethyl benzene process since the temperatures of process is operated at quite temperature.

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

There is no particular necessary to establish any additional control loops. The flowsheet with the controllers installed is given in Figure 5.19-5.21. The controlled, variables, manipulated variables, types of controller, nominal value and the tuning parameters for all the controllers are given in Table B.3 to B.5. The control valves are all designed for 50% valve opening under initial steady-state conditions. All the flow and pressure loops are tuned based on initial tuning values. The level loops are proportional-only. The composition and temperature control loops are tuned as PI controllers using the auto tuner. In the benzene recycle column, fixed reflux to feed ratio cannot be used to infer composition of benzene and ethyl benzene are very close. Next, the dual temperature control is controlled as this scheme is found to handle changes in feed disturbances better than a fixed reflux to feed scheme. As for the product column, Temperature cannot be used in this case as the temperature profile in the stripping section is very flat. Fixed reflux to feed is controlled as this scheme.

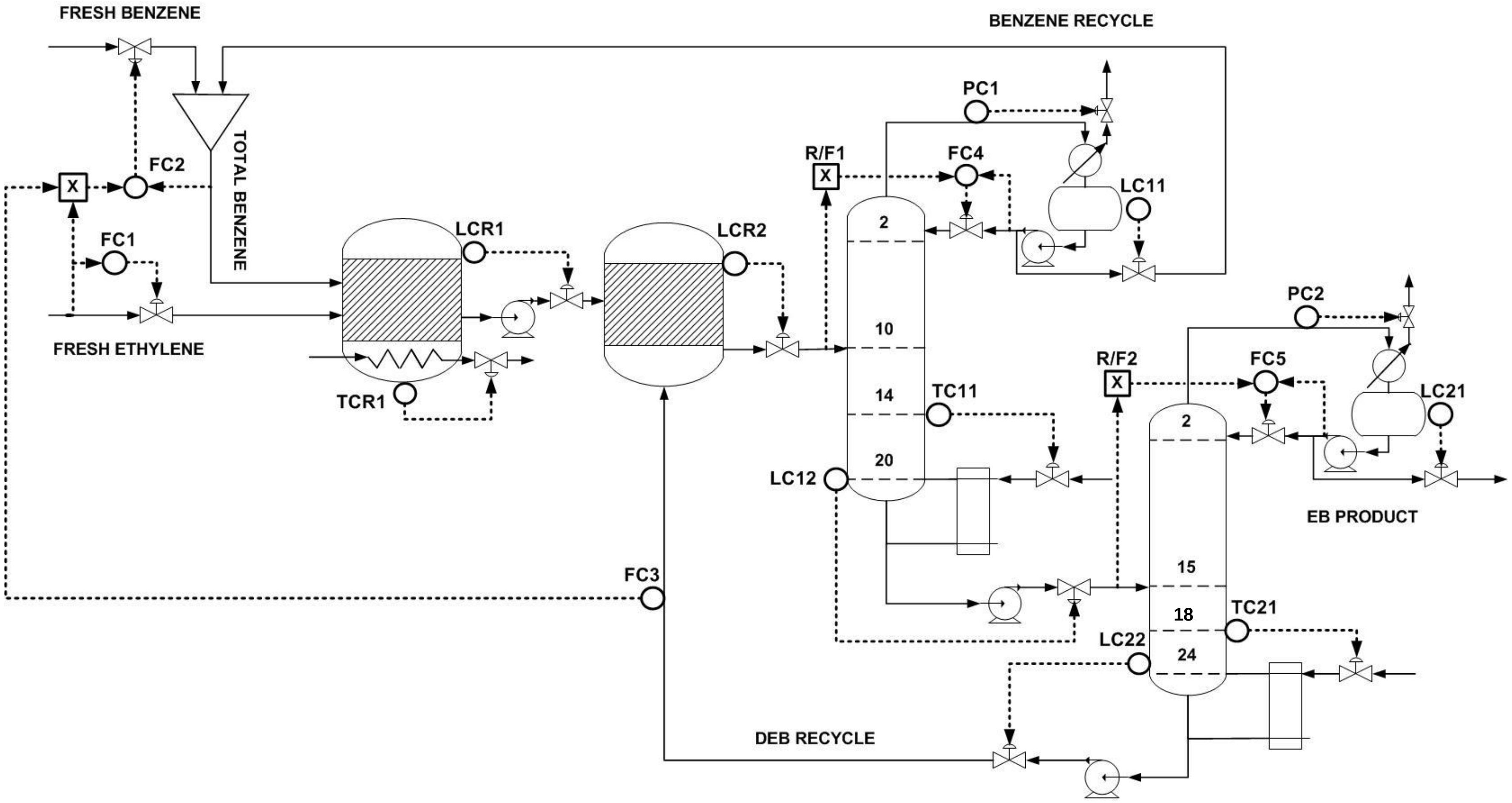


Figure 5.19 Ethyl benzene plantwide control structure CS0

Table 5.10 Control structure lists of CS0

Equipment	Controller	Controlled Variables	Manipulated Variables	Type	Action
Reactor 1	TCR1	Reactor 1 temperature	Heat load of R1	PI	Reverse
	LCR1	Reactor 1 level	Flowrate out of R1	P	Direct
	FC1	Fresh ethylene flow	Fresh ethylene flow	PI	Reverse
	FC2	Total benzene flow	Fresh benzene flow	PI	Reverse
Reactor 2	LCR2	Reactor 2 level	Flowrate out of R1	P	Direct
Column 1	R/F1	Ratio of reflux to feed	Reflux of C1	PI	Direct
	TC11	Stage 14 C1 temp.	Heat load of QR1	PI	Reverse
	LC11	Reflux drum 1 level	Flowrate out of D1	P	Direct
	LC12	Bottom 1 level	Flowrate out of B1	P	Direct
	PC1	Column 1 pressure	Heat load of QC1	PI	Reverse
Column 2	R/F2	Ratio of reflux to feed	Reflux of C2	PI	Direct
	TC21	Stage 18 C2 temp.	Heat load of QR2	PI	Reverse
	LC21	Reflux drum 2 level	Flowrate out of D2	P	Direct
	LC22	Bottom 2 level	Flowrate out of B2	P	Direct
	PC2	Column 2 pressure	Heat load of QC2	PI	Reverse
	FC3	DEB flowrate	Ratio of BTOT/FFE	P	Direct

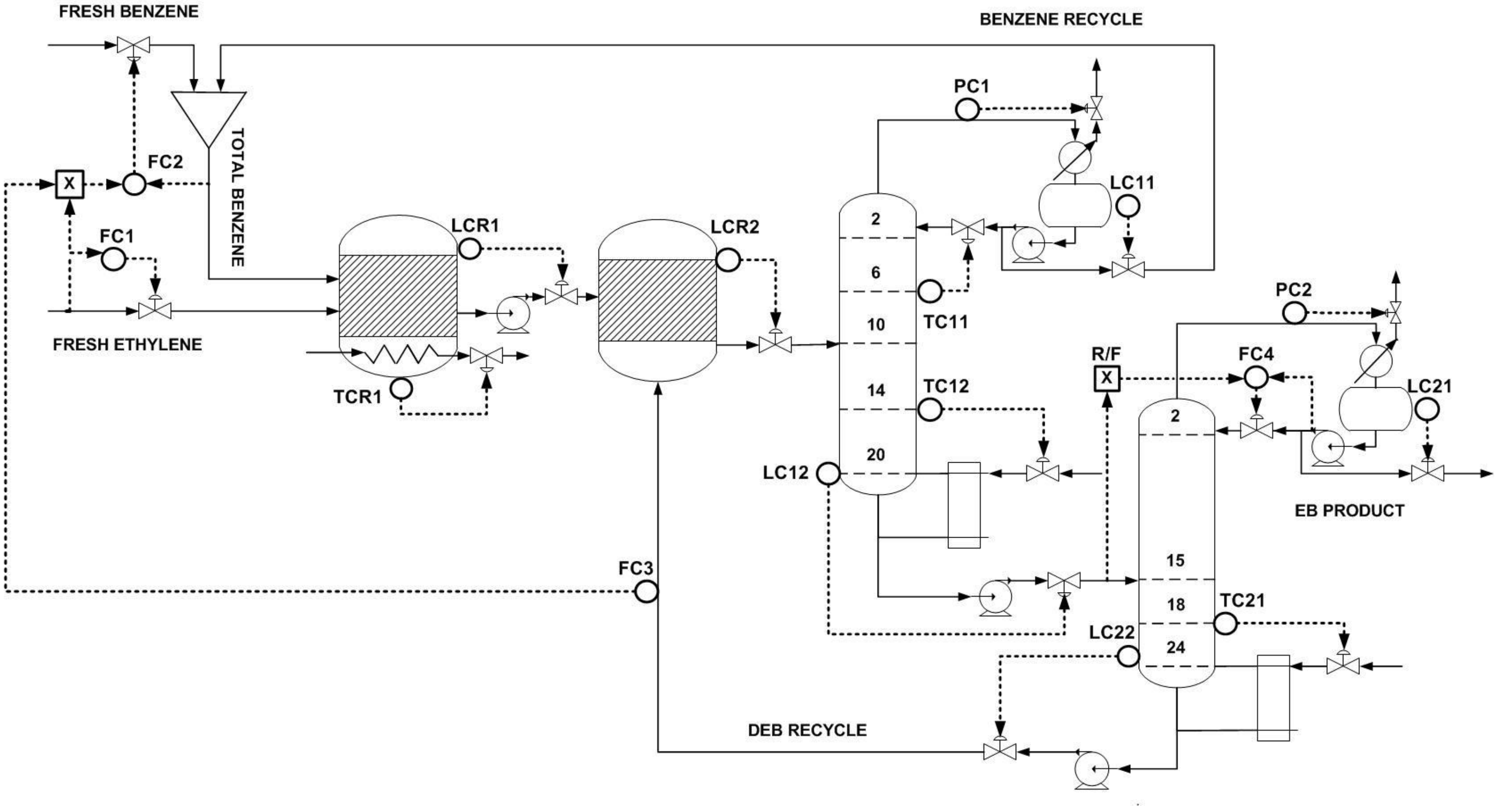


Figure 5.20 Ethyl benzene plantwide control structure CS1

Table 5.11 Control structure lists of CS1

Equipment	Controller	Controlled Variables	Manipulated Variables	Type	Action
Reactor 1	TCR1	Reactor 1 temperature	Heat load of R1	PI	Reverse
	LCR2	Reactor 1 level	Flowrate out of R1	P	Direct
	FC1	Fresh ethylene flow	Fresh ethylene flow	PI	Reverse
	FC1	Total benzene flow	Fresh benzene flow	PI	Reverse
Reactor 2	LCR2	Reactor 2 level	Flowrate out of R1	P	Direct
Column 1	TC11	Stage 6 C1 Temp.	Reflux flowrate	PI	Direct
	TC12	Stage 14 C1 Temp.	Heat load of QR1	PI	Direct
	LC11	Reflux drum 1 level	Flowrate out of D1	P	Direct
	LC12	Bottom 1 level	Flowrate out of B1	P	Direct
	PC1	Column 1 pressure	Heat load of QC1	PI	Reverse
Column 2	R/F1	Ratio of reflux to feed	Reflux flowrate	PI	Direct
	TC21	Stage 18 C2 Temp.	Heat load of QR2	PI	Reverse
	LC21	Reflux drum 2 level	Flowrate out of D2	P	Direct
	LC22	Bottom 2 level	Flowrate out of B2	P	Direct
	PC2	Column 2 pressure	Heat load of QC2	PI	Reverse
	FC3	DEB flowrate	Ratio of BTOT/FFE	P	Direct

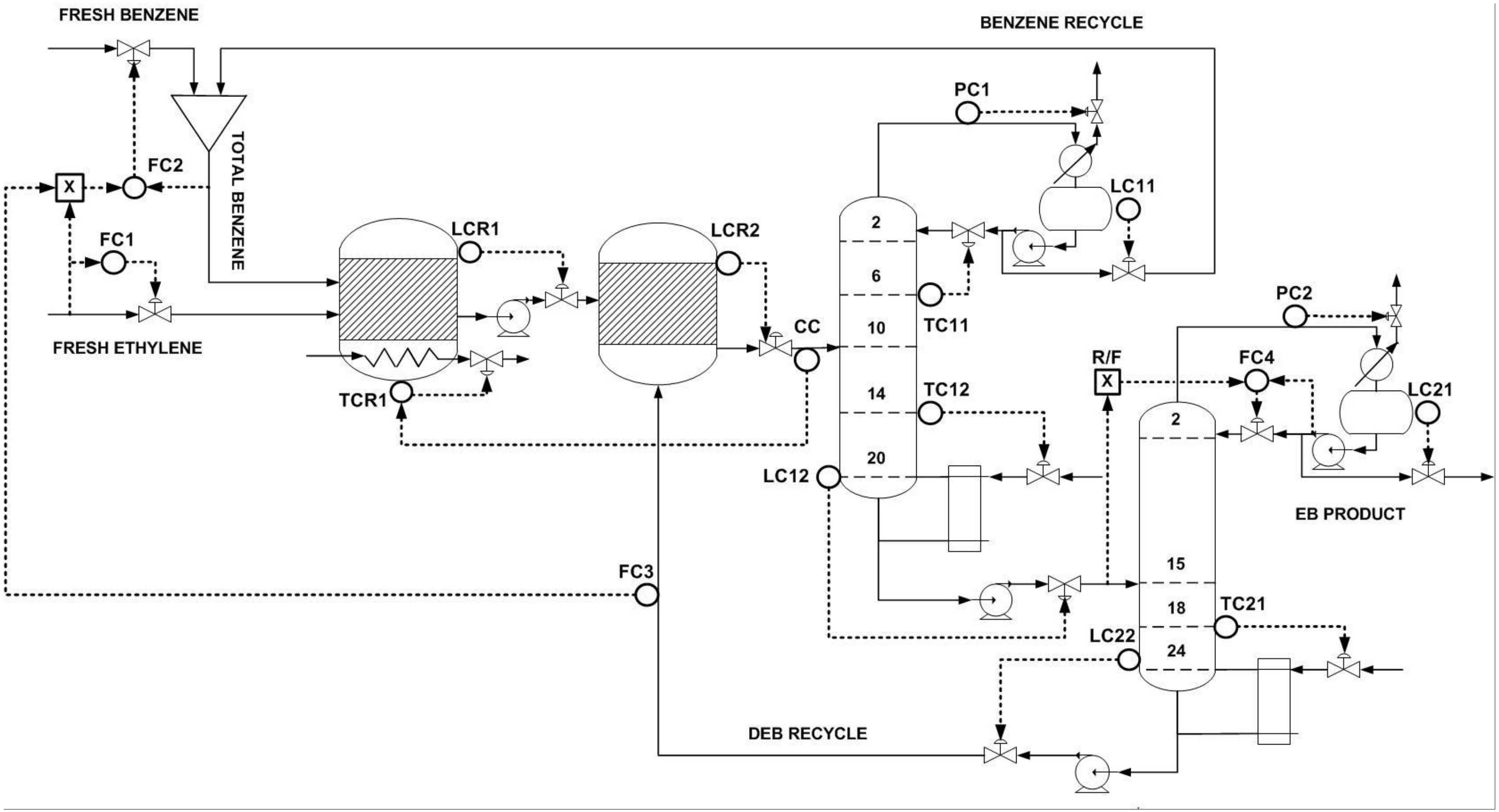


Figure 5.21 Ethyl benzene plantwide control structure CS2

Table 5.12 Control structure lists of CS2

Equipment	Controller	Controlled Variables	Manipulated Variables	Type	Action
Reactor 1	TCR1	Reactor 1 temperature	Heat load of R1	PI	Reverse
	LCR1	Reactor 1 level	Flowrate out of R1	P	Direct
	FC1	Fresh ethylene flow	Fresh ethylene flow	PI	Reverse
	FC2	Total benzene flow	Fresh benzene flow	PI	Reverse
Reactor 2	LCR2	Reactor 2 level	Flowrate out of R1	P	Direct
	CC	Ethylene mole fraction	R1 Temperature	PI	Direct
Column 1	TC11	Stage 6 C1 temp.	Reflux flowrate of C1	PI	Direct
	TC12	Stage 14 C1 temp.	Heat load of QR1	PI	Reverse
	LC11	Reflux drum 1 level	Flowrate out of D1	P	Direct
	LC12	Bottom 1 level	Flowrate out of B1	P	Direct
	PC1	Column 1 pressure	Heat load of QC1	PI	Reverse
Column 2	R/F1	Ratio of reflux to feed	Reflux flowrate of C2	PI	Direct
	TC21	Stage 18 C2 temp.	Heat load of QR2	PI	Reverse
	LC21	Reflux drum 2 level	Flowrate out of D2	P	Direct
	LC22	Bottom 2 level	Flowrate out of B2	P	Direct
	PC2	Column 2 pressure	Heat load of QC2	PI	Reverse
	FC3	DEB flow	Ratio of BTOT/FFE	P	Direct

Step 8: Validate the designed control structures by rigorous dynamic simulation.

