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PLANTWIDE CONTROL STRUCTURE DESIGN FOR CUMENE PROCESS

The logo of Chulalongkorn University, featuring a central emblem with a sunburst and a tiered structure, surrounded by a circular arrangement of rays.

Mr. Saiyawit Korprasert

จุฬาลงกรณ์มหาวิทยาลัย

CHULALONGKORN UNIVERSITY

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering

Department of Chemical Engineering

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ศัยวิทย์ ขอประเสริฐ : การออกแบบโครงสร้างการควบคุมทั้งโรงงานสำหรับกระบวนการคิวมีน. (PLANTWIDE CONTROL STRUCTURE DESIGN FOR CUMENE PROCESS) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ผศ. ดร. มนตรี วงศ์ศรี, 109 หน้า.

การออกแบบโครงสร้างการควบคุมทั้งโรงงานอาศัยหลักการพื้นฐานสองข้อ ได้แก่ การรักษาสภาวะการดำเนินการที่เหมาะสมตามค่าที่ได้ออกแบบไว้ และการกำจัดสิ่งรบกวนได้อย่างรวดเร็ว และ/หรือกำกับสิ่งรบกวนให้ไปยังเส้นทางที่เหมาะสม วัตถุประสงค์ของงานวิจัยนี้เพื่อสาธิตวิธีการออกแบบโครงสร้างการควบคุมทั้งโรงงานของวงศ์ศรี (2012) สำหรับกระบวนการคิวมีน วิธีการออกแบบประกอบด้วย 5 ช่วงซึ่งแบ่งเป็น 8 ขั้นตอน ซึ่งเน้นที่การทำให้โรงงานมีสภาวะคงที่โดยการควบคุมอัตราการไหลของแต่ละสารที่จุดที่มีการระบุปริมาณสารแต่ละชนิด และสามารถปรับเปลี่ยนได้อย่างรวดเร็ว และการจัดการกับสภาวะรบกวนได้อย่างเหมาะสม โครงสร้างการควบคุมใหม่ถูกประเมินโดยใช้โปรแกรมจำลองกระบวนการเชิงพลวัต Aspen HYSYS และเปรียบเทียบประสิทธิภาพกับกรณีอ้างอิงที่ถูกเลือก (W. L. Luyben, Design and Control of the Cumene Process, Ind. Eng. Chem. Res., Vol. 49, No. 2, 2010: 719-734) โครงสร้างที่ออกแบบใหม่ 2 โครงสร้าง (CS2 และ CS3) ให้ประสิทธิภาพที่ดีกว่ากรณีอ้างอิง เนื่องจากสามารถรักษาสภาวะการดำเนินการของกระบวนการได้ดีและสามารถจัดการกับสภาวะรบกวนได้ดีกว่า

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Plantwide control structure design relies on two basic principles, namely, maintaining operating conditions at designed values and quick rejecting disturbance and/or directing disturbances to appropriate paths. The purpose of this research is to illustrate the application of the plantwide control structure design procedure of Wongsri (2012) for cumene process. The design procedure consists of 5 stages with 8 steps which emphasis on the establishment of a fixture plant by regulating material component flow rates using their quantifiers and handlers, and proper disturbance management. The new control structure designs are evaluated using Aspen HYSYS dynamic simulator and compared their performance with the selected base case (W. L. Luyben, Design and Control of the Cumene Process, Ind. Eng. Chem. Res., Vol. 49, No. 2, 2010: 719-734). Two new design structures (CS2 and CS3) give better performance than the base case because of their good maintaining plant conditions and better disturbance handlings.



Department: Chemical Engineering Student's Signature

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CONTENTS

	Page
THAI ABSTRACT	iv
ENGLISH ABSTRACT	v
ACKNOWLEDGEMENTS	vi
CONTENTS	vii
LIST OF TABLES	ix
LIST OF FIGURES	x
CHAPTER I INTRODUCTION.....	1
1.1 Importance and Reasons of Research.....	1
1.2 Research Objectives	1
1.3 Scopes of research	1
1.4 Contributions of Research.....	2
1.5 Research Procedure	2
1.6 Research Framework.....	3
CHAPTER II LITERATURE REVIEW	4
2.1 Literature Review of Plantwide Control Structure Design.....	4
2.2 Literature Review of Cumene Production Process	6
CHAPTER III THEORY	8
3.1 Principle of plantwide control	8
3.2 Steps of Plantwide Control Design Procedure of Luyben.....	9
3.3 Wongsri's Plantwide Control Design Procedure	11
CHAPTER IV CUMENE PROCESS.....	20
4.1 Introduction to Cumene Process.....	20
4.2 Kinetics and Thermodynamic Model.....	20
4.2.1 Reaction Kinetics.....	20
4.2.2 Phase Equilibrium	21
4.3 Cumene Process Descriptions	22
CHAPTER V CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION RESULT	25

	Page
5.1 Introduction	25
5.2 Application of Wongsri's design procedure.....	25
5.3 Dynamic simulation results.....	65
5.3.1 The fresh feed flow rate of mixed C3 disturbances.....	66
5.3.2 The composition of propylene feed disturbances	73
5.3.3 The catalyst deactivation disturbances.....	79
5.4 Control Structure Performance Evaluation	85
CHAPTER VI CONCLUSIONS AND RECOMMENDATIONS	87
6.1 Conclusion.....	87
6.2 Recommendations.....	87
REFERENCES	88
APPENDIX.....	91
APPENDIX A EQUIPMENTS DATA AND PROCESS STREAMS	92
APPENDIX B CONTROLLER TYPE AND TUNING PARAMETERS.....	98
APPENDIX C Research Review of Wongsri.....	106
VITA.....	109

LIST OF TABLES

	Page
Table 4.1 Reaction kinetics.....	21
Table 5.1 The control degree of freedom for the cumene process.....	26
Table 5.2 Quantifiers and handlers of components.....	30
Table 5.3 Surplus and deficit disturbances shifting direction.....	34
Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3.....	68
Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3.....	74
Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3.....	80
Table 5.7 Summation of the IAE results for handle mixed C3 fresh feed flow rate disturbance.....	85
Table 5.8 Summation of the IAE results for handle propylene composition feed disturbance.....	86
Table 5.9 Summation of the IAE results for handle catalyst deactivation Disturbance.....	86
Table A.1 Equipment sizing data of benzene process.....	90
Table A.2 Stream table of cumene process in steady state mode operation.....	92
Table B.1 Tuning parameters for cumene process of CS0.....	97
Table B.2 Tuning parameters for cumene process of CS1.....	98
Table B.3 Tuning parameters for cumene process of CS2.....	100
Table B.4 Tuning parameters for cumene process of CS3.....	101