The simulation of this process is analyzed by using the commercial process simulator. All liquid level controllers and pressure loops are proportional control, liquid level with $K_C = 5$ for reactor level loops, $K_C = 2$ for column base and reflux drum level loops and $K_C = 2$, $\tau_I = 10$ for pressure loops. Temperature loops are containing 1 min deadtime. Deadtimes of 3 min are assumed in the reactor temperature loop and composition loops. The product quality and safety loops are tuned by using a relay-feedback test to determine ultimate gains and periods. The Tyreus-Luyben tuning rules are implemented. Table 5.13 gives the variation of setpoint and disturbances changes in feed stream.

Table 5.13 Setpoint changes and disturbances

No.	Type	Description	Change
1	Setpoint changes	Ethylene feed flowrates	±20%
2	Disturbances	EB feed composition	+5%
		DEB feed composition	+5%
		Feed temperatures	±20 K

5.3 Dynamic simulation results

The effectiveness of the plantwide control structures are demonstrated by subjecting the process to disturbances. The important plantwide disturbances in the ethyl benzene process have three feed disturbances. The several types of feed disturbances are introduced into the system to test and evaluate the dynamic performance of the control structure. The first one is the step change in ±20% throughput changes. This can be done by changing the set point of the ethylene feed flow control loop. The second disturbance is the tougher benzene feed composition changes. It is assumed that the benzene feed is not pure but contains 5% of the other reactant, which including ethyl benzene and di-ethylbenzene in this stream. These two variables are the manipulators for ethyl benzene production rate. The third disturbance is the ±20K feed temperature changes. It is assumed that the feed temperature is not nominal value but contains ±20K of both feed streams. This variable is the disturbance, which agitates to smoothly operation of ethyl benzene process.

The control structure efficiency is interested in two topics. First, how do these design variables and control loops affect the control of product quality (ethyl benzene purity in the distillate of the product column) and ethyl benzene loses (ethyl benzene impurity in the distillate of benzene column)? Second, how do they affect the robustness of the control structures? All control structures can be made to fail if they are upset with a large enough disturbances. It is desirable for a process and control structure to handle relatively large disturbances. In order illustrate the dynamic of control structure designed using new design procedure of Wongsri.

5.3.1 Ethylene feed flowrate disturbance

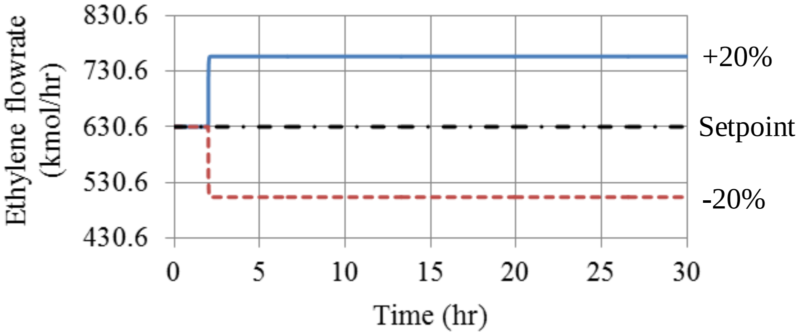


Figure 5.22 Step changes for ±20% ethylene flowrate.

The control structures are tested for the responses of the entire process. Step changes for ±20% ethylene flowrate in the setpoint of the ethylene flowrate controller shown in Figure 5.22. All control structures, there are changed from nominal value is 630.6 kmol/h to 504.5 kmol/h and 756.7 kmol/h as same as the feed of basecase. Table 5.9 shows the responses of the whole process for ethylene feed flowrate disturbance. The setpoint of the ethylene fresh feed flow controller are changed. The step changes are made at time = 2 hr. and finished at time = 30 hr. The fresh feed ethylene can be changed ±20%. The solid lines are responses of a 20% increase and the dashed lines are a 20% decrease. Table 5.14 shown responses for disturbances in ethylene feed flowrate. The total benzene flowrate is ratioed to the fresh feed ethylene flowrate. So the total benzene flowrate increases when the ethylene fresh feed is increased. The benzene fresh feed stream rapidly changes in control structure 1 and 2, while fresh feed benzene gradually changes in basecase. The ethyl benzene product flowrate gradually increased, while flowrate of all streams increase throughout of plant. Notice, the response result differences that because basecase is used R/F to handle disturbances. When feed flowrate changes, reflux flow is manipulated before disturbances fed into the column. So the distillate flowrate gradually changes; on the other hand, the distillate flowrate of control structure 1 and 2 rapidly changes when disturbances enter the distillation column. Responses shown that as results of dual temperature control, which controller are operated after disturbances enter the column or temperature at stage sensor controller changes. If temperature changes, the controller gradually manipulates and reaches to the setpoint.

Outlet temperature of reactor R1 is not significantly different in basecase and control structure 1, since outlet temperature is controlled. As a results, outlet temperature of reactor R1 changes from steady state value. After a period of time, its temperature is turned to its nominal value again in basecase and control structure 1 case. For control structure 2, the temperature reaches to new setpoint depend on ethylene composition at outlet reactor R2. The outlet temperature of reactor R1 is disturbed about for basecase. Duty of the reactor R1 must be increased or decreased to hold the outlet temperature in basecase and control structure 1 and hold ethylene composition in control structure 2. For the temperature control loops in column C1 and C2 are quite well controlled. Duties of the columns have the same results for adjusting their duties to hold the temperature setpoint.

All Cases, dynamic response of the benzene purity related to the amount of feed flowrate. Change of benzene purity in the benzene recycle stream of basecase cannot be controlled by reflux to feed. In ethylene flowrate case is decreased, the benzene composition is still maintained at high purity for the first 4 hr. but becomes less pure after that time. The purity of the ethyl benzene distillate product decreases to 0.987 during this disturbance, which is below the nominal value. More ethyl benzene is lost in the benzene recycle stream. Purity of benzene cannot maintain at desired value since reflux flow is insufficient amount to handle disturbance. The way to maintain the compositions at their specifications is to control dual temperature or adjust the temperature setpoints of the tray temperature loops.

For the benzene recycle stream, single end control should be sufficient as the main objective is not to lose ethyl benzene from the distillate stream. However, from the disturbance propagation through the recycle stream is also as important as minimizing the ethyl benzene loss. Hence, perception is given due importance and dual temperature control is chosen for the first column. Control structure 1 and 2 can be kept benzene purity well since the amounts of vapor depend on temperature at top stage, which benzene composition can be directly controlled. The desired distillate impurity is 0.1 mol% EB. The responses of the distillates composition are adjusted to their setpoint value in new designed control structure. All control structures can handle the composition of di-ethyl benzene escaping out the product stream well. In basecase, the response of ethyl benzene purity decreases because more benzene creeping from the bottom, which as a result from control structure of column C1.

For responses of control structure 1 and 2 shown, the purity of the ethyl benzene distillate product is kept quite close to the desired value, The di-ethylbenzene recycle stream (Bottom C2) can be controlled by adjusting the ratio of total benzene/ethylene fresh feed, which change of di-ethylbenzene quantities related to ratio of BTOT/FFE. So, the amount of di-ethylbenzene gradually increases when the reactants (ethylene and benzene) are increased and decreases when the reactants are decreased. Notice, the amount of di-ethylbenzene in control structure 2 is smaller than other cases. As a result, the amount of di-ethylbenzene has a little bit oscillated. There is only very small deviation (less than 0.16%) from correct temperature of reaction by controlling ethylene composition at outlet of the second reactor.

Conclusion, Table 5.14, it is found that the overall control structures performed nicely in maintaining high purity of the ethyl benzene products. The product flowrate is desirably increased/decreased to new values. The disturbances of ethylene feed flowrate change have very little effect on the ethyl benzene composition at the top of the column C2 in all cases. Only very small offset is observed for the benzene composition at the bottom of the column C1, which basecase is quite disturbed from these disturbances than new control structure designed. However, the new control structure can manage with changes of the ethylene feed flowrate quite well.

Table 5.14 The dynamic responses for the ethylene feed flowrate disturbances.

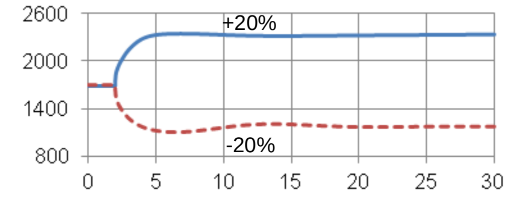
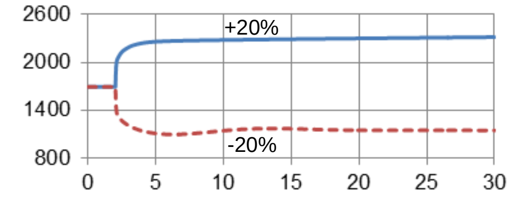
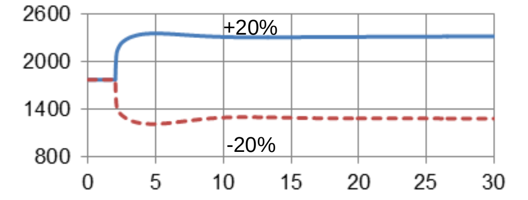
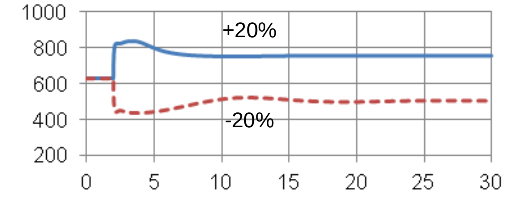
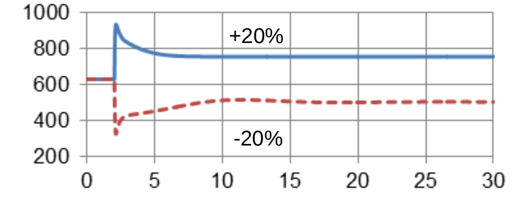
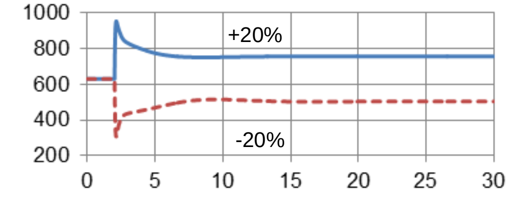
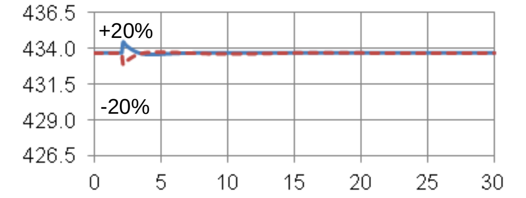
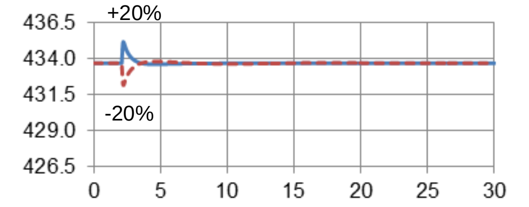
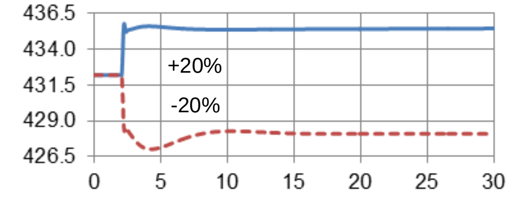
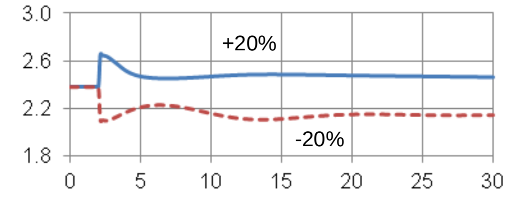
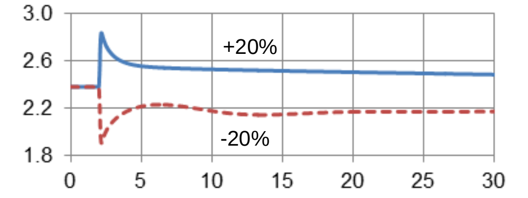
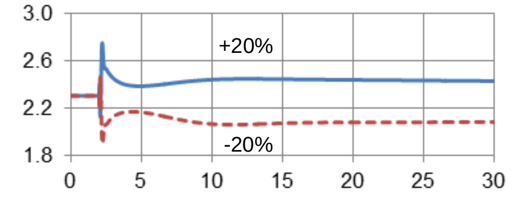
	BASECASE	**CS1**	**CS2**
BTOT (kmol/hr)			
FFB (kmol/hr)			
TR1 (K)			
Q react (Mcal/s)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.14 The dynamic responses for the ethylene feed flowrate disturbances (continued).

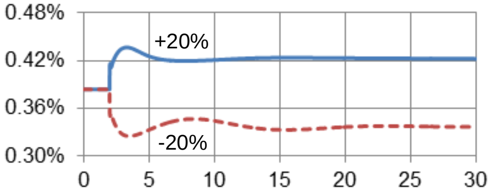
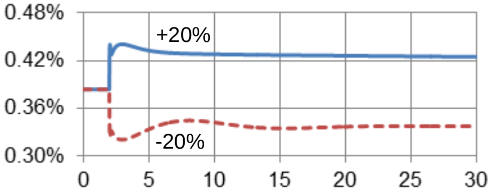
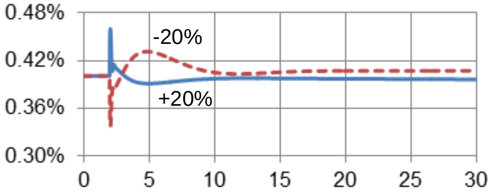
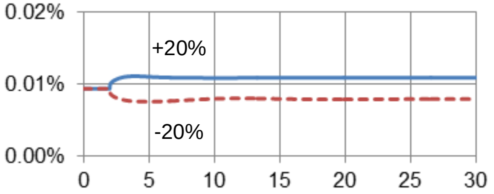
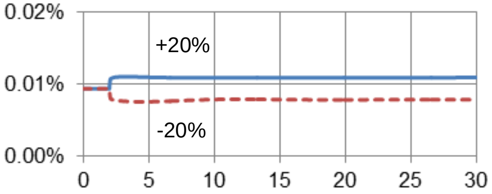
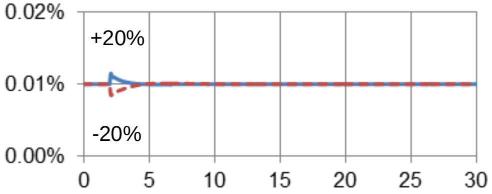
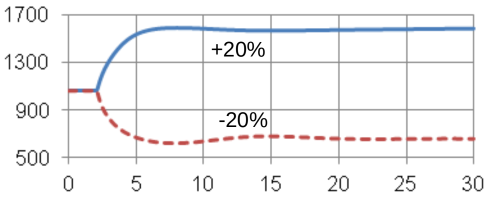
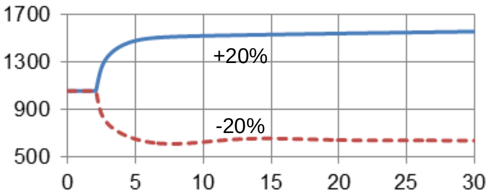
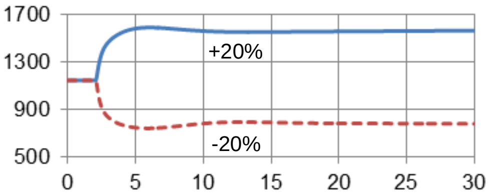
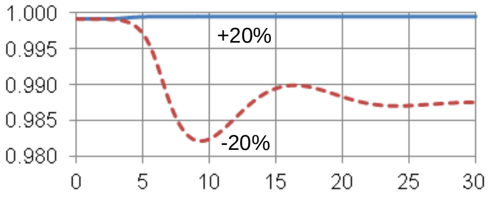
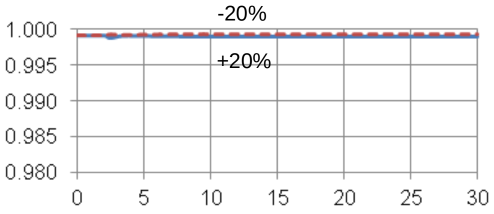
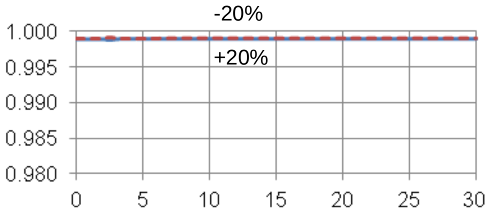
	BASE CASE	**CS1**	**CS2**
xR1 (%E)			
xR2 (%E)			
D1 (kmol/hr)			
xD1 (B)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.14 The dynamic responses for the ethylene feed flowrate disturbances (continued).

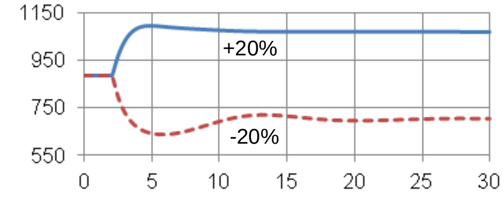
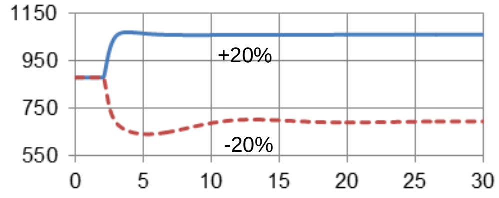
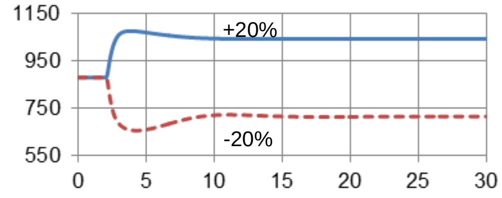
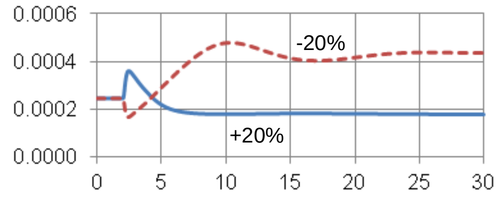
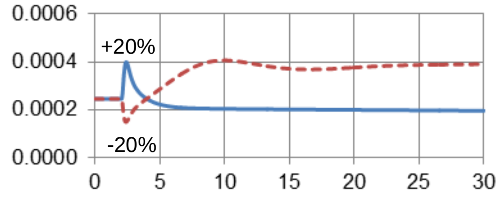
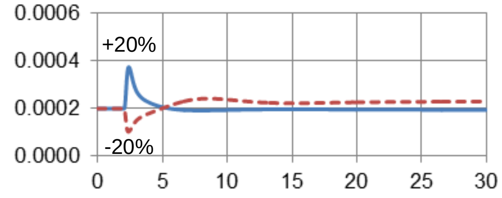
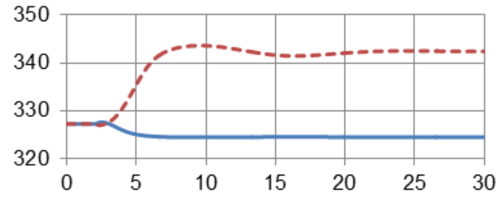
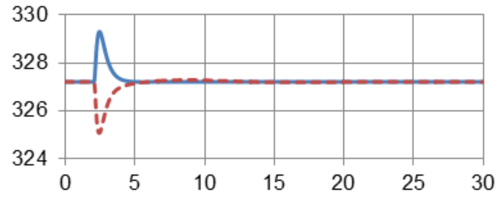
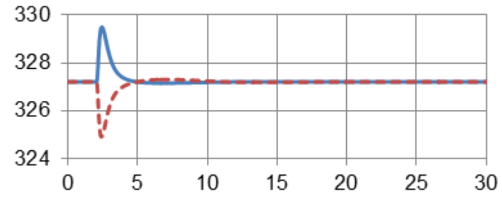
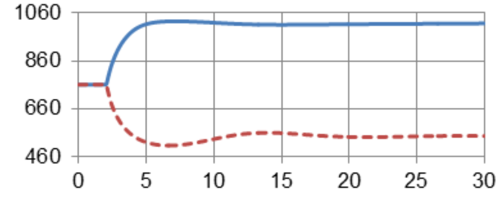
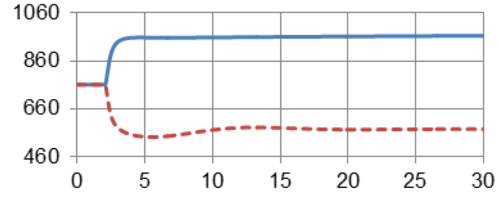
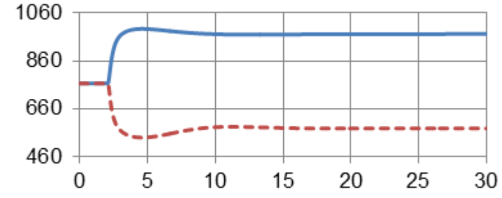
	BASECASE	**CS1**	**CS2**
B1 (kmol/hr)			
xB1 (B)			
T6 (K)			
R1 (kmol/hr)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.14 The dynamic responses for the ethylene feed flowrate disturbances (continued).

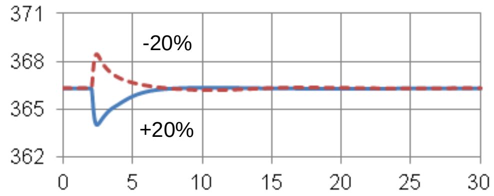
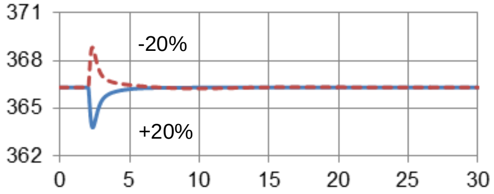
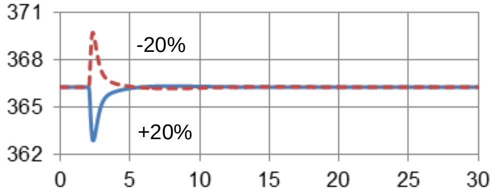
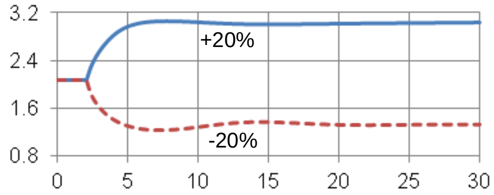
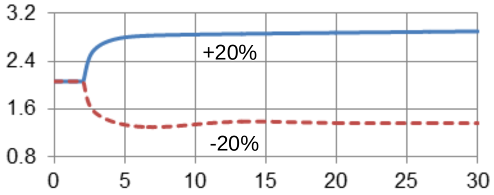
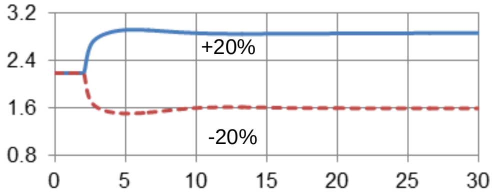
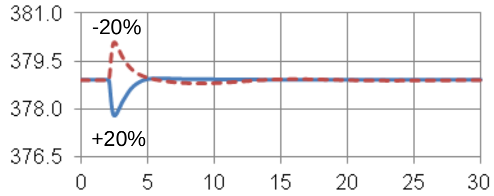
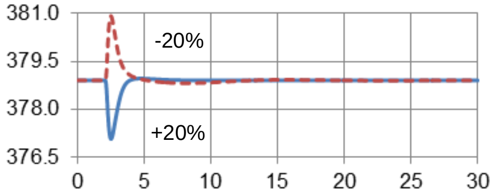
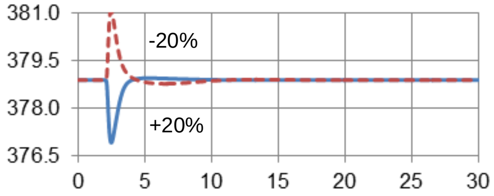
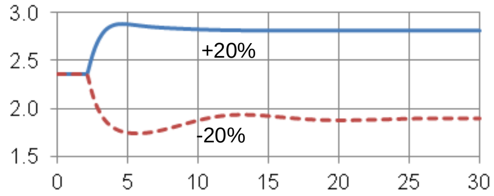
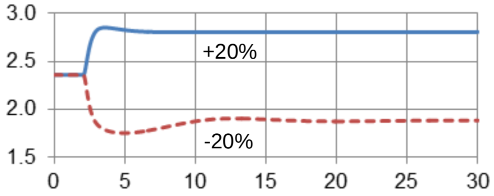
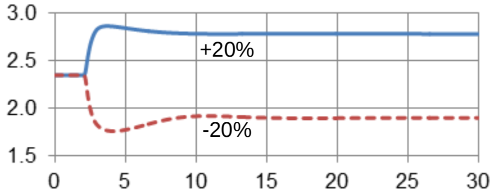
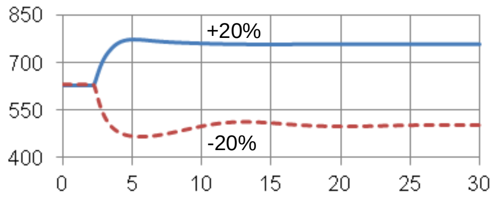
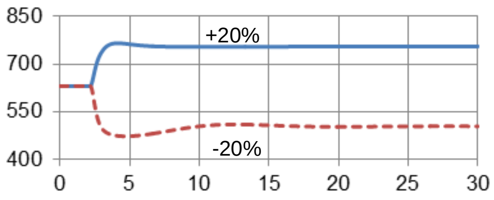
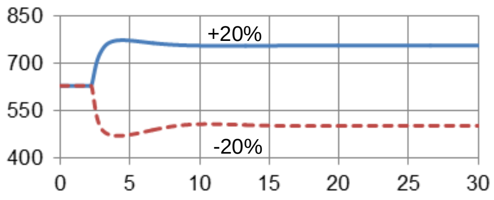
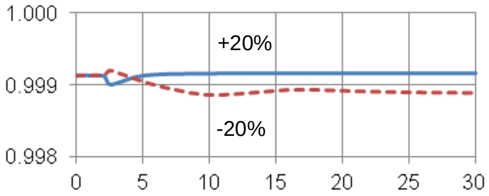
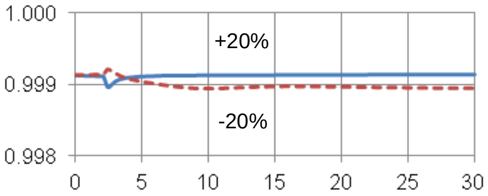
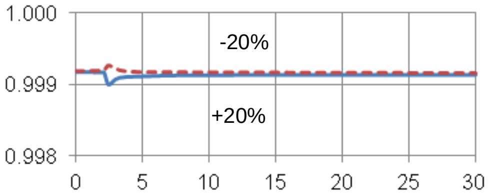
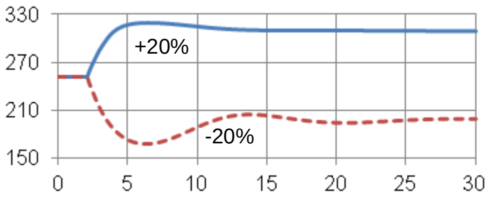
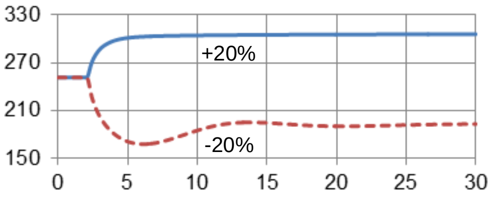
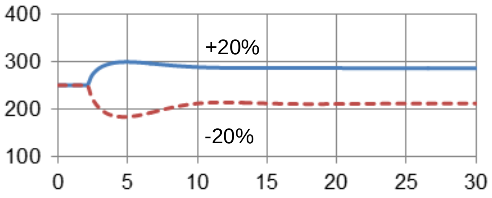
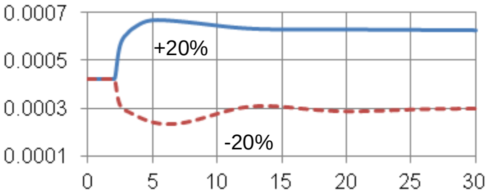
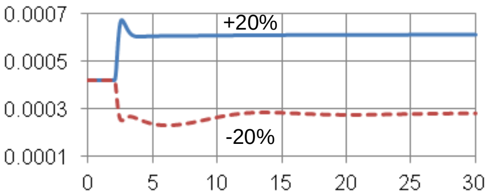
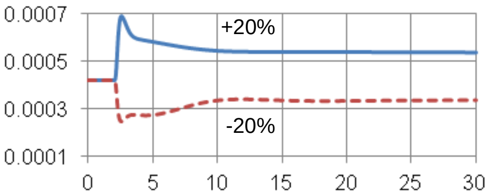
	BASECASE	**CS1**	**CS2**
T14 (K)			
QR1 (Mcal/s)			
T18 (K)			
QR2 (Mcal/s)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.14 The dynamic responses for the ethylene feed flowrate disturbances (continued).

	BASECASE	**CS1**	**CS2**
D2 (kmol/hr)			
xD2 (EB)			
B2 (kmol/hr)			
xB2 (EB)			
	Time (hr)	**Time (hr)**	**Time (hr)**

5.3.2 Benzene feed purity disturbances

Table 5.10 shows the dynamic responses for disturbances in two different benzene feed purity. The solid lines are when more di-ethylbenzene is added. The fresh benzene composition is changed from pure benzene to 95% mol benzene with a corresponding increase in DEB from 0 to 5% mol DEB. The dashed lines are when ethyl benzene is putted. The fresh benzene composition is changed from pure benzene to 95% mol benzene and 5% mol EB. All control structures are changed from nominal value at time = 2 hr. and then finished at time = 30 hr.

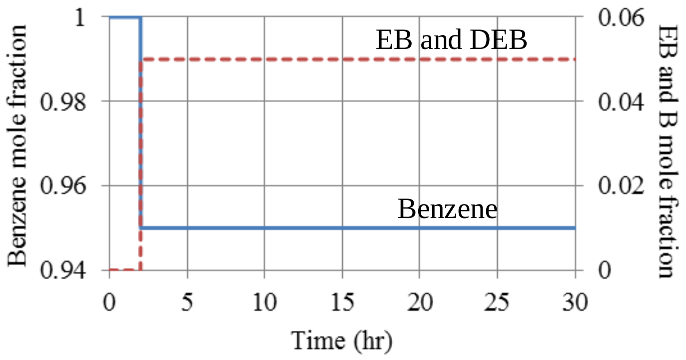


Figure 5.23 Step changes for +5% EB and DEB mole fraction

5.3.2.1 Ethyl benzene feed composition disturbance

The unmeasured feed benzene composition disturbances will be used to test all control structures with +5% ethyl benzene changes in the benzene feed stream in the fresh feed composition. Table 5.15 shows the closed-loop results for this unmeasured disturbance. From the bottom table, it is found that the temperature control loops perform well in bringing the temperatures back to their setpoints. For control structure 2, the setpoint of the loop as a controlled variable is changed under cascade control. The temperature is gradually settled at its new operating value and ethylene composition from the outlet of the second reactor can return to its corresponding specified value. Other the temperature control loops which including temperature at stage 14 of column C1 and at stage 18 of column C2, there are gradually settled at its setpoint value.

For these disturbances, when more ethyl benzene are loaded into the process. The fresh feed benzene must be increased to arrange the desired benzene by stoichiometry reaction, while the ethylene fresh feed is constant. Some ethyl benzene must be converted into di-ethyl benzene but di-ethylbenzene would be reacted again become two ethyl benzene. As a result, the flowrate of all streams increases throughout of plant. The components purity in all streams is also kept small in whole control structures, which is held very close to its specified value. If quality of component streams are considered, the ethyl benzene feed composition disturbance has a little bit effect to process operation.

In conclusions, product purities can quickly return to their desired values. From results of bottom table, much improved control performance, especially for that of ethylbenzene composition disturbance can be observed for control structure 1 and 2 but the best is control structure 1. They demonstrate that control performance improvement can also be made when there are feed purity changes.