LIST OF FIGURES

	Page
Figure 3.1 Heat pathways.....	13
Figure 4.1 T_{xy} diagram: (a) for benzene/cumene; (b) for cumene/PDIB.....	22
Figure 4.2 Flow sheet of the cumene process (Luyben 2010).....	24
Figure 5.1 Heat pathways of cumene process.....	27
Figure 5.2 Material pathways of cumene process.....	29
Figure 5.3 Material pathways and material quantifiers.....	30
Figure 5.4 Steady state simulation results in reactor section analysis.....	32
Figure 5.5 The directions of material disturbances predetermined.....	33
Figure 5.6 Selecting temperature control tray location of C1 by keeping the reboiler heat duty (Q_r) and reflux	34
Figure 5.7 Selecting temperature control tray location of C1 by keeping the reboiler heat duty (Q_r) and reflux ratio.....	35
Figure 5.8 Selecting temperature control tray location of C2 by keeping the reboiler heat duty (Q_r) and reflux	35
Figure 5.9 Selecting temperature control tray location of C2 by keeping the reboiler heat duty (Q_r) and reflux ratio.....	36
Figure 5.10 On supply design structure.....	37
Figure 5.11 Keep the materials entered of cumene process.....	38
Figure 5.12 Adjust the flow of exit material streams.....	39
Figure 5.13 Maintain the production rate.....	40
Figure 5.14 Direct the heat disturbances that are not directly related to quality.....	41
Figure 5.15 The heat disturbance that related to quality in order to maintain the product constraints.....	42
Figure 5.16 The control structure for handle disturbances in separation section.....	44
Figure 5.17 Column dynamic results for $\pm 10\%$ changes of benzene component feed flow.....	46

Figure 5.18 Column dynamic results for $\pm 10\%$ changes of Cumene component feed flow.....	47
Figure 5.19 Column C1 dynamic results for ± 5 mole % benzene changes in column feed.....	48
Figure 5.20 Column C1 dynamic results for $\pm 10\%$ temperature changes in column feed.....	49
Figure 5.21 Column C1 dynamic results for $\pm 10\%$ total flow changes in column Feed.....	50
Figure 5.22 Column dynamic results for $\pm 10\%$ changes of cumene component feed flow.....	52
Figure 5.23 Column dynamic results for $\pm 10\%$ changes of DIPB component feed flow.....	53
Figure 5.24 Column C2 dynamic results for ± 2 mole % cumene changes in column feed.....	54
Figure 5.25 Column C2 dynamic results for $\pm 10\%$ temperature changes in column feed.....	55
Figure 5.26 Column C2 dynamic results for $\pm 10\%$ total flow changes in column Feed.....	56
Figure 5.27 Material disturbance structure.....	57
Figure 5.28 The control loops for the remaining control variables.....	58
Figure 5.29 Enhanced control structure 1 (CS1).....	59
Figure 5.30 Enhanced control structure 2 (CS2).....	60
Figure 5.31 Enhanced control structure 3 (CS3).....	60
Figure 5.32 The base case control structure (CS0).....	63
Figure 5.33 The new control structure 1 (CS1).....	64
Figure 5.34 The new control structure 2 (CS2).....	64
Figure 5.35 The new control structure 3 (CS3).....	65

Figure 5.36 Dynamic results for $\pm 10\%$ fresh feed flow rate of mixed C3 Disturbances.....	66
Figure 5.37 Dynamic results for $\pm 2\%$ propylene composition feed disturbance.....	73
Figure 5.38 Dynamic results for 95% catalyst deactivation disturbances.....	79
Figure A.1 Cumene process flow sheet for steady state simulation.....	95



CHAPTER I

INTRODUCTION

1.1 Importance and Reasons of Research

Industrial chemical plants include many types of operations and items of equipment operating at different conditions. The safety and stability of process operations of industrial chemical plants must to maintain operating conditions (temperature, pressure and level) at their optimal values as well as within safe limits. This challenging task has to be achieved in the presence of known disturbances such as throughput and product specification changes arising from variations in the market demand and requirements, as well as unknown and unmeasured disturbances in raw material composition, catalyst activity, equipment conditions and environment. Hence, a reliable and extensive monitoring and control system is essential for the safe and optimal operation of modern chemical plants.

The purpose of this research is to apply the new plantwide control structure design procedure of Wongsri (2012) for cumene process. This research will design plantwide control structures of cumene process and simulate them by using HYSYS simulation software to study about dynamic behavior and evaluate the performance of the designed structures.

1.2 Research Objectives

The Research objectives are to design, optimization and evaluate the plantwide control structures of a cumene process by using a new design procedure of Wongsri (2012).

1.3 Scopes of research

1. Steady-state and dynamic simulation of cumene process by using a commercial process simulator.
2. Information and description of cumene process is given by Luyben (2010).

3. New control structures of cumene process are designed by using Wongsri's procedure (2012).
4. Compare the new design control structures of cumene process with the work proposed by Luyben (2010).

1.4 Contributions of Research

1. Steady state and dynamic modes of cumene process is obtained by using HYSYS simulation software.
2. The new plantwide control structures of cumene process are designed by using Wongsri's procedure (2012).
3. Evaluated the performance of the new design plantwide control structures and compared with the control structure of base case given by Luyben (2010).

1.5 Research Procedure

1. Study the cumene process and concerned information by Luyben (2010).
2. Simulate steady-state operation of the reference structure is obtained from Luyben (2010) by using HYSYS simulation software.
3. Simulate steady-state operation of the new structure by using HYSYS simulation software.
4. Study the Wongsri's plantwide control structures and design procedure (2012).
5. Design the new plantwide control structures of cumene process followed the Wongsri's procedure (2012).
6. Simulate the dynamic operation of cumene process with the new design control structures and the base case control structure.
7. Evaluate the dynamic performance of the new control structures based on the external disturbance loads.
8. Analyze and discuss of the design and simulate results.
9. The research provides conclusions.

1.6 Research Framework

This the thesis consisting of six chapters as follows:

Chapter I: presents importance and reasons for research, research objectives, scopes of research, and contributions of research, research procedures, research framework and research plan.

Chapter II: presents literature reviews related to plantwide control structures design procedure, review of previous work on the cumene process design, and control structure design.

Chapter III: purposes the fundamental of process control, plantwide control structures design principle, and the new plantwide control structure design procedure.

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

Chapter V: presents the control structure of base case (Luyben 2010) and new control structures designed by Wongsri's design procedures (2012), its dynamic response when load and thermal disturbances arise, and evaluated dynamic performance index to compare the performance of control structures designed by both procedures.

Chapter VI: presents the conclusions of research and recommendations.