5.3.2.2 Di-ethyl benzene feed composition disturbance

More di-ethylbenzene added to the process that must be converted into ethyl benzene, which is recycled to extinction in the second reactor. All control structures, when more di-ethylbenzene added in the fresh feed benzene. The di-ethylbenzene increased affects to the reaction section. Duty of the reactor R1 must be increased to hold the outlet temperature and to hold ethylene composition for control structure 2.

The large flowrate increases in bottom stream B2 and flowrate of all streams increases everywhere of plant, since di-ethylbenzene becomes ethyl benzene from react with benzene. The compositions of benzene in the benzene recycle stream highs well above its nominal value in basecase because this control structure uses reflux to feed to handling disturbances. So, when feed flowrate increases would affect to reflux flowrate increases, purity of benzene would increases. For control structure 1 and 2, there are fairly small change of the benzene in benzene recycle stream and benzene in the bottom, which it is kept very close to its specification. Since these control structures have been temperature controlled in two sections (top stage at 6th and bottom stage 14th). For temperature control loops of both columns are well controlled and steadily maintained at setpoint values under feed composition disturbances without the problem exhibited under basecase and the control structure designed.

The purity of the ethyl benzene in product stream of column C2 can maintain well above the desired value. In the bottom of column, there is more ethyl benzene dropping out the bottom of column but a little bit.

Conclusion, from the closed-loop responses shows under overall control structures with the unmeasured feed composition disturbance. It is noticed that the product compositions are maintained much closer to high purity in control structure 1 and 2, which performance better than basecase. The deviations in product purities are less than that in the base case.

Table 5.15 The dynamic responses for the EB and DEB composition disturbances.

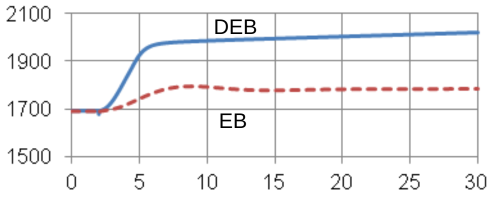
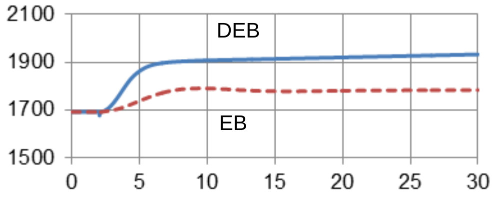
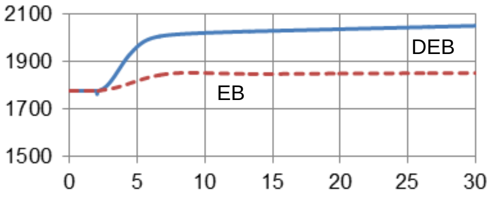
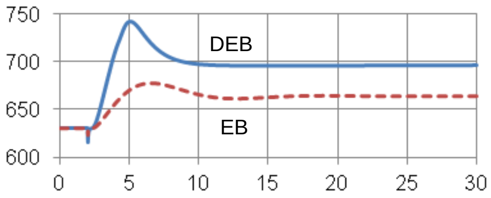
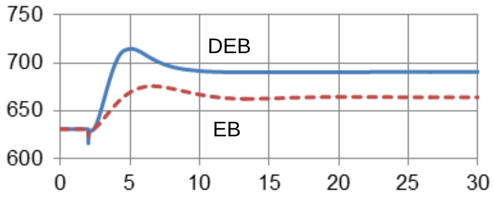
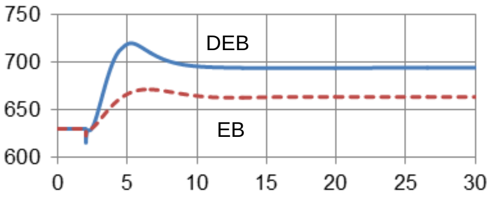
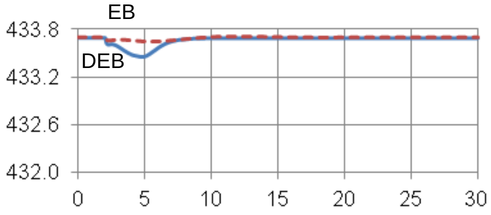
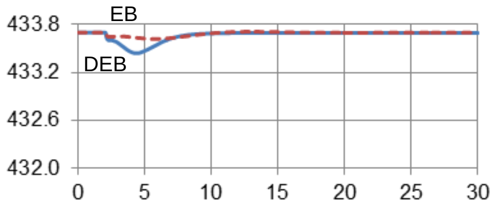
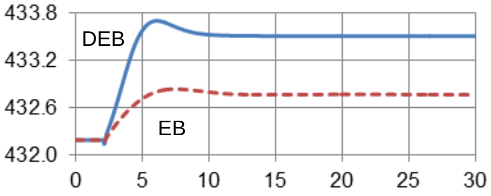
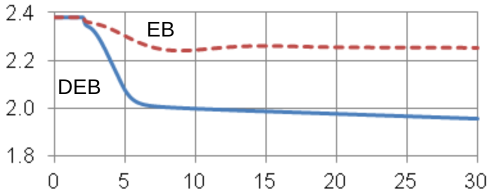
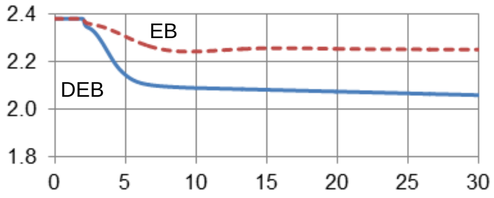
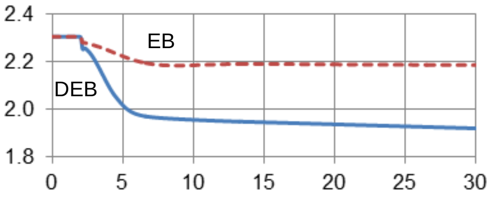
	BASECASE	**CS1**	**CS2**
BTOT (kmol/hr)			
FB (kmol/hr)			
TR1 (K)			
Q react (Mcal/s)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.15 The dynamic responses for the EB and DEB composition disturbances (continued).

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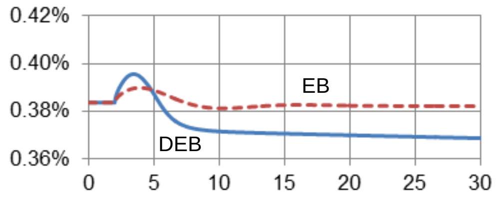
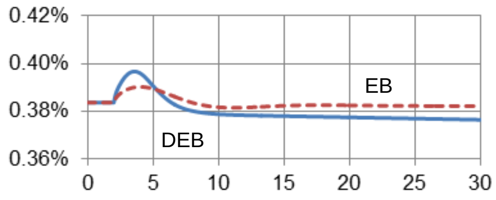
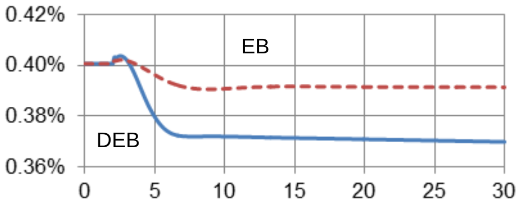
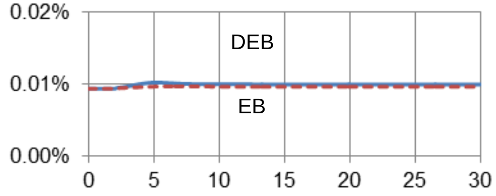
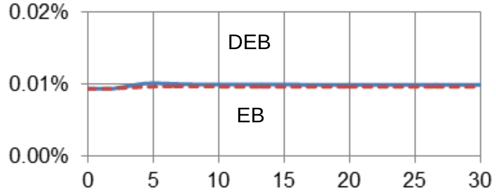
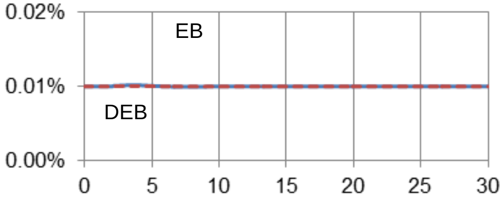
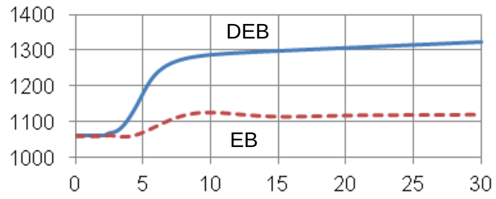
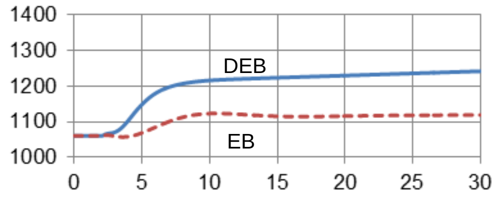
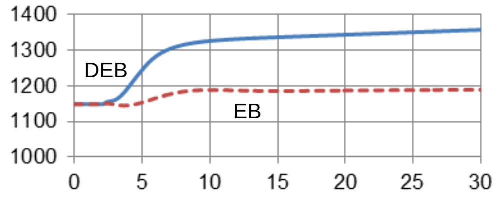
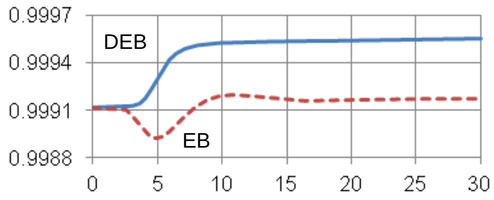
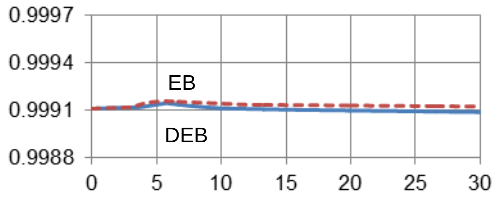
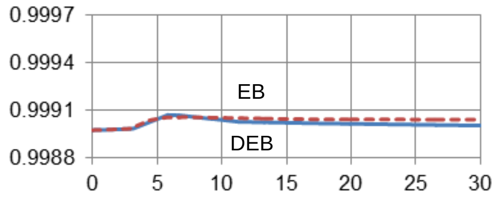
xR1 (%E)			
xR2 (%E)			
D1 (kmol/hr)			
xD1 (B)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.15 The dynamic responses for the EB and DEB composition disturbances (continued).

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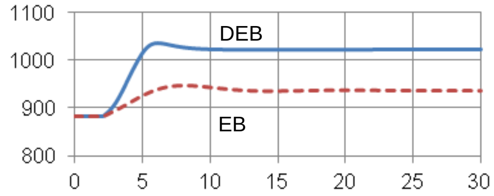
<tr><td>B1 (kmol/hr)</td>
<td>
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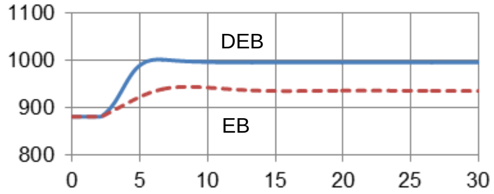
<td>
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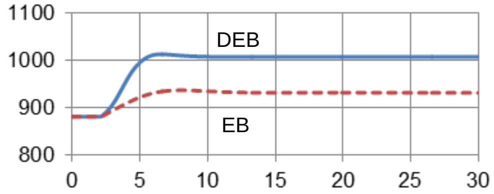
<td>
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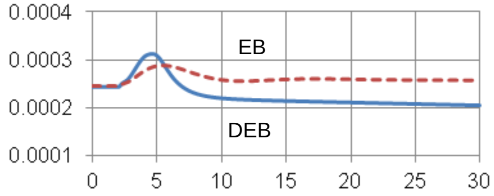
<td>
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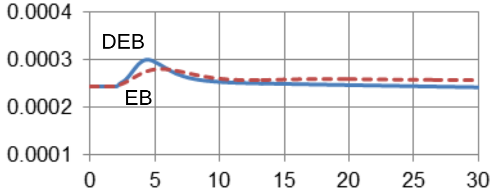
<td>
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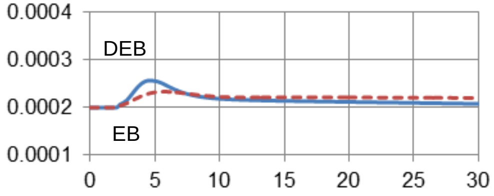
<td>
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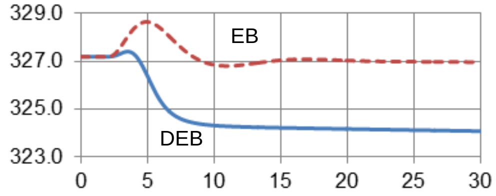
<tr><td>T6 (K)</td>
<td>
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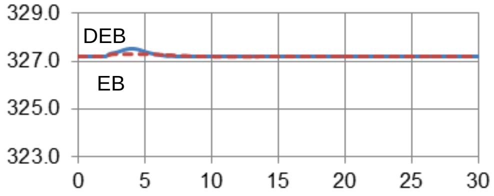
<td>
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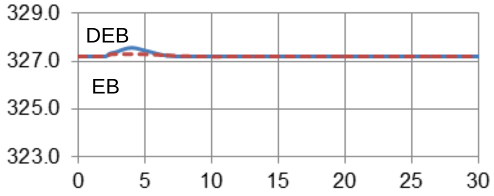
<td>
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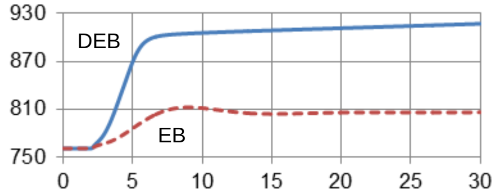
<td>
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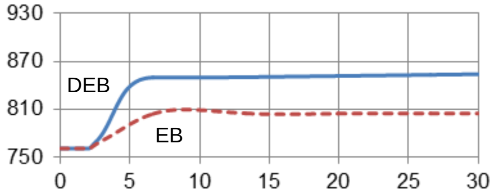
<td>
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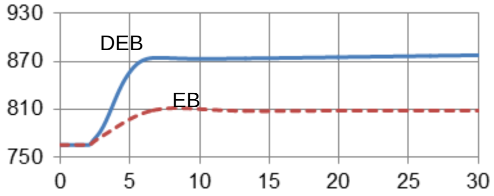
<td>
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<tr><td></td><td>Time (hr)</td><td>Time (hr)</td><td>Time (hr)</td></tr>
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Table 5.15 The dynamic responses for the EB and DEB composition disturbances (continued).