CHAPTER II

LITERATURE REVIEW

2.1 Literature Review of Plantwide Control Structure Design

Buckley (1984) proposed a plantwide control design procedure that consisted of two levels. The first level is the material balance control to regulate inventories of vessel for low-frequency disturbances. The second level is the product quality control to handle high-frequency disturbances. However, the Buckley's procedure does not discuss the main point that it is the center of the plantwide control design problem. The material balanced control is the first level control hierarchy which interacts directly with the process. Since the manipulated variable of inventory and quality loops are not quite in conflict and if the duplicity of manipulated variables should occur, the conflicts are reconciled. (Buckley 1984)

Price and Georgakis (1993) identified two frameworks for plantwide process control design (modular and tiered). A CSTR/column process example and a procedure for the plantwide control design of the coupled system regulatory structure has been developed. The plantwide control system design procedure is based on a tiered framework and is evaluated performance by a dynamic simulation. The guidelines for inventory control structure design are presented. The best structures are shown to be those which are "self-consistent" and designed to minimize the propagation of disturbances through the system. (Price 1993)

Price, Lyman and Georgakis (1994) presented a well-designed process plant control system that it can effectively manage of the production rate and regulate the inventories within the process. Price and Georgakis have introduced guidelines for the improvement of the production rate and inventory controls. This guideline is applied using the complex test problem provided by the Tennessee Eastman Company. There are three steps to regulate the production rate and inventory controls. Firstly, applying the throughput control guidelines; identify the primary process path, and list throughput manipulators. Secondly, applying the inventory control guidelines;

Identify inventories which may need control, Identify inventory control manipulators, Determine which inventories can be controlled, and Construct a self-consistent chain of inventory controls along the primary process path. Finally, testing and evaluation by using commercial simulation software. (Price 1994)

Luyben (1997) presented the plantwide control structure design procedure to control an entire plant that includes many interconnected unit operations. The control structure design procedure of Luyben (1997) includes nine steps to propose procedure center around the principles of plantwide control: thermal management, production rate, quality of product, operational, environment and safety, level of liquid and gas pressure inventories, makeup of fresh feed reactants, material balances, and economic or process optimization. Luyben applied his procedures with three industrial such as the vinyl acetate monomer process, the Eastman plantwide-control process, and the HDA process. (Luyben 1997)

Skogestad et al. (2004) presented the plantwide control design procedure that it is expanded from five steps in 2000 (Skogestad 2000) to eight steps. The change in procedure is an emphasis on degree of freedom analysis, selection of controlled variables, control system complexity, inventory control, and loss in performance by bottom-up design. The procedure is presented in 2 main parts. The first four steps are top-down analysis including of operational objectives and consideration of degrees of freedom. And the last four steps are bottom-up design of the control system for stabilizing control layer. Step 5 and step 6 are the analysis of control layer using a linear multi-variable dynamic mode. Step 3 and step 7 are the analysis of optimization layer using a non-linear steady-state mode. This procedure is based on the mathematical analysis method. (Skogestad 2004)

Konda et al. (2005) presented the plantwide control design procedure that it is important for chemical processes and recycle stream for reasons of safety, environmental, and economics. In this work, simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The proposed framework is applied to the hydrodealkylation (HDA) process. An analysis of results shows that the proposed framework builds synergies between the

powers of both the simulation and the heuristics, thereby resulting in a practical PWC methodology that leads to a viable control system. (N.V.S.N. M. Konda 2005)

2.2 Literature Review of Cumene Production Process

Luyben (2010) presented to optimize the economics of capital costs, energy costs, and raw material costs and to improve a plantwide control structure that can be handle large disturbances in production rate. The design optimization variables are reactor size (number of tube) and amount of benzene recycle flow rate. Design optimization variables affect both energy costs and capital costs because they have affected the amount of reactants required to produce the design product (cumene). The economic effect of reactant consumption is very large, an order of magnitude greater than the impact of energy or capital. (Luyben 2010)

Mahapatra and Khanam (2010) presented about design of the cumene production process that it can significantly reduce production cost and make the process safe and reduce environmental damages. They used the ASPEN PLUS simulation software to design and optimize a cumene process in steady state mode. The operating temperature of the reactor system on being optimised as 360 C and the ratio value of benzene and propylene in feed was 6:1. The distillation columns were optimised and the number of trays for benzene column was found to be 20 by 8 and that for cumene column to be 20 by 10. The reflux ratio values were found to be 0.5 and 0.8 respectively for the columns. The optimized temperature in the flash tank was identified as 92.5 C. (Mahapatra 2010)

Gera et al. (2011) applied Skogestad (2004)'s plantwide control design procedure to the cumene process. A top-down analysis is used to select the set of self-optimizing primary controlled variables which when kept constant lead to acceptable economic loss without re-optimize the process when disturbances happen. 2 modes of operation are considered (given feed rate and optimized throughput). (Gera 2011)

Maity et al. (2013) presented the systematic top-down economic plantwide control of the cumene process by synthesizing a control system for maximize the plant operating profit at maximum throughput via the top-down pairing approach. First, obtain active constraints and self-optimizing CVs for unconstrained degree of freedoms via a steady state optimization for maximum throughput. Then, loop pairings are implemented in the order of the top-down control objective prioritization. Loops are paired for tight control of the active constraints. Next, pairings for appropriate self-optimizing CVs corresponding to unconstrained degree of freedoms are chosen. Finally, regulatory loops (inventories) are considered to complete the control system. The control structure of two level loops on the recycle column are unconventional and long ones because the inventory loops are paired by only using the remaining control valves after pairing the active constraint and self-optimizing CV loops. However, the dynamic simulations show that acceptable regulatory control is achieved for large disturbances. (D. Maity 2013)

CHAPTER III

THEORY

3.1 Principle of plantwide control

One of the biggest challenges to the successful development of a chemical process is finding an effective plantwide control structure. All of the units in a process must “dance together” in a stable harmonious manner. Small ripples in the reaction section should not be transmitted into the separation section, and vice versa.

The development of a plantwide control structure is not a trivial task. Typical processes can have many variables that must be controlled and many valves that must be driven by some control signal. Single-input-single-output proportional-integral controllers are widely used in industry. A process may have 30 to 50 loops to configure (select controlled/manipulated variable pairings and controller tuning constants). With 30 loops there are 30-factorial possible combinations of the variables. So an exhaustive enumeration of all possible pairings is untenable. Common sense, experience, and process control wisdom can reduce the possible pairings to a manageable number with dynamic performance that can be evaluated using dynamic simulation.

There are several alternative plantwide control structures that do work. The best structure depends on the control objectives of the plant, which in turn depend on the business objectives of the company. For example, if the product from the plant is to be provided to a downstream customer at whatever flowrate the customer desires at any point in time, an “on-demand” plantwide control structure must be developed. The inventory loops (liquid levels and pressures) would be set up to work their way backwards from the product leaving the process to the fresh feed streams coming into the process.

3.2 Steps of Plantwide Control Design Procedure of Luyben

The design procedure of Luyben is carried out in nine steps, which contented the two fundamental of the overall conservation of energy and mass. Each of steps is as follows:

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.

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. 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.

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

Select the “best” valves to control each of the product quality, safety and environmental variables. We want tight control of these important quantities for economic and operational reasons. Hence we should select manipulated variables such that 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 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.

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.

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 (Shinsky 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 or to improve dynamic response.

3.3 Wongsri's Plantwide Control Design Procedure

Wongsri (2012) presented the new plantwide control design procedure carried out in five stages with eight steps, the major steps deal with plant level design; establishing a fixture plant. The component balances are accounted by identifying the material quantifiers that indicate the amounts of the components and using their handlers to control them. The disturbances entering into the process must be directed by using the proposed material and energy disturbance management for avoiding disturbance propagation throughout the plant. Each step is as follows:

Stage 1 Plant Information and Analysis

Step 1: Gather of relevant plant information and control objectives including constraints for control.

It is necessary to obtain all information relevant to process control, such as product quality, production rate, smooth operation, process and equipment constraints, plant safety, and environmental regulations.

Step 2: Plant analysis.

Several tasks to assist design decision in Step 3 are:

2.1 Control degree of freedom (CDOF).

Each single independent stream, physical or virtual, material or energy, must have a handle or one control degree of freedom.

2.2 Heat pathways.

The first pathway is heat generated by exothermic reactions and flows out to the environment. This pathway is from inside the process and flows out. A second pathway carries heat from utilities into the process and to the environment. This pathway is from the environment passing through the process and out to the environment. The third pathway is internal to the process. Here heat flows circularly through all process units in the process loops. The fourth pathway is accounted for the enthalpies entered and left the plant.

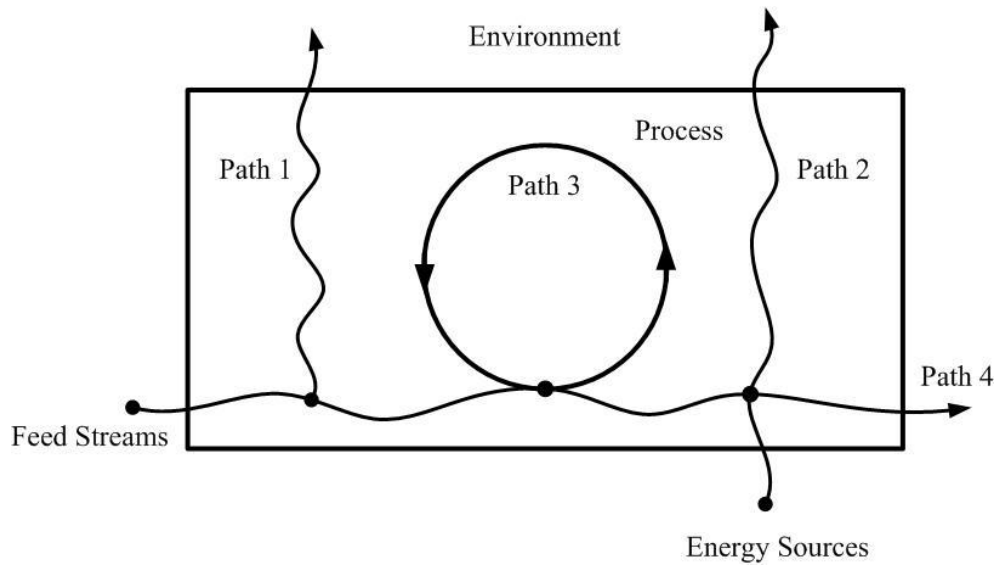


Figure 3.1 Heat pathways.

2.3 Material pathways.

The pathway is the main flow path of a component from its entry point or its originated point to its exit point or its end point (completely consumed in the reactor).

2.4 Material quantifier.

A material quantifier is the place indicating the significant amounts of a chemical component (or a group of components) in the plant which can be handled quite readily by regulating at their handlers. In the case that the quantifier is a flow, it is, but not necessarily, the place that has the highest gain of component flow is the total flow.

2.5 Reaction section.

It is necessary to obtain required information for control design of reactor section. In general, what kind of controlled variables used to regulate the reaction yield and where to measure such controlled variables? What is the best control strategy and all? If feeds and recycled streams are fixed, the only places that the material (total or component) flow rates altered are a reactor and also a separator.

2.6 Separation section.

The appropriate directions of disturbances are analyzed and specified. A surplus disturbance, D^+ is the surplus deviation of the mass load from the nominal load and the deficit disturbance, D^- is the deficit deviation of the mass load. The paths of D^+ and D^- in the separation section are analyzed and then designed in order to shift surplus or deficit mass loads to the desired targets to achieve the plant operation objective, e.g. maintaining product quality and avoiding disturbance propagation and recycling. The paths of D^+ and D^- in the separation section must be shifted to the proper exits. In the case that there is no proper exit for D^+ or shifting it through available exits will disturb the product quality, recycling it would be allowed.

Next, a good location of temperature control is the tray with the largest changes in the temperature from the initial steady state by changing of composition, total flow, temperature, and component flow during keeping the reboiler heat duty and reflux flow or reflux ratio or reflux fraction or boil up ratio constants.

2.7 Mode of operation: On-supply, On-demand, and on-internal.

The mode of operation is dictated by a business objective and the mode of operation, such as on-supply (fixed feed rate), on-demand (fixed product rate), and on-internal (fixed internal flow rate) based on throughput manipulator (TPM) decision Price and Georgakis (1994). For on-internal control scheme, the throughput manipulator (where the production rate is set) is located inside the plant downstream of this location (normally at the bottleneck), the plant has to process whatever comes in, and upstream of this location the plant has to produce the desired quantity. The selection of on-supply, on-demand or on-internal should depend on the completeness of total control of components.

In some processes, the separation section is placed before the reactor section, there are two locations to fix the material flows into the process: at the entrances of the reactor section or of the separation section. In the case that the reactor influent is fixed, the quantifiers (inventories) prior to this point must be controlled as 'on-demand production'.

2.8 Production rate control.

Throughput changes achieved by altering the reactor conditions: temperature, reactant concentrations, liquid holdup, or pressure would be somehow limited. The production rate is normally set at the throughput manipulator. The quantifier/inventory control structure is set as discussed in 2.7.

Stage 2 Fixture Plant and Disturbance Management (Plant Level Loop Design)

This stage is a major design stage; plant control structure is created at plant level in two steps: Step 3 and Step 4. The plant control loop design procedure presented in this paper is explicit and systematic while the Luyben design procedure has some shortcomings, Konda (2005). There are two objectives: the plant nominal material balance is maintained; the heat and material disturbances must be rejected to the nearest exits or directed to less significant streams.

Step 3: Establish fixture plant.

The principal idea of establishing a fixture plant is first to have a material-balanced in the plant by controlling each component at its quantifier, i.e. fixture point.

3.1 Keep the materials entered and/or reentered fixed.

A fresh feed and/or a combined stream of make-up feed and recycle stream must be kept constant to maintain the plant inventory by flow/composition controls. A recycle flow should not be fixed. This leaves the recycle flow free to be adjusted; one degree of freedom is restored to the plantwide control design process. If the composition of the recycled stream differs from the fresh feed stream significantly, each recycled stream may be flow-controlled. However, in the case that the composition of the recycled reactant can be measured, the composition of the combined stream is controlled to keep the combined reactant flow in check.