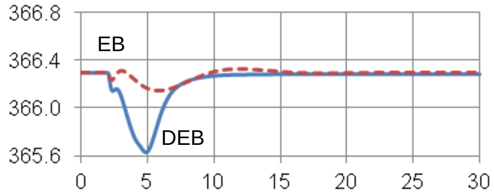
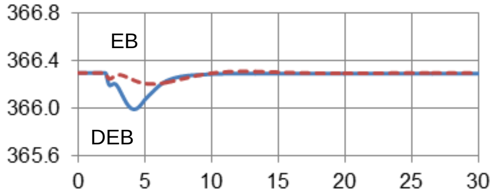
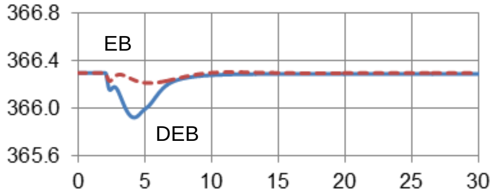
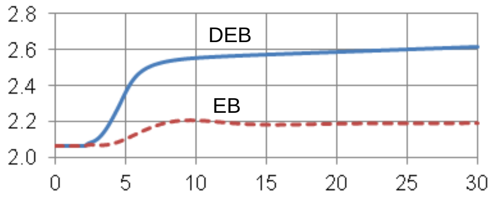
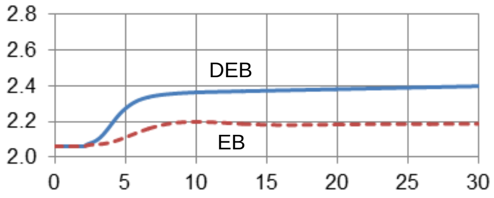
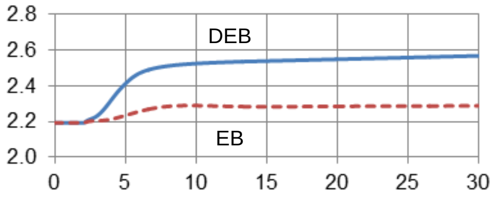
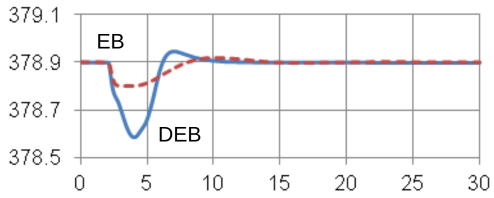
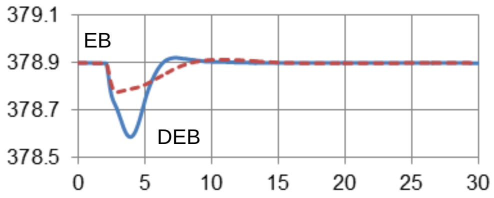
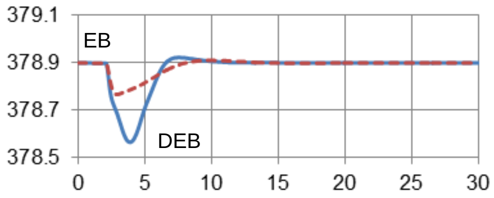
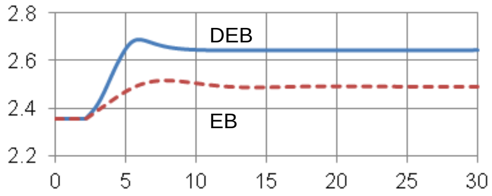
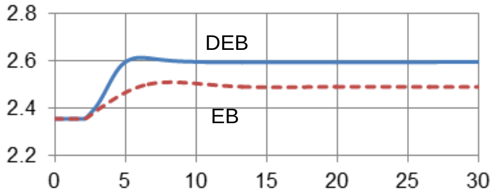
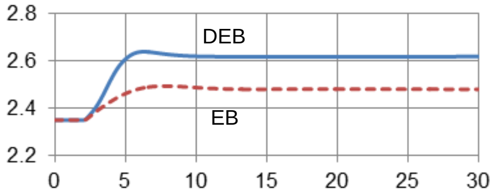
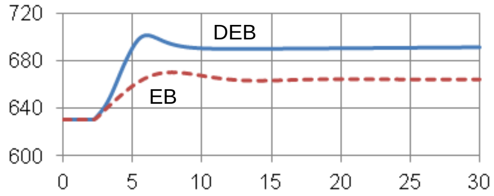
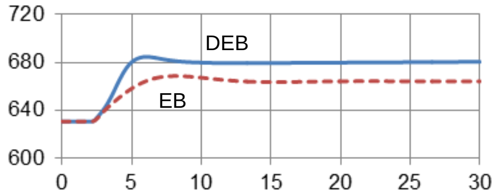
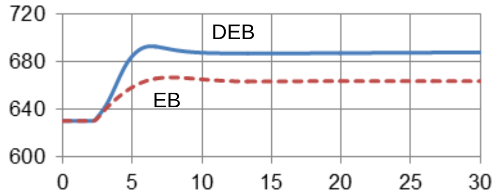
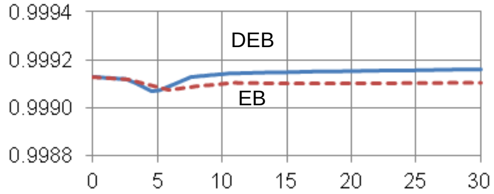
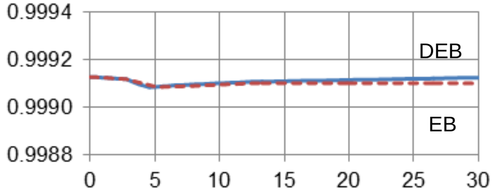
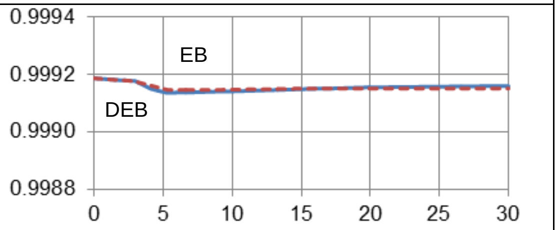
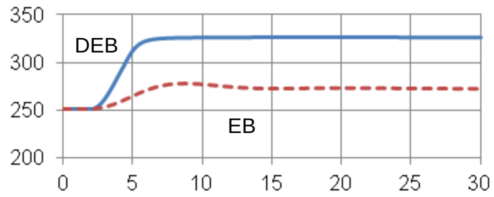
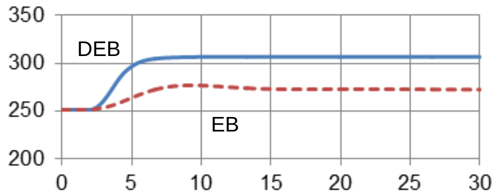
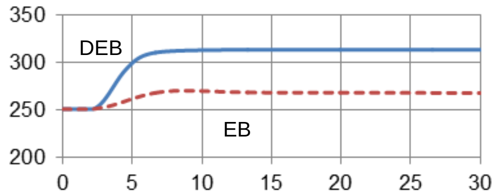
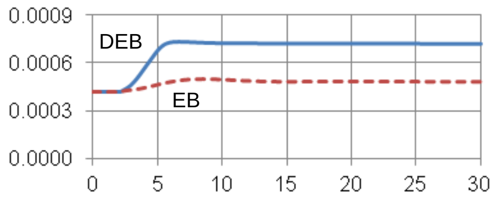
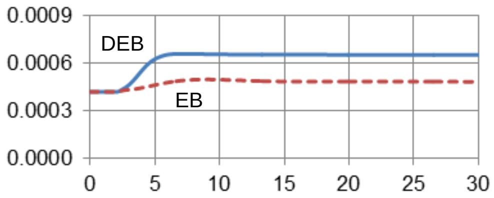
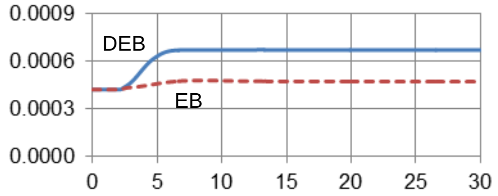
	BASECASE	**CS1**	**CS2**
T14 (K)			
QR1 (Mcal/s)			
T18 (K)			
QR2 (Mcal/s)			
	Time(hr)	**Time(hr)**	**Time(hr)**

Table 5.15 The dynamic responses for the EB and DEB composition disturbances (continued).

	BASECASE	**CS1**	**CS2**
D2 (kmol/hr)			
xD2 (EB)			
B2 (kmol/hr)			
xB2 (EB)			
	Time (hr)	**Time (hr)**	**Time (hr)**

5.3.3 Temperature of feed streams disturbance

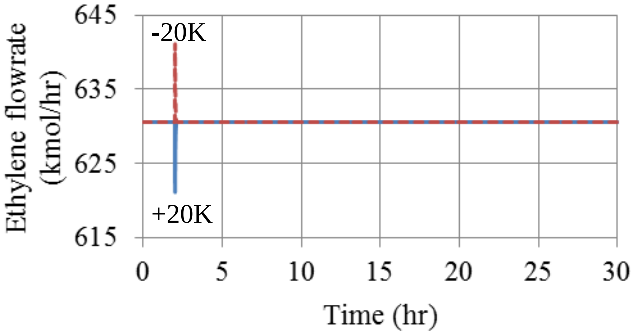


Figure 5.24 Effect of feed temperature changes to ethylene flowrate

The final disturbance is a change in temperature of feed streams. Table 5.16 shown responses for a change ±20 K. Step changes +20 K from 320 to 300 K (dashed lines) and -20 K from 320 to 340 K (solid lines) at time 2 hr. and are finished at time 30 hr., as expected, increasing and decreasing feed temperature produces more reaction and separation. There is small change in all streams and controller. The duties in the reactor R1 must be decreased or increased to hold the outlet temperature, when feed temperature changes. All control structures can handle this disturbance very well.

Table 5.16 The dynamic responses for the temperature disturbances.

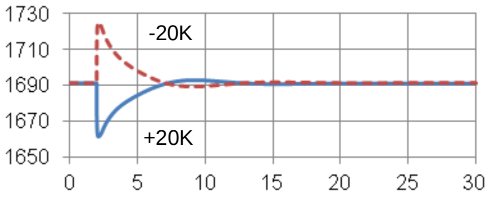
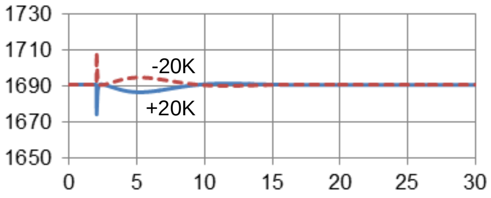
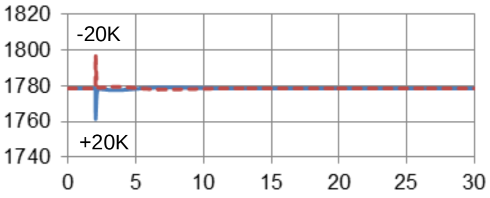
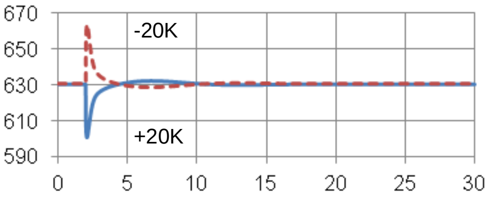
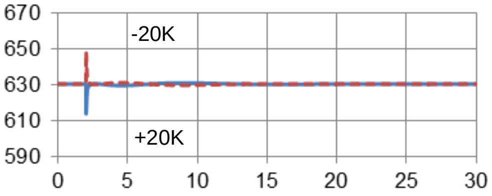
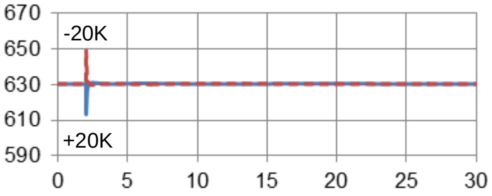
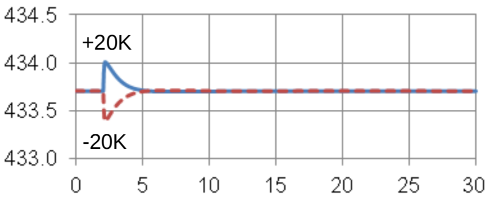
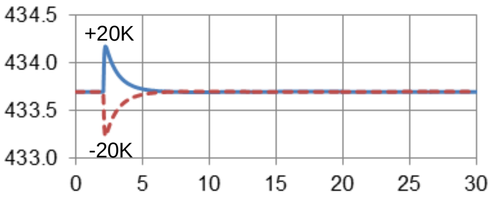
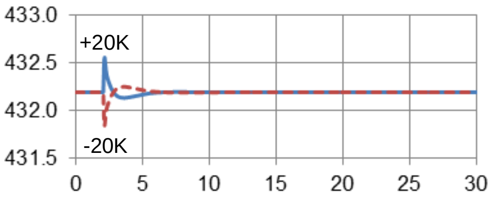
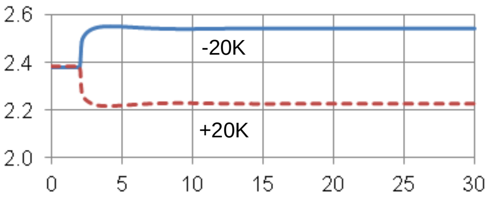
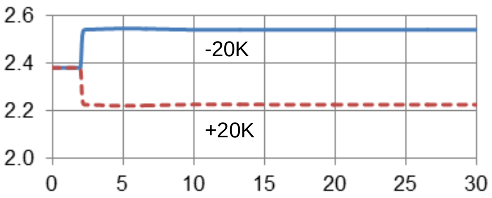
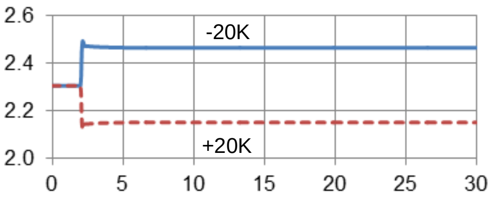
	BASECASE	**CS1**	**CS2**
BTOT (kmol/hr)			
FFB (kmol/hr)			
TR1 (K)			
Q react (Mcal/s)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.16 The dynamic responses for the temperature disturbances (continued).

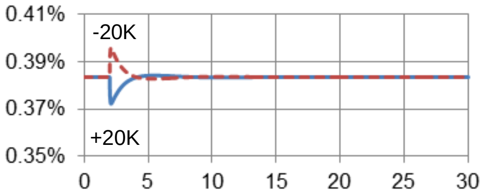
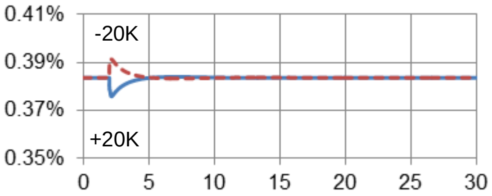
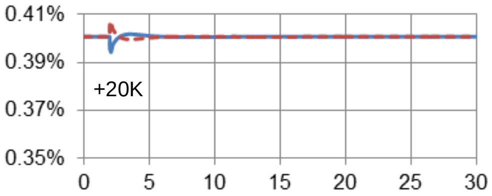
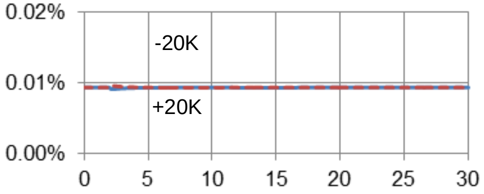
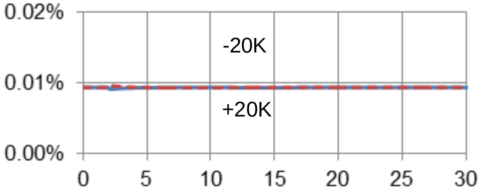
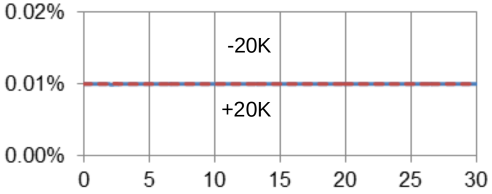
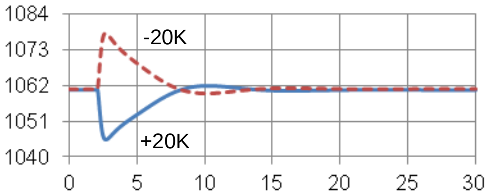
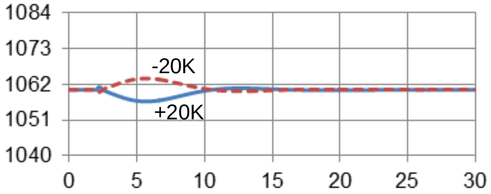
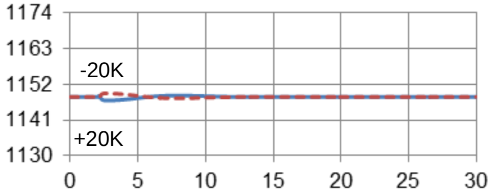
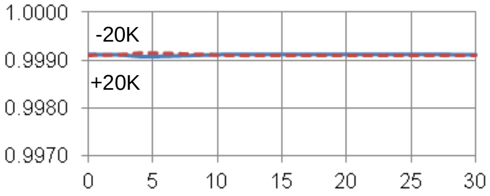
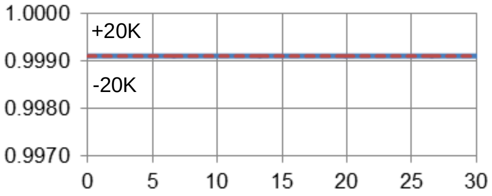
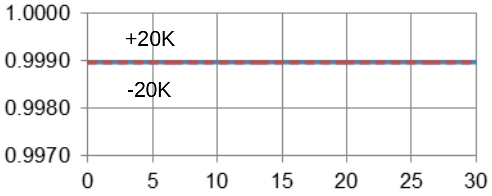
	BASECASE	**CS1**	**CS2**
xR1 (%E)			
xR2 (%E)			
D1 (kmol/hr)			
xD1 (B)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.16 The dynamic responses for the temperature disturbances (continued).