In the case of changing throughput, the combined stream of make-up feed and recycle or the recycle stream is adjusted accordingly to maintain the material balance principle. Normally, the liquid recycle is adjusted automatically by its level

somewhere in the process. However, it might be not the case for the gaseous recycle flow, the additional ratio loop of the recycle and the feed is recommended.

3.2 Adjust the flow of exit material streams (products, byproducts, and inert) according to their accumulations.

If the flows of the products are controlled (mode of operation is on-demand) the quantifiers of the products, e.g. levels of reflux drums indicating the surplus/deficit will be used to control the feeds.

3.3 Handle the material that not leaving the process.

The reactor is the logical place to regulate a component fed or formed in the process and not leaving the process. If there is only one reactor and there is more than one component that not leaving the process, their kinetics must be similar, e.g. increasing the reactor temperature reduces or increases the amount of both components. Handlers of these components must be identified. If their kinetics are not compatible, we must provide exits for the incompatible components.

3.4 Control the amount of the rest of the component at their quantifiers.

This step assures the rest of component inventory is regulated from a plantwide perspective. Setting the control at the specified quantifiers is like providing coordination over different sections of the plant to ensure that the rate of accumulation of each component in the overall process is zero.

3.5 Maintain the production rate.

3.5.1 Consume the limiting reactant.

Determine the most appropriate manipulate variable to control the limiting reactant for the economic reason, i.e. the reactor temperature, the reactor pressure, or the reactor holdup.

3.5.2 Maintain 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. However, the design constraints may limit this strategy concerning increasing the reactant feed rate.

Step 4: Disturbance management for quality control.

The nominal conditions of process streams are maintained by specifying the disturbance shifting directions. The principles of disturbance management are following:

4.1 Heat disturbance management.

The heat disturbance is divided into two categories. Heat disturbance of category 1 (HDC1) is the heat disturbance that does not instantly effect on the qualities of process streams, such as heat disturbance in a process stream toward a heater, a cooler, or a process-to-process heat exchanger. Heat disturbance of category 2 (HDC2) is the heat disturbance that will affect the process stream qualities where an additional phase is created or introduced, and the equilibrium is altered; or where chemical reactions are undergoing, such as separators and reactors.

4.1.1 Direct the HDC1 to the environment via the next and nearest exit points, usually heaters or coolers, to keep the thermal conditions of the process stream fixed.

4.1.2 Direct the HDC2 to less significant output streams of separators. This rule is generally apt to a separator using heat as a separating agent.

4.2 Material disturbances management (MDM).

The configurations of the control loops are decided base on the desired material pathways. As in the case of heat disturbance management, we should direct the material disturbances to the environment via the next and nearest exit points to avoid disturbance recycling and propagation.

Many industrial distillation columns use some type of single-end temperature control because of its simplicity and low maintenance cost. This step presents a procedure to determine the control structure of a distillation column with desired material disturbances (D^+ and D^-) following step 2.6 by using a dynamics process simulator for various single-end control structures, namely constant reflux flow (R), constant reflux ratio (Arrayasinlapathorn), constant reflux-to-feed ratio (R/F), constant reflux fraction ($R/(R+D)$), constant boil-up ratio (V/B). Several kinds of material disturbances in feed, such as temperature, flow rate, composition, and component flow rate are generated to test the disturbance shifting ability of these control structures. In addition, the principals of the material disturbance management are as follows:

4.2.1 Direct the material disturbances of byproducts, inerts, and unconverted raw materials to the environment via the next and nearest exit points.

4.2.2 For the main products, the deficit disturbances should follow Rule 4.2.1. However, the main product surplus disturbances should be allowed to propagate to their exits.

4.2.3 MDM rule for the recycled streams: their surplus disturbances of unreacted raw materials are permitted, however, their deficit disturbances must not be allowed to economize the make-ups.

The selection of the distillation control structures is carried out in two steps: preliminary screening using steady-state simulation and the selected candidates are further tested by rigorous dynamic simulation.

Stage 3 Unit Level Loop and Enhanced Loop Designs

Control loop design at this stage is solely based on individual unit operations.

Step 5: Design the rest of the control loops.

Normally, the rest of the control loops is inventory loops which are self-regulating and less crucial. They can be designed using unit-based approach.

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

5.2 Adding simple enhanced controls, e.g. cascade, feed forward controls.

Stage 4 Energy Management and Optimization

The supplementary design activities involve heat exchanger network design and control, and plant operation and design optimization.

Step 6: Energy management via heat exchanger networks.

In the case that the exothermic heat of reaction is large enough to heat some process cold streams, i.e. potential heat exchanger networks or alternative heat integrated processes (Thipsukhum) exist, a heat exchanger network must be designed and a HEN must be resilient, i.e. delivering the exchange streams to their target temperature. The resilient heat exchanger network with specified load disturbances can be designed using Wongsri's method.

Step 7: Optimize economics or improve control performance.

The design and control issue remains an open research area regarding the plantwide control design, so the opportunity to alter the process design is possible.

Stage 5 Design Validation

The validation of the design control structures using rigorous nonlinear simulation is inevitable; whatever may be the design procedure.

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

The measures would be costs, raw material and energy consumptions, control performances of the total plant or some selected loops, etc. Expected disturbances must be listed to perform the disturbance test on the plant with designed control structures.

CHAPTER IV

CUMENE PROCESS

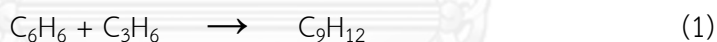
4.1 Introduction to Cumene Process

Cumene can be found in crude oil and is a part of processed high-octane gasoline. Cumene is an important intermediate for industrial products such as phenolic resins, epoxy, nylon-6 and polycarbonate resins etc. Generally, processes for cumene manufacture consist of a packed bed reactor (liquid or vapor phase) followed by a separation train that removes the light inerts (propane), recycles the unreacted benzene and separates the cumene product from heavies generated by further alkylation of cumene to diisopropylbenzene.

4.2 Kinetics and Thermodynamic Model

4.2.1 Reaction Kinetics

The production of cumene (isopropylbenzene) involves the reaction of benzene with propylene in a high-temperature, high-pressure gas-phase reactor.



There is also a side reaction of propylene and cumene to form diisopropylbenzene (DIPB).

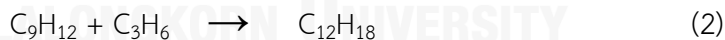


Table 4.1 gives the reaction kinetics provided by Turton et al. All reaction rates have units of $\text{kmol s}^{-1} \text{m}^{-3}$. Concentration units are molarity. The reactions occur in the vapor phase in the presence of a solid catalyst (assumed to have 0.5 void fractions and a 2000 kg/m^3 solid density). The reactor is run at high pressure (25 bar) since the moles of reactants are more than the moles of product (LeChatier's principle).