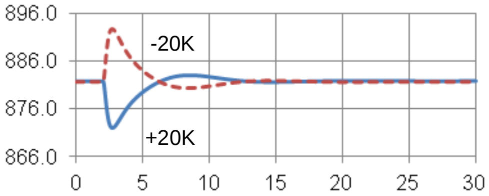
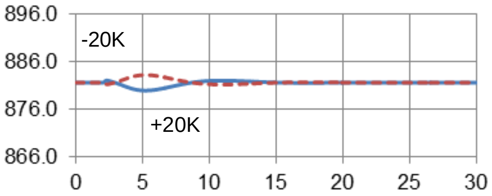
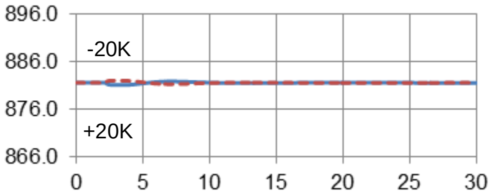
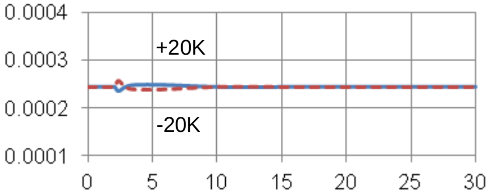
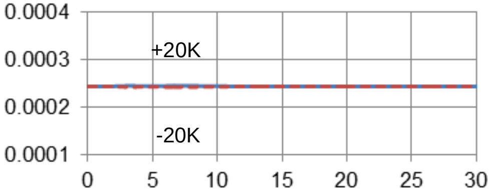
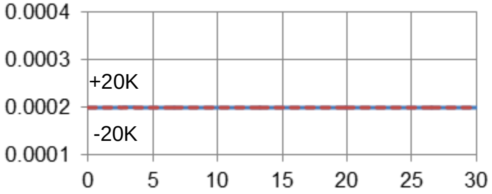
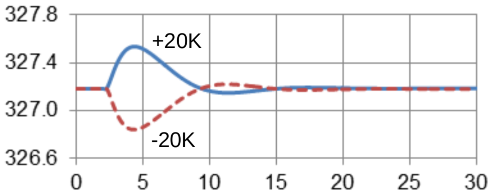
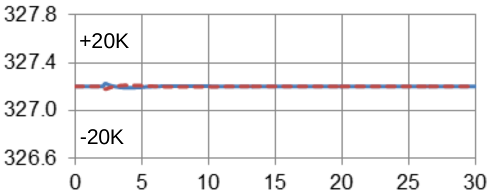
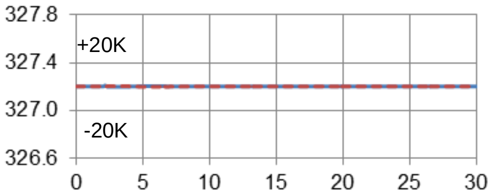
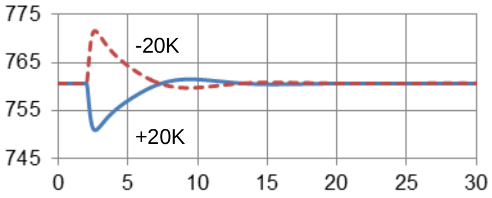
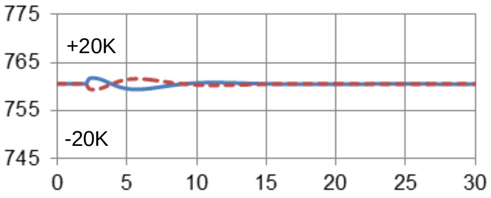
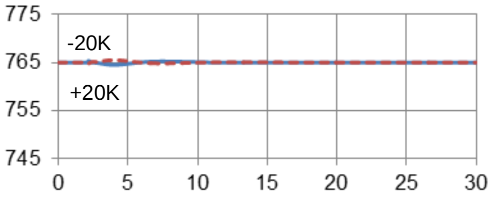
	BASECASE	**CS1**	**CS2**
B1 (kmol/hr)			
xB1 (B)			
T6(K)			
R1 (kmol/hr)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.16 The dynamic responses for the temperature disturbances (continued).

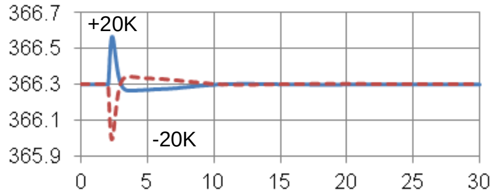
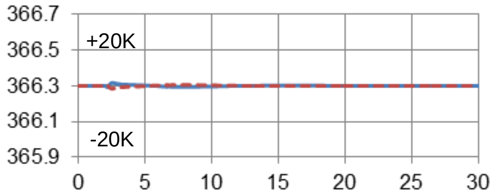
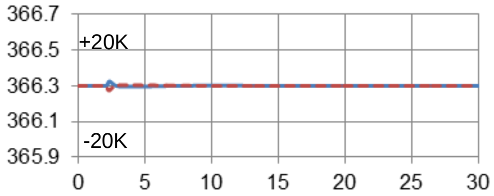
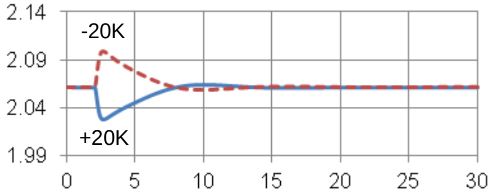
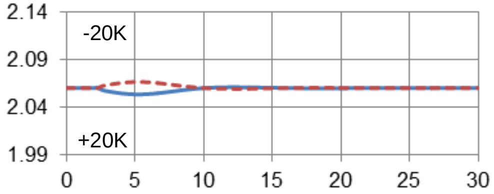
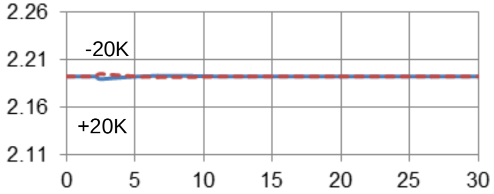
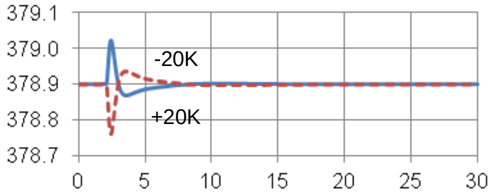
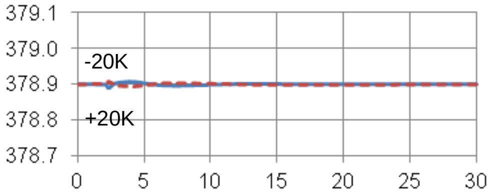
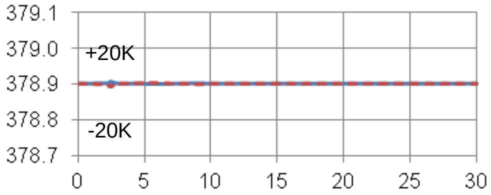
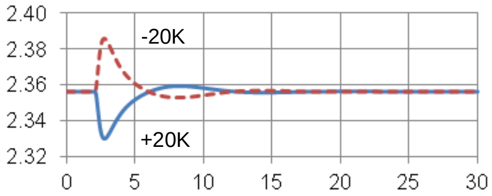
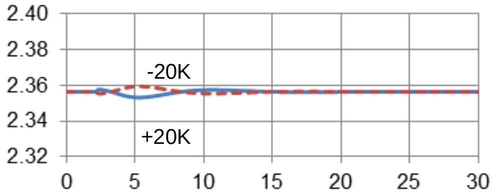
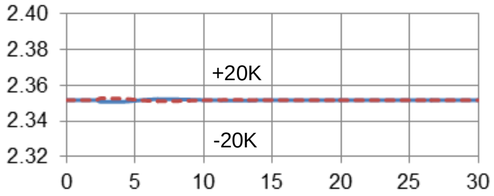
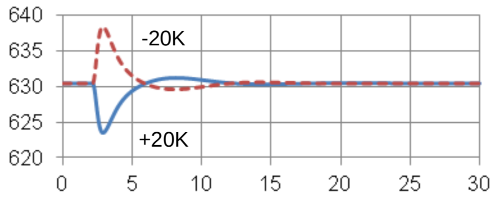
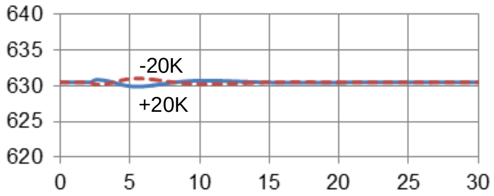
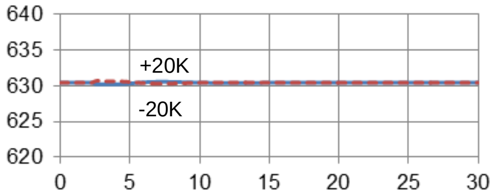
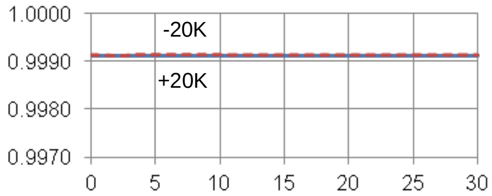
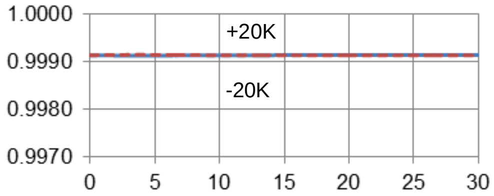
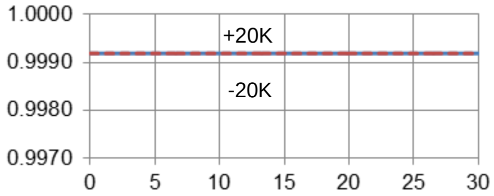
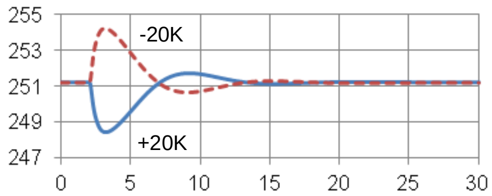
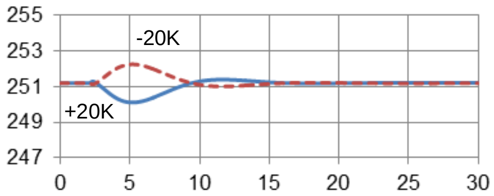
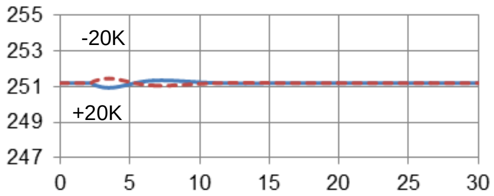
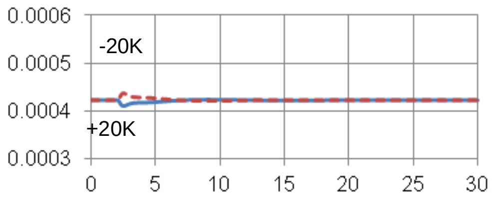
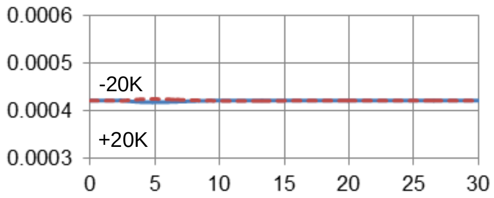
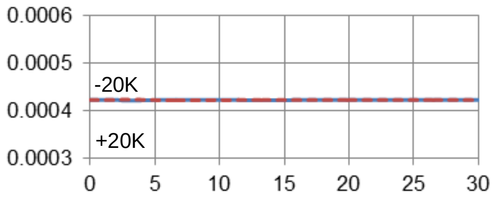
	BASECASE	**CS1**	**CS2**
T14 (K)			
QR1 (Mcal/s)			
T18 (K)			
QR2 (Mcal/s)			
	Time (hr)	**Time (hr)**	**Time (hr)**

Table 5.16 The dynamic responses for the temperature disturbances (continued).

	BASECASE	**CS1**	**CS2**
D2 (kmol/hr)			
xD2 (EB)			
B2 (kmol/hr)			
xB2 (EB)			
	Time (hr)	**Time (hr)**	**Time (hr)**

The simulation results shown in Table 5.14-5.16 demonstrate that product compositions can return to or be settled around their desired values under temperature control. The control structure designed can maintain product quality and provide a robust operation even though the desired temperature profiles change under external and internal disturbances.

5.4 Control Structure Performance Evaluation

A common problem in control system design is establishing the appropriate value of controller gain. In general a low value of gain produces a slow system response, while high gain values can cause an excessively-oscillatory response with the possibility of instability. Somewhere between these extremes is a value of gain that produces the best system response.

The tuning of different parameters in a controller is not exact, which is usually a compromise that is largely dependent on the process control. There are a methods used to evaluate and compare the control structure performance for different parameters. One method is using quantitative performance for dynamic process simulations. This type of performance assessment is usually used in an academic research and uses different criteria to minimize the value of error from the setpoint. One of the four basic criteria are in common use (IAE, ISE, ITAE and ITSE) is integral absolute error (IAE). Use for systems that need to suppress all errors equally.

In this research, IAE method and IAE results are used to evaluate the dynamic performance of whole control structures. Variables in the process have different variable types, (temperature, pressure, composition, level and molar flowrate). Control loops which are considered are safety loops and quality loops.

Integral absolute error is well known and widely used. For the formulation of a dynamic performance as written below:

$$\mathrm{IAE} = \int |e\ (t)|\ dt \tag{5.1}$$

Note that $e(t) = y_{sp}(t) — y(t)$ is the deviation (error) of the response from the desired setpoint.

For change in material disturbances consists of ethylene feed flowrate, benzene feed purity and feed temperatures. The IAE results for handles each disturbance and maintain product quality are shown in Table 5.17, 5.18 and 5.19.

Table 5.17 Summation of the IAE results for handle disturbance to the change in ethylene feed flowrate

Control Structures	**Control loops**		
	Temperature	**Pressure**	**Composition**
Basecase	14.1997	0.0301	0.3188
CS1	**11.5791**	**0.0266**	0.0234
CS2	12.6344	0.0312	**0.0118**

Table 5.18 Summation of the IAE results for handle disturbance to the change in benzene purity

Control Structures	**Control loops**		
	Temperature	**Pressure**	**Composition**
Basecase	5.6949	0.0102	0.0234
CS1	**4.3157**	**0.0075**	**0.0102**
CS2	4.6604	0.0090	0.0132

Table 5.19 Summation of the IAE results for handle disturbance to the change in feed temperature

Control Structures	**Control loops**		
	Temperature	**Pressure**	**Composition**
Basecase	1.6405	0.0021	0.0008
CS1	1.2407	0.0005	**0.0000**
CS2	**0.7786**	**0.0002**	**0.0000**

The IAE values in the pressure control and temperature control loops are not significantly different. In composition loops, the IAE values are significantly different because new control structure has been designed to handles disturbances (temperature controller). The little IAE values of new control structure indicate that the control of average temperature of column C2 give high performance for material disturbances. In addition, the IAE results of thermal disturbances for CS0 are smaller values because temperature of this control structure has been controlled in all units.

Conclusion, The minimum IAE value is the value of case CS2, which can handle disturbances well when compared with other control structures.

5.5 Evaluation of Cost

In this topic, the evaluation cost of benzene process is discussed. The utilities cost includes the energy cost of reactor, columns and work of pumps. The costs of energy used operate follow as:

- Cooling water used in condenser of columns is $0.354/GJ.
- The boiling feed water is 414 K, which is assumed to be provided at a price of $6/GJ.
- The low pressure stream used in the columns is $7.78/GJ.
- The electric costs $16.8/GJ used in pumps.

The utilities cost used to handles each disturbance has been presented in Table 5.20-5.22.

Table 5.20 Summation of utilities cost for handle disturbance to the change in ethylene feed flow

Control Structures	Energy		Work		Utilities Cost
	GJ/h	m$/year	kW	m$/year	(m$/year)
CS0	206.93	6.8025	323.97	0.1674	6.9699
CS1	205.22	6.7601	324.42	0.1676	**6.9277**
CS2	208.45	6.8214	325.00	0.1679	6.9893

Table 5.21 Summation of utilities cost for handle disturbance to the change in benzene feed purity

Control Structures	Energy		Work		Utilities Cost
	GJ/h	m$/year	kW	m$/year	(m$/year)
CS0	220.17	7.1248	331.02	0.1711	7.2959
CS1	216.06	7.0201	329.66	0.1703	**7.1905**
CS2	220.40	7.0967	330.00	0.1705	7.2672

Table 5.22 Summation of utilities cost for handle disturbance to the change in feed temperature

Control Structures	Energy		Work		Utilities Cost
	GJ/h	m$/year	kW	m$/year	(m$/year)
CS0	203.64	6.7411	325.71	0.1683	6.9094
CS1	199.97	6.5496	326.30	0.1686	**6.7182**
CS2	207.44	6.8209	325.81	0.1684	6.9893

The utilities cost for basecase (CS0) is $21,175,220.18. For CS1 and CS2 are $20,836,373.09 and $21,245,766.49, respectively. The utilities cost required to handling all disturbances of CS1 are smaller cost. In control structure CS2, The utilities cost is highest cost for all disturbances.