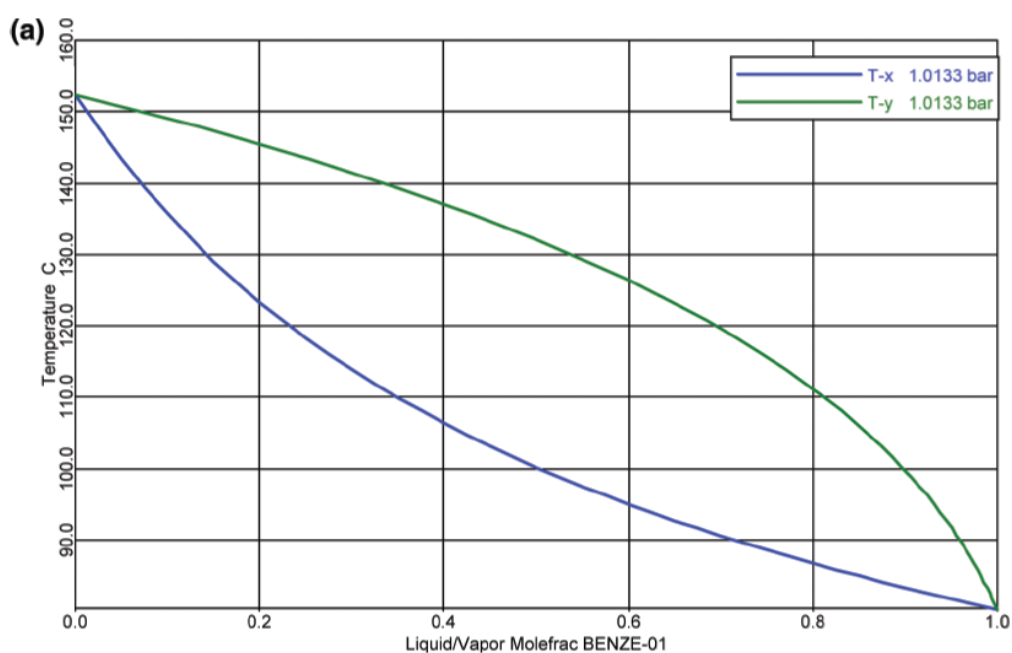
Notice that the activation energy of the undesirable reaction is larger than that of the desirable reaction. Therefore low reactor temperatures improve selectivity. In addition selectivity is improved by keeping the concentration of cumene and propylene low in the reactor. This can be achieved by using a large excess of benzene, but the excess must be recovered and recycled.

Table 4.1 Reaction kinetics

	R1	R2
K	2.8×10^7	2.32×10^9
E (kJ/kmol)	104174	146742
Concentration terms (kmol/m ³)	$C_P C_B$	$C_C C_P$

4.2.2 Phase Equilibrium

The normal boiling points of benzene, cumene, and DIPB are 80.1, 152.4, and 209.8 °C, respectively. The NRTL fluid package is used in the HYSYS simulations software used in this thesis. Figure 4.1 gives the Txy diagrams for the benzene/cumene system and the cumene/DIPB system at atmospheric pressure.



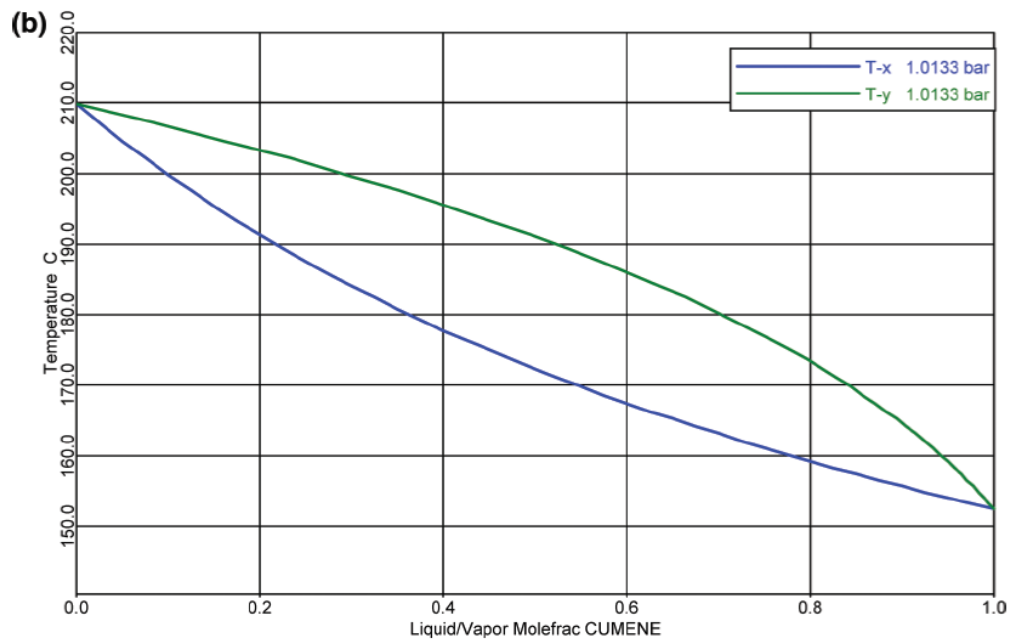


Figure 4.1 Txy diagram: (a) for benzene/cumene; (b) for cumene/PDIB.

4.3 Cumene Process Descriptions

Fixture 4.2 shows the flowsheet of the cumene process that it includes the stream data and equipment size information from Luyben (2010).

The fresh feed of mixed C3 (propylene and propane) is combined with the total benzene as liquids. The fresh feed flow rate of the mixed C3 is set at 101.93 kmol/h and 25 °C. The composition of mixed C3 includes propylene (limiting reactant) 95 mol% and propane (inert) 5 mol%. Since propane is an inert, it is purged at the gas stream of flash tank about 5.1 kmol/h. The fresh feed benzene is set at 98.78 kmol/h and the production rate of cumene product is set at 92.86 kmol/h in the Luyben design.

The fresh feeds of benzene are combined with a liquid recycle stream from benzene distillation column and fed into a vaporizer. The total benzene fed to the vaporizer is 208.93 kmol/h. The gas stream leaves from the top of the vaporizer at 210 °C and 25 bars and it is preheated in the feed effluent heat exchanger (FEHE). Then, the second preheating is preheated in heater to bring the reactor inlet temperature up to 358 °C.

The Cooled Tubular Reactor: The tubular reactor operates at high-pressure stream and reaction is the exothermic reactions. There are 1500 tubes, 0.0763 m in diameter, and 6 m in length. The tubular reactor is filled with a solid catalyst with 0.5 of a void fraction and a solid density of 2000 kg/m^3 . An overall heat-transfer coefficient is $0.065 \text{ kW m}^{-2} \text{ K}^{-1}$.