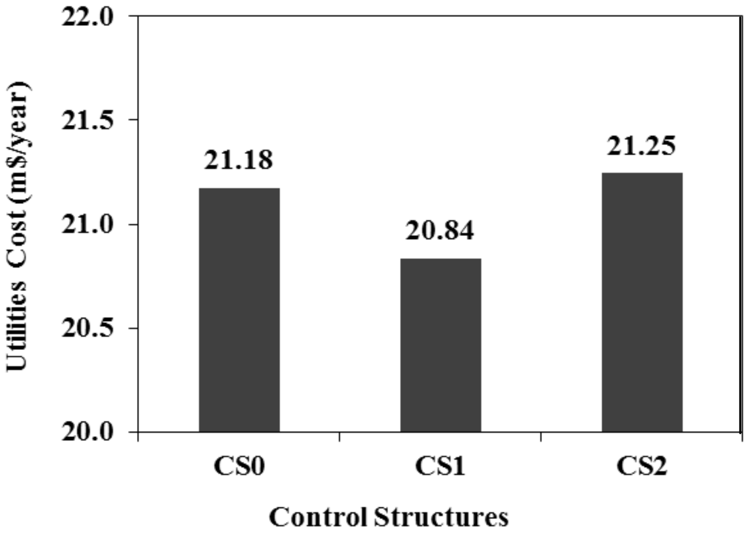


Figure 5.25 Utility costs for each control structure for the change in all disturbances testing

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

This research illustrated another fairly complex chemical process involving multiple interconnected unit operations. The two liquid recycle streams can present steady state and dynamic difficulties. The new plantwide control structures design procedure of Wongsri has been applied to design the control structures for ethyl benzene process. The Wongsri's procedure can apply easily and can be catch up easily even for those who is not in the control field.

When disturbances enters the process, the best control structure should be handle disturbances, kept product quality at the desired condition and minimize energy during process operating. Three designed control structures can be used to handle disturbances well, irrespective of the feed flow changes, composition change or temperature change. For all disturbances are tested, control structure of CS2 can handle disturbances, keep product quality well, when compared with basecase and CS1. In utilities cost section, CS1 is the minimize energy used. Although, the simulation results of all control structures can achieve the objective of the design.

The performance of each control structure is evaluated by analyzing the IAE value and the utilities cost. As a result, CS1 is appropriate control structure for the ethyl benzene process.

6.2 Recommendations

Study and control structure design should be applied to other process via design procedure of Wongsri (2012).

REFERENCES

Buckley, P.S. Techniques of Process Control. New York: Wiley, 1964.

Detjareansri, S. Plantwide Control Structures Design for Alkylation Process. Master's Thesis. Department of Chemical Engineering, Engineering, Chulalongkorn University, 2009.

Douglas, J.M. Conceptual Design of Chemical Processes, New York, McGraw-Hill: 1988.

Downs, J.J., and Skogestad, S. An industrial and academic perspective on plantwide control. Annual Reviews in Control 35 (2011): 99-110.

Konda, N.V.S.N.M., Rangaiah, G.P., and Krishnaswamy P.R. Plantwide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics, Ind. Eng. Chem. Res., 44, 8300-8313 (2005).

Larsson, T., and Skogestad, S. Plantwide control-A review and a new design procedure. Modeling, Identification and Control , 21 (2000): 209-240.

Luyben, W.L. Snowball Effects in Reactor/Separator Processes with Recycle, Ind. Eng. Chem. Res., 33, 299-305 (1994).

Luyben, W.L. Design and Control Degrees of Freedom, Ind. Eng. Chem. Res., 35, 2204-2214 (1996).

Luyben, M.L. and Tyreus, B.D. Plantwide Control Design Procedure, AIChE J., 43, 3161-3174 (1997).

Luyben, W.L., Tyreus, B.D., and Luyben, M.L. Plantwide Process Control, McGraw-Hill, New York (1999)

Luyben, W.L. Plantwide Dynamic Simulators in Chemical Processing and Control, Marcel Dekker, New York, (2002).

Luyben, W.L. Distillation Design and Control Using Aspen Simulation, John Wiley & Sons, Hoboken, New Jersey, (2006).

Luyben, W.L. Design and Control of the Ethyl Benzene Process, AIChE J., 57, 655-670 (2011).

Ng, C., and Stephanopoulos, G. Synthesis of Control systems for Chemical plants., Computers & Chemical Engineering 20 (1996): 999-1004.

Price, R.M., and Georgakis, C. Plantwide Regulatory Control Design Procedure Using a Tiered Framework. Ind. Eng. Chem Res., 32 (1993): 2693- 2705.

Saowani, D. Plantwide Control Structure Design for Hydrodealkylation Process, Master's Thesis. Department of Chemical Engineering, Engineering, Chulalongkorn University, 2009.

Skogestad, S., and Larsson, T. A review of plantwide control, Department of Chemical Design, Doctoral dissertation, Norwegian University of Science and Technology, Norwegian, (1998).

Skogestad, S. Conrol Structure Design for Complete Chemical Plants, Computers and Chemical Engineering., 21, 219-234 (2004).

Stephanopoulos, G., and Ng, C. Perspectives on the synthesis of plant-wide control structures. Journal of Process Control 10 (2000): 97-111.

Suchada, S. Plantwide Control Structure Design Applied to the Hydrodealkylation Process using Fixture Point Theorem, Master's Thesis. Department of Chemical Engineering, Engineering, Chulalongkorn University, 2008.

Suntisrikomol, S. Plantwide Control Structures Design Procedure Applied to the Hydrodealkylation Processusing Fixture Point Theorem. Master's Thesis. Department of Chemical Engineering, Engineering, Chulalongkorn University, 2008.

Turton, R., Bailie R.C., Whiting W.B., Shaeiwitz J..A. Analysis, Synthesis and Design of Chemical Processes, 2nd Ed. Upper Saddle River, NJ: Prentice Hall, 2008.

Wongsri, M. Private Communication, (2009).

Wu, K.L., and Yu, C.C. Reactor/Separator Processes with Recycle-1. Candidate Control structure for Operability. Computers & Chemical Engineering 20 (11) (1996): 1291-1316.

Wu, K.L., Yu, C.C., Luyben, W.L., and Skogestad, S. Reactor/Separator Processes with Recycle-2. Design for Composition control. Computers & Chemical Engineering, 27 (2002): 401-421.

APPENDICES

APPENDIX A

PROCESS STREAMS AND EQUIPMENTS DATA

The two columns and two reactors must be sized for dynamic simulation and results are summarized in Table A.1

Table A.1 Equipment data of ethylbenzene process

Section	Equipment	Specifications	
Reaction	Both Reactor	Diameter (m)	5.03
		Length (m)	10.1
		Volume (m^3)	200
Separation	Benzene column (C1)	Number of trays	21
		Feed to tray	10
		Condenser Pressure (atm)	0.3
		Reboiler Pressure (atm)	0.438
		Diameter (m)	4.80
		Reflux drum volume (m^3)	11.9
		Column base volume (m^3)	17.9
		Reflux ratio	0.774
		Mole fraction of Distillate (EB)	0.001
		Mole fraction of Bottom (B)	0.0003
	Ethyl benzene column (C2)	Number of trays	25
		Feed to tray	15
		Condenser Pressure (atm)	0.1
		Reboiler Pressure (atm)	0.23
		Diameter (m)	5.61
		Reflux drum volume (m^3)	10.1
		Column base volume (m^3)	14.5
		Reflux ratio	0.661
		Mole fraction of Distillate (EB)	0.999
		Mole fraction of Bottom (EB)	0.001

Table A.2 Duty table of steady state operating for ethyl benzene process

Variables	**R1**	**R2**	**C1**		**C2**	
			Condenser	**Reboiler**	**Condenser**	**Reboiler**
Outlet Temperature (K)	434	432	314	390	338	403
Heat duty (MW)	-10.3	0	-15.6	8.13	-11.7	10

Table A.3 Stream table for steady state operating of ethyl benzene process

	1	2	3	4	5	6
Temperature (K)	320.0	319.1	320.0	320.0	318.6	434.0
Pressure (atm)	21	20	21	20	20	20
Vapor Fraction	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000
Mole Flow (kmol/hr)	630.6	630.6	630.6	630.6	1600.0	1606.1
Mass Flow (kg/hr)	17690.7	17690.7	49258.5	49258.5	125004.8	142695.5
Volume Flow (l/min)	11763.2	12375.6	966.0	966.0	2447.2	3299.3
Mole Flow (kmol/hr)						
E	630.6	630.6	0.0	0.0	0.1	6.2
B	0.0	0.0	630.6	630.6	1598.9	1054.8
EB	0.0	0.0	0.0	0.0	1.0	464.6
DEB	0.0	0.0	0.0	0.0	0.0	80.4
Mole Fraction						
E	1.0000	1.0000	0.0000	0.0000	0.0001	0.0039
B	0.0000	0.0000	1.0000	1.0000	0.9993	0.6568
EB	0.0000	0.0000	0.0000	0.0000	0.0006	0.2893
DEB	0.0000	0.0000	0.0000	0.0000	0.0000	0.0501

Table A.3 Stream table for steady state operating of ethyl benzene process (continued)

	7	8	9	10	11	12	13
Temperature (K)	434.2	434.3	432.0	352.0	314.5	316.8	390.0
Pressure (atm)	23.49	19.00	19.00	0.3621	0.30	40.00	0.4380
Vapor Fraction	0.0000	0.0000	0.0000	0.4859	0.0000	0.0000	0.0000
Mole Flow (kmol/hr)	1606.1	1606.1	1882.2	1882.2	969.4	969.4	912.8
Mass Flow (kg/hr)	142695.5	142695.5	180569.0	180569.0	75746.3	75746.3	104822.6
Volume Flow (l/min)	3300.5	3301.0	4131.1	1204634.6	1475.6	1479.7	2226.9
Mole Flow (kmol/hr)							
E	6.2	6.2	0.1	0.1	0.1	0.1	0.0
B	1054.8	1054.8	968.6	968.6	968.3	968.3	0.3
EB	464.6	464.6	631.1	631.1	1.0	1.0	630.1
DEB	80.4	80.4	282.4	282.4	0.0	0.0	282
Mole Fraction							
E	0.0039	0.0039	0.0001	0.0001	0.0001	0.0001	0.0000
B	0.6568	0.6568	0.5146	0.5146	0.9989	0.9989	0.0003
EB	0.2893	0.2893	0.3353	0.3353	0.0010	0.0010	0.6903
DEB	0.0501	0.0501	0.1500	0.1500	0.0000	0.0000	0.3093

Table A.3 Stream table for steady state operating of ethyl benzene process (continued)

	14	15	16	17	18	19	20
Temperature (K)	390.2	362.1	403.0	404.7	405.0	337.8	338.2
Pressure (atm)	5.0	0.1758	0.23	29.0	19.0	0.10	3.0
Vapor Fraction	0.0	0.1710	0.0	0.0	0.0	0.00	0.0
Mole Flow (kmol/hr)	912.8	912.8	282.2	282.2	282.2	630.6	630.6
Mass Flow (kg/hr)	104822.6	104822.6	37873.1	37873.1	37873.1	66949.5	66949.5
Volume Flow (l/min)	2227.6	437938.8	800.4	801.9	802.2	1345.5	1346.0
Mole Flow (kmol/hr)							
E	0.0	0.0	0.0	0.0	0.0	0.0	0.0
B	0.3	0.3	0.0	0.0	0.0	0.3	0.3
EB	630.1	630.1	0.1	0.1	0.1	630.0	630.0
DEB	282.4	282.4	282.1	282.1	282.1	0.3	0.3
Mole Fraction							
E	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B	0.0003	0.0003	0.0000	0.0000	0.0000	0.0005	0.0005
EB	0.6903	0.6903	0.0005	0.0005	0.0005	0.9990	0.9990
DEB	0.3093	0.3093	0.9995	0.9995	0.9995	0.0005	0.0005

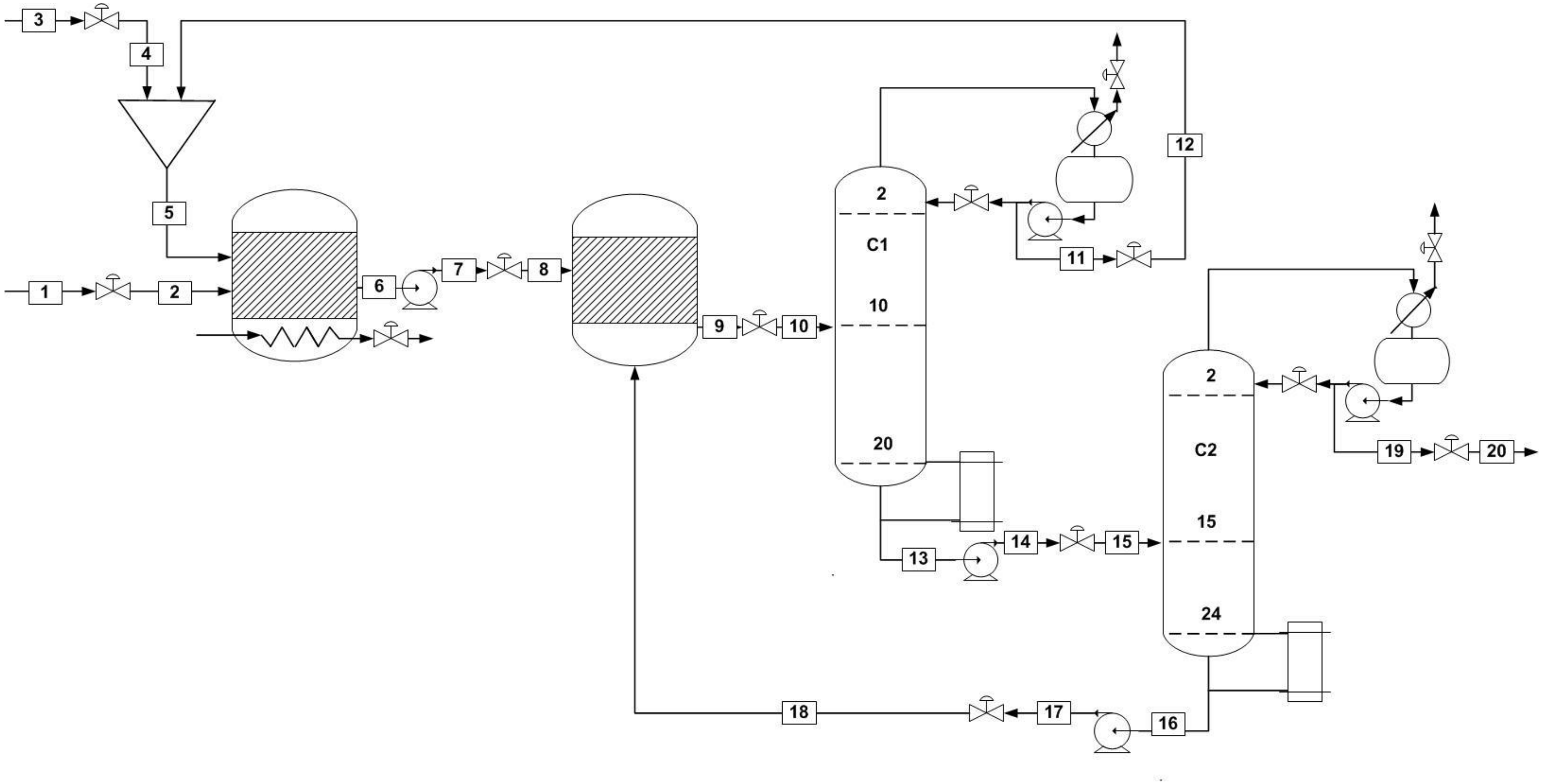


Figure A.1 Ethyl benzene process flowsheet for steady state simulation

APPENDIX B

CONTROLLER TYPE AND TUNING PARAMETERS

B.1 Tuning Controller

Each process has its own dynamic characteristics that condition the tuning condition. If we do not have any preliminary tuning constant we have to find some start with. Each tuning method will end up with a different of tuning parameter. The first widely used technique for PID tuning was published by Ziegler-Nichols in 1942.

Flow controllers: The dynamic of flow measurement are fast processes. Therefore use PI with small gain and fast integral time.

Level controllers: These controllers are integrating processes, use P or PI controller.

Pressure controllers: These controllers are normally very fast loops that normally require PI, which high gain and fast integral time.

Temperature controllers: These controllers are normally very slow loops that normally require derivative time.

B.2 Tuning Parameter

Åström and Hägglund presented a relay feedback system to generate sustained oscillation as an alternative to the conventional continuous cycling technique for controller tuning in 1984. This relay feedback test was soon referred as auto-tune variation via the system as shown in Figure. B.1. Luyben popularizes the relay feedback method and calls this method “ATV” (Auto-Tune Variation). The auto-tune variation techniques are used to determine the ultimate period and the ultimate gain, which applied to Ziegler–Nichols (ZN) and Tyreus and Luyben (TL). Tuning values for proportional, integral and derivative controller parameters has been determined from the ultimate period and the ultimate gain.

Theoretical Analysis:

Read off the amplitude of PV signal wave “a” and OP signal wave “h”, it is used to calculate ultimate gain (Ku) from equation:

$$K_u = \frac{4h}{\pi a} \qquad \text{B-1}$$

When Pu is period taken from limit cycle (ultimate period)

Ku is controller gain that produces the limit cycle (ultimate gain)

Kc is the controller path gain

Ti is the controller's integrator time constant

Td is the controller's derivative time constant

given two measured feedback loop parameters derived from measurements:

1. The period Pu of the oscillation frequency at the stability limit.
2. The gain margin Ku for loop stability

with the goal of achieving good regulation (disturbance rejection).

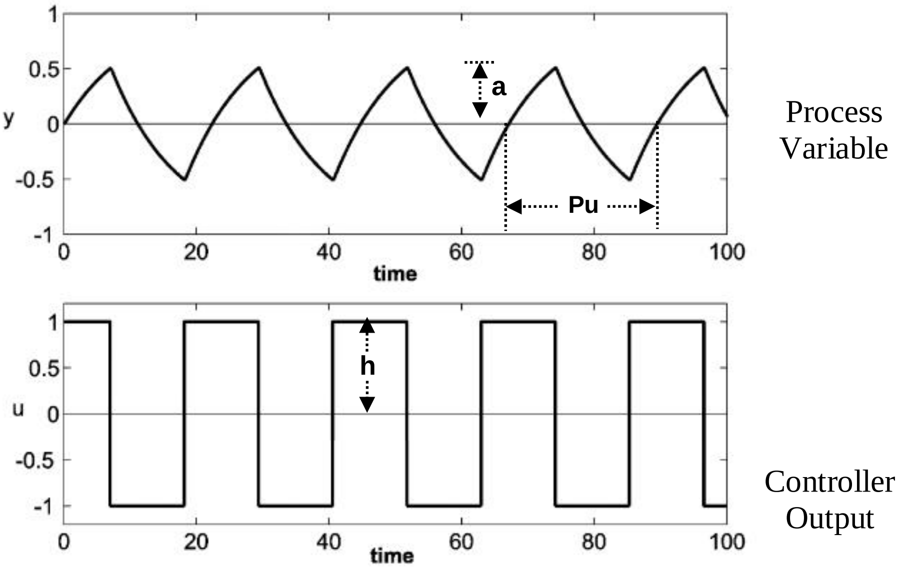


Figure B.1 Input and Output from Relay-Feedback Test.

B.2.1 Ziegler-Nichols Method

. Ziegler and Nichols published a classic paper in 1942, which introduced the continuous cycling method for controller tuning. They explained two empirical methods, which are used for obtaining controller parameters of P, PI, and PID controllers. These are the Ziegler-Nichols closed loop and open loop method. The closed-loop method is the most useful, and it is described below.

The Ziegler-Nichols rule is a heuristic tuning. The Ziegler-Nichols method is perhaps the first rigorous method to tune PID controllers. It is based on the following trial-and-error procedure. The ultimate gain (Ku) of a controller (which is the gain which causes sustained oscillations in the signals in the control system without the control signal reaching the maximum or minimum limits) must be found, and the ultimate (or critical) period (Pu) of the sustained oscillations is measured. Then, the controller is tuned by using Ku and Pu to calculate the controller gain, Kc. This method can be used in P-only, PI and PID controllers. The formulas for this method shown in Table B.1

For drawbacks of the Ziegler-Nichols method are small stability margin that the method may not be quick to use because it requires trial and error. The closed-loop behavior of this technique tends to be oscillatory and sensitive to uncertainty. The user has to make sure that the control signal does not reach its maximum and minimum values during the experiment.

Table B.1 Formulas for the controller parameters in the Ziegler-Nichols method

Controller	K_C	τ_I	τ_D
P	K_U / 2.0	-	-
PI	K_U / 2.2	P_U / 1.2	-
PID	K_U / 1.7	P_U / 2.0	P_U / 8

B.2.2 Tyreus and Luyben Method

Tyreus and Luyben have suggested tuning parameter rules that result in less oscillatory responses, improves robustness and that are less sensitive to changes in the process condition, often called the TLC tuning rules. They formulas for the controller parameters are shown in Table B.2.

The Tyreus and Luyben tuning method is based on oscillations as in the Ziegler-Nichols method, but with modified formulas for the controller parameters to obtain better stability in the control loop compared with the Ziegler-Nichols method.

Table B.2 Formulas for the controller parameters in the Tyerus-Luyben method

Controller	K_C	τ_I	τ_D
PI	K_U / 3.2	2.2 P_U	-
PID	K_U / 2.2	2.2 P_U	P_U / 6.3

Drawbacks of Tyreus-Luyben tuning method are sluggish disturbance compensation that the method may not be quick to use because it requires trial and error. The user has to make sure that the control signal does not reach its maximum and minimum values during the experiment.

Table B.3 Parameter tuning for ethyl benzene process of CS0

Equipment	Controllers	Controlled variables	Manipulate Variables	Controller Types	Action	Nominal value	PV Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor 1	TCR1	Reactor 1 temperature	Heat load R1	PI	Reverse	433.7 K	400-500 K	1.65	26.4	-
	LCR1	Reactor 1 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
	FC1	Fresh ethylene flow	Fresh ethylene flow	PI	Reverse	630.6 kmol/h	0-1,261.2 kmol/h	0.5	0.3	-
	FC2	Total benzene flow	Fresh benzene flow	PI	Reverse	1,600 kmol/h	0-3,200 kmol/h	0.5	0.3	-
Reactor 2	LCR2	Reactor 2 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
Column 1	R/F1	Ratio of reflux to feed	Reflux flowrate	PI	Direct	0.3238	-	-	-	-
	TC12	Stage 14 temperature	Heat load QR1	PI	Reverse	366.3 K	320-420 K	0.77	10.6	-
	LC11	Reflux drum 1 level	Distillate flowrate D1	P	Direct	50%	0-100%	2	9999	-
	LC12	Bottom 1 level	Bottom flowrate B1	P	Direct	50%	0-100%	2	9999	-
	PC1	Column 1 pressure	Heat load QC1	PI	Reverse	0.3 atm	0-0.6 atm	2	10	-
Column 2	R/F2	Ratio of reflux to feed	Reflux flowrate	PI	Direct	0.4222	-	-	-	-
	TC21	Stage 18 temperature	Heat load QR2	PI	Reverse	393.9 K	350-450 K	1.51	9.2	-
	LC21	Reflux drum 2 level	Distillate flowrate D2	P	Direct	50%	0-100%	2	9999	-
	LC22	Bottom 2 level	Bottom flowrate B2	P	Direct	50%	0-100%	2	9999	-
	PC1	Column 2 pressure	Heat load QC2	PI	Reverse	0.1 atm	0-0.2	2	10	-
	FC3	DEB flowrate	Ratio of BTOT/FFE	P	Direct	251.2 kmol/h	0-500 kmol/h	0.6	9999	-

Table B.4 Parameter tuning for ethyl benzene process of CS1

Equipment	Controllers	Controlled variables	Manipulate variables	Controller Types	Action	Nominal value	PV Range	Tuning parameter		
								K_C	τ_I	τ_D
Reactor 1	TCR1	Reactor 1 temperature	Heat load R1	PI	Reverse	433.7 K	400-500 K	1.33	31.7	-
	LCR1	Reactor 1 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
	FC1	Fresh ethylene flowrate	Fresh ethylene flowrate	PI	Reverse	630.6 kmol/h	0-1,261.2 kmol/h	0.5	0.3	-
	FC2	Total benzene flowrate	Fresh benzene flowrate	PI	Reverse	1,600 kmol/h	0-3,200 kmol/h	0.5	0.3	-
Reactor 2	LCR2	Reactor 2 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
Column 1	TC11	Stage 6 temperature	Reflux flowrate	PI	Direct	327.2 K	280-380 K	1.91	15.8	-
	TC12	Stage 14 temperature	Heat load QR1	PI	Reverse	366.3 K	320-420 K	0.78	10.6	-
	LC11	Reflux drum C1 level	Distillate flowrate D1	P	Direct	50%	0-100%	2	9999	-
	LC12	Bottom C1 level	Bottom flowrate B1	P	Direct	50%	0-100%	2	9999	-
	PC1	Column C1 pressure	Heat load QC1	PI	Reverse	0.3 atm	0-0.6 atm	2	10	-
Column 2	R/F2	Ratio of reflux to feed	Reflux flowrate	PI	Direct	0.4222	-	-	-	-
	TC21	Stage 18 temperature	Heat load QR2	PI	Reverse	378.9 K	330-430 K	0.95	10.6	-
	LC21	Reflux drum C2 level	Distillate flowrate D2	P	Direct	50%	0-100%	2	9999	-
	LC22	Bottom C2 level	Bottom flowrate B2	P	Direct	50%	0-100%	2	9999	-
	PC2	Column C2 pressure	Heat load QC2	PI	Reverse	0.1 atm	0-0.2	2	10	-
	FC3	DEB flowrate	Ratio of BTOT/FFE	P	Direct	251.2 kmol/h	0-500 kmol/h	0.6	9999	-

Table B.5 Parameter tuning for ethyl benzene process of CS2

Equipment	**Controllers**	**Controlled variables**	**Manipulate variables**	**Controller Types**	**Action**	**Nominal value**	**PV Range**	**Tuning parameter**		
								K_C	τ_I	τ_D
Reactor 1	TCR1	Reactor 1 temperature	Heat load R1	PI	Reverse	433.7 K	400-500 K	2.72	25.1	-
	LCR1	Reactor 1 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
	FC1	Fresh ethylene flow	Fresh ethylene flow	PI	Reverse	630.6 kmol/h	0-1,261.2 kmol/h	0.5	0.3	-
	FC2	Total benzene flow	Fresh benzene flow	PI	Reverse	1,600 kmol/h	0-3,200 kmol/h	0.5	0.3	-
Reactor 2	LCR2	Reactor 2 level	Outlet flowrate	P	Direct	50%	0-100%	5	9999	-
	CC	Ethylene mol fraction	R1 temperature	PI	Direct	0.0001	0-0.0002	0.43	38.3	-
Column 1	TC11	Stage 6 temperature	Reflux flowrate	PI	Direct	327.2 K	280-380 K	2	15.8	-
	TC12	Stage 14 temperature	Heat load QR1	PI	Reverse	366.4 K	320-420 K	0.73	10.6	-
	LC11	Reflux drum 1 level	Distillate flowrate D1	P	Direct	50%	0-100%	2	9999	-
	LC12	Bottom 1 level	Bottom flowrate B1	P	Direct	50%	0-100%	2	9999	-
	PC1	Column 1 pressure	Heat load QC1	PI	Reverse	0.3 atm	0-0.6 atm	2	10	-
Column 2	R/F2	Ratio of reflux to feed	Reflux flowrate	PI	Direct	0.4222	-	-	-	-
	TC21	Stage 18 temperature	Heat load QR2	PI	Reverse	378.9 K	330-430 K	0.93	10.6	-
	LC21	Reflux drum 2 level	Distillate flowrate D2	P	Direct	50%	0-100%	2	9999	-
	LC22	Bottom 2 level	Bottom flowrate B2	P	Direct	50%	0-100%	2	9999	-
	PC2	Column 2 pressure	Heat load QC2	PI	Reverse	0.1 atm	0-0.2	2	10	-
	FC3	DEB flowrate	Ratio of BTOT/FFE	P	Direct	251.2 kmol/h	0-500 kmol/h	0.6	9999	-

APPENDIX C

IAE Results Data

Table C.1 The IAE Results for handle disturbance to the change in ethylene feed flowrate

Control Structures	Changes	Control loops											
		Temperature			Sum IAE	Pressure		Sum IAE	Composition			Sum IAE xD1&xB2	Sum IAE xD2
		TCR1	TC12	T21		PC1	PC2		xD1(B)	xD2(EB)	xB2(DEB)		
CS0	+20%	0.7775	4.5226	1.4474	14.1997	0.0125	0.0022	0.0301	0.0103	0.0008	0.0059	0.3090	0.0098
	-20%	0.9845	4.2760	2.1915		0.0123	0.0032		0.2922	0.0058	0.0039		
CS1	+20%	1.1185	2.5342	1.5506	**11.5791**	0.0105	0.0020	**0.0266**	0.0028	0.0004	0.0053	0.0139	0.0095
	-20%	1.3990	2.7001	2.2767		0.0113	0.0028		0.0065	0.0042	0.0042		
CS2	+20%	0.9602	3.0538	1.7573	12.6344	0.0132	0.0022	0.0312	0.0015	0.0015	0.0037	**0.0054**	**0.0063**
	-20%	1.5840	3.0188	2.2602		0.0130	0.0028		0.0019	0.0005	0.0027		

Table C.2 The IAE Results for handle disturbance to the change in benzene purities

Control Structures	Changes	Control loops											
		Temperature			Sum IAE	Pressure		Sum IAE	Composition			Sum IAE xD1&xB2	Sum IAE xD2
		TCR1	TC12	T21		PC1	PC2		xD1(B)	xD2(EB)	xB2(DEB)		
CS0	+5% DEB	0.8814	2.3146	0.9132	5.6949	0.0061	0.0013	0.0102	0.0104	0.0007	0.0079	0.0137	0.0097
	+5% EB	0.3523	0.7605	0.4729		0.0021	0.0007		0.0019	0.0008	0.0018		
CS1	+5% DEB	1.0298	1.0050	0.7863	**4.3157**	0.0040	0.0010	**0.0075**	0.0004	0.0005	0.0061	**0.0024**	**0.0078**
	+5% EB	0.5053	0.4801	0.5092		0.0019	0.0006		0.0007	0.0008	0.0017		
CS2	+5% DEB	1.0919	1.3767	0.8928	4.6604	0.0057	0.0011	0.0090	0.0013	0.0010	0.0066	0.0052	0.0080
	+5% EB	0.4445	0.3980	0.4564		0.0017	0.0006		0.0019	0.0010	0.0014		

Table C.3 The IAE Results for handle disturbance to the change in feed temperatures

Control Structures	Changes	Control loops											
		Temperature			Sum IAE	Pressure		Sum IAE	Composition			Sum xD1&xB2	Sum IAE xD2
		TCR1	TC12	T21		PC1	PC2		xD1(B)	xD2(EB)	xB2(DEB)		
CS0	+20 K	0.3738	0.2892	0.1375	1.6405	0.0008	0.0002	0.0021	0.0003	0.0000	0.0001	0.0006	0.0002
	-20 K	0.3626	0.3214	0.1560		0.0009	0.0002		0.0003	0.0001	0.0001		
CS1	+20 K	0.5483	0.0480	0.0304	1.2407	0.0002	0.0000	0.0005	0.0000	0.0000	0.0000	**0.0000**	**0.0000**
	-20 K	0.5322	0.0437	0.0380		0.0002	0.0000		0.0000	0.0000	0.0000		
CS2	+20 K	0.3615	0.0257	0.0070	**0.7786**	0.0001	0.0000	**0.0002**	0.0000	0.0000	0.0000	**0.0000**	**0.0000**
	-20 K	0.3508	0.0246	0.0091		0.0001	0.0000		0.0000	0.0000	0.0000		

VITA

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