The exit stream of the reactor leaves at $358.5 \text{ }^\circ\text{C}$ and it is cooled to $279 \text{ }^\circ\text{C}$ in the FEHE, and sent to a cooler that it is cooled to $90 \text{ }^\circ\text{C}$. The two phase stream from the cooler is fed to a flash tank. The gas stream from the top of flash tank is used as fuel. The liquid stream from the bottom of flash tank is fed into the benzene distillation column C1.

Benzene Recycle Column C1: The benzene column has 15 stages and is fed on stage 6, which is the optimum feed stage to minimize reboiler heat input. The operating pressure at the top of benzene column is operated at 1.75 bars, which gives a reflux-drum temperature of $60 \text{ }^\circ\text{C}$. The reflux ratio (Arrayasinlapathorn) is 0.44 and the benzene column diameter is 1.36 m. The distillate stream includes mostly benzene and it is recycled back to the process. The composition of benzene in the benzene recycle stream is 95.6 mol% with small amounts of propylene and propane.

The specify design is to maintain benzene from dropping out of the bottom and affecting the concentration of the cumene product that leaving in the distillate stream of the cumene column (C2). Since the specified cumene purity is 99.9 mol% so the benzene concentration in C1 bottoms must be maintain at 0.05 mol%.

Cumene Product Column C2: The cumene column has 20 stages and is fed on stage 12. The operating pressure at the top of cumene column is operated at 1.75 bars, which gives a reflux-drum temperature of $152 \text{ }^\circ\text{C}$. The reflux ratio (Arrayasinlapathorn) is 0.63 and the cumene column diameter is 1.26 m.

The specify design is to maintain high-purity of cumene in the distillate stream and minimize the loss of cumene in the bottoms so the cumene composition at the bottoms is set at 0.1 mol%. The cumene composition in distillate stream is 99.9 mol % using the 0.63 reflux ratio.

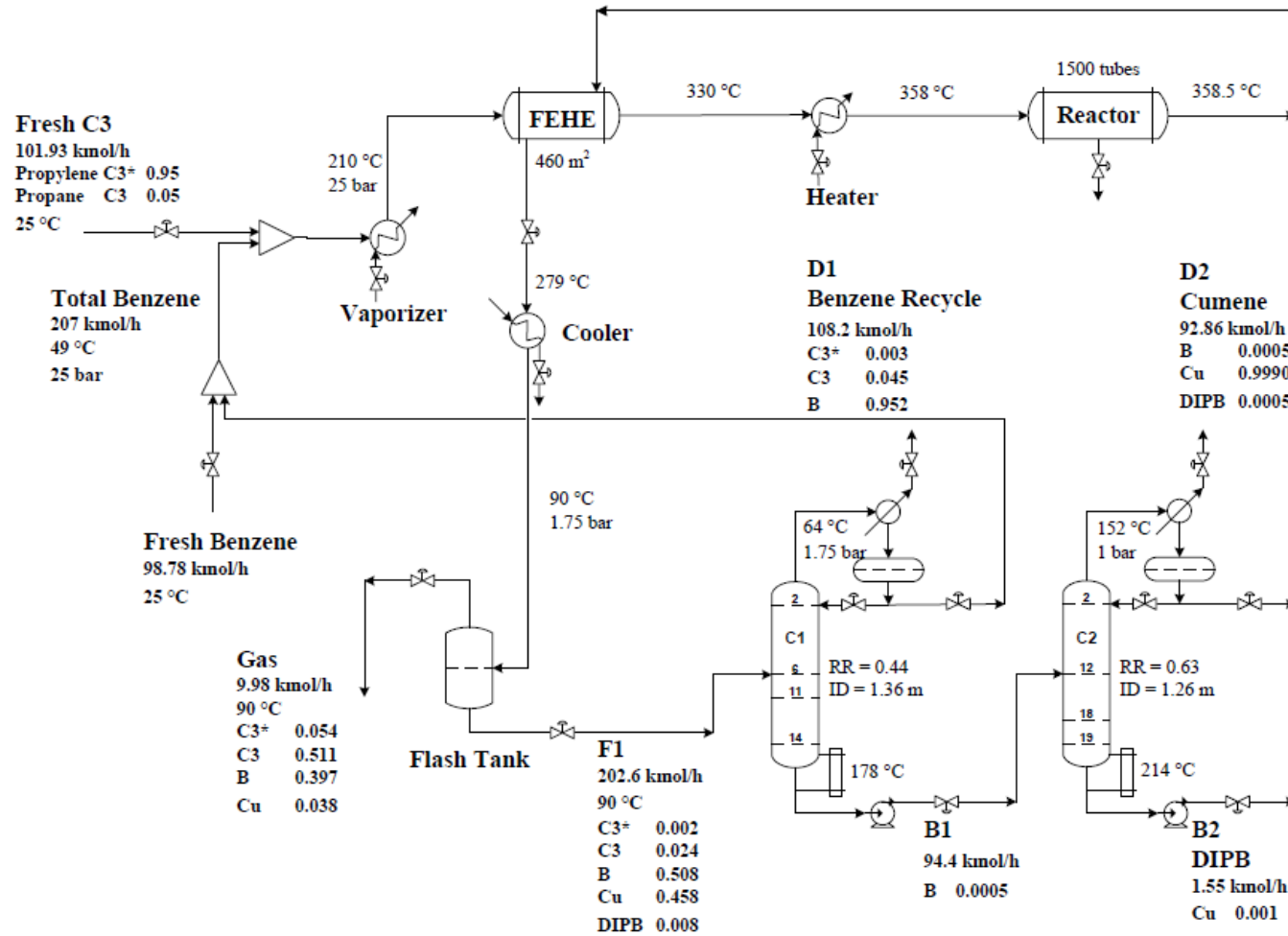


Figure 4.2 Flow sheet of the cumene process (Luyben 2010)

CHAPTER V

CONTROL STRUCTURES DESIGN AND DYNAMIC SIMULATION RESULT

5.1 Introduction

The plantwide control structure design for the cumene process is designed base on the new plantwide control structure design procedure of Wongsri (2012). The disturbances entering into the process must be directed by using the proposed material and energy disturbance management for avoiding disturbance propagation throughout the plant. The new plantwide control design procedure emphasis on maintaining the plant operating conditions.

5.2 Application of Wongsri's design procedure

In this section, the new design procedure of Wongsri (2012) is applied to design the plantwide control structures of cumene process. The five stages with eight steps of new plantwide control structure design are discussed in each step as follows:

Stage 1 Plant Information and Analysis

Step 1: Gather of relevant plant information and control objectives including constraints for control.

The information mentioned in Section 3 is used in control structure design and simulation. The performances of control structure must satisfy the four control objectives, we want to maintain the purity of the cumene more than 99.9 mol%. The benzene distillation column C1 operates pressure at 1.75 bar and the cumene distillation column C2 operates pressure at 1 bar. The inlet temperature of the reactor is 358 °C and pressure about 25 bars. Since, we want to keep high conversion of propylene and reduce the production of the undesired product. The recycle benzene is maintained flow rate at 108.2 kmol/h.

Step 2: Plant analysis

2.1 Control degree of freedom (CDOF)

Each single independent stream, physical or virtual, material or energy, must have a handle or one control degree of freedom. There are total of 19 independent streams, hence 19 CDOFs, according to Assertion 2.1 of Wongsri's procedure. The CDOFs are listed in Table 5.1

Table 5.1 The control degree of freedom for the cumene process

Entities	Independent Streams	Quantity	CDOF
Streams	Fresh C3, Fresh benzene feeds, and FEHE effluent	3	3
Vaporizer	Vaporizer duty	1	1
Heater	Heater duty	1	1
Coolers	Cooler duties	1	1
Tubular reactor	Reactor effluent	1	1
Separator	Separator top and bottom flows	1	2
Distillation columns, C1 and C2	Distillate flows, Bottom flows, Reflux flows, Reboiler duties, Condenser duties.	2	10
Total degrees of freedom			19

2.2 Heat pathways

The heat pathways are used to design control loops to regulate thermal condition of the process streams and reject the thermal disturbances. The heat pathways are presented in Figure 5.1. The first pathway is heat generated by exothermic reactions (9.33 GJ/h) and out to the environment via reactor cooling media. The second pathway is heat from heaters, reboilers, and pumps into the process (24.34 GJ/h) and to coolers, condenser to the environment (22.62 GJ/h). The third pathway is heat in the process loop (5.29 GJ/h). The fourth pathway is the enthalpies entered (6.36 GJ/h) and left the plant (1.25 GJ/h) via exit process streams, cooler, reactor jacket, and condensers.

Heat disturbances are rejected or introduced at vaporizer, heater, cooler, jacket at the reactor, two condensers, and two reboilers to maintain the thermal conditions of the process streams.

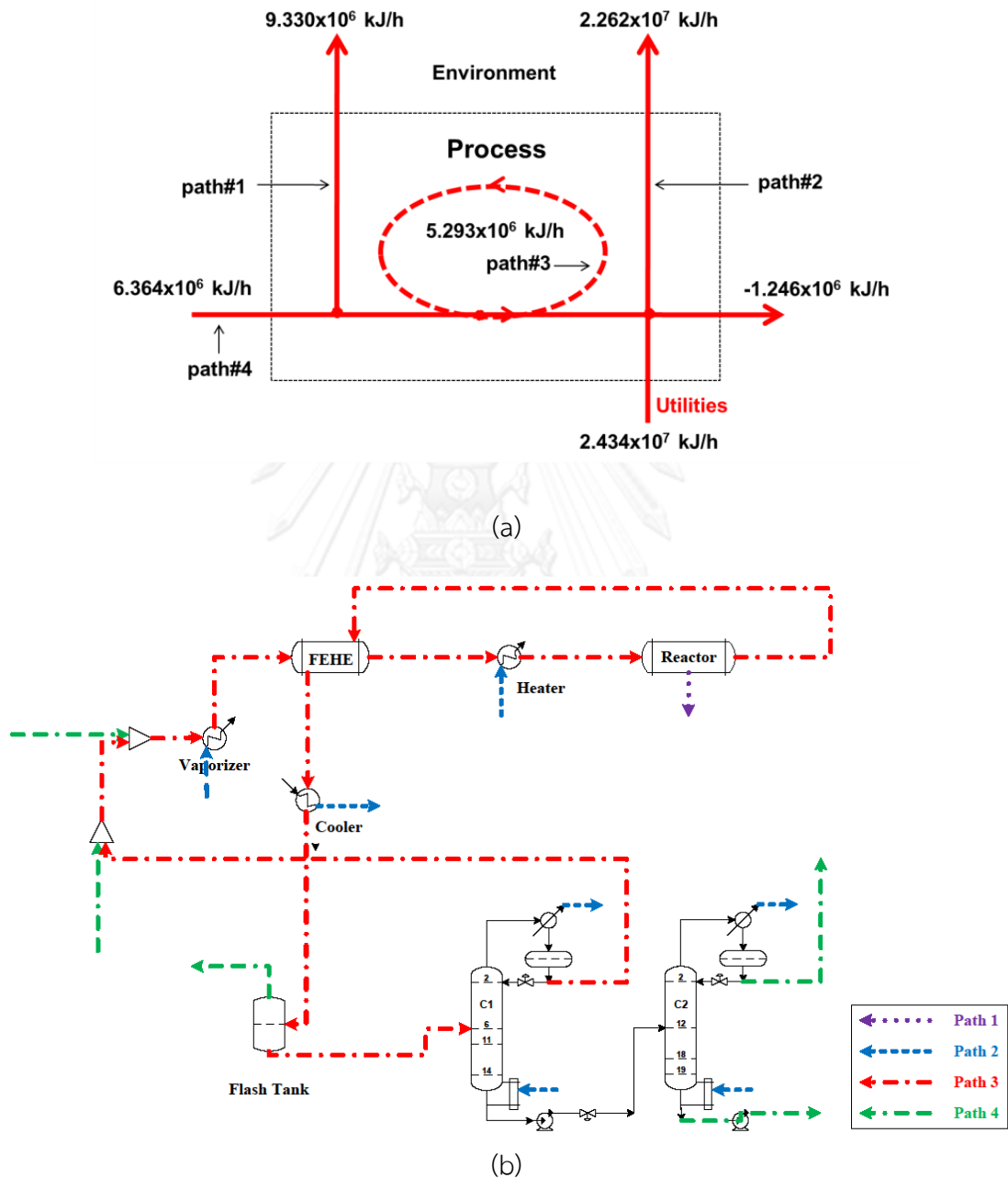


Figure 5.1 Heat pathways of cumene process

2.3 Material pathways

The material pathways are useful in identifying the material quantifiers as discussed in Section 2.4. Five material pathways for propylene, propane, benzene, cumene, and di-isopropylbenzene are depicted in Figure 5.2.

Propylene and benzene are raw materials that affects to the reaction and quality of cumene. The first pathway is propylene. Propylene is fed to the process by the fresh feed of mixed C3 stream into the vaporizer to become the saturated gas. Then, it is fed into the FEHE and heater for preheating before into the reactor. After that it is consumed in the reactor. The second pathway is propane. Propane has the same pathway as propylene but propane is an inert. So it is purged in the gas stream of flash tank. The third pathway is benzene. Benzene is fed to the process by the fresh feed benzene stream. Since benzene is an excess reactant, it is fed into the flash tank and into the benzene column C1 for separate excess benzene from product and recycle benzene to the process. The fourth pathway is cumene. Cumene is generated at the reactor. Then, it is fed into the flash tank, benzene column C1, and out of the process in the distillate stream at the cumene column C2. The fifth pathway is DIPB. DIPB has the same pathway as cumene but it is separated from cumene and out of the process in the bottom stream at the cumene column C2.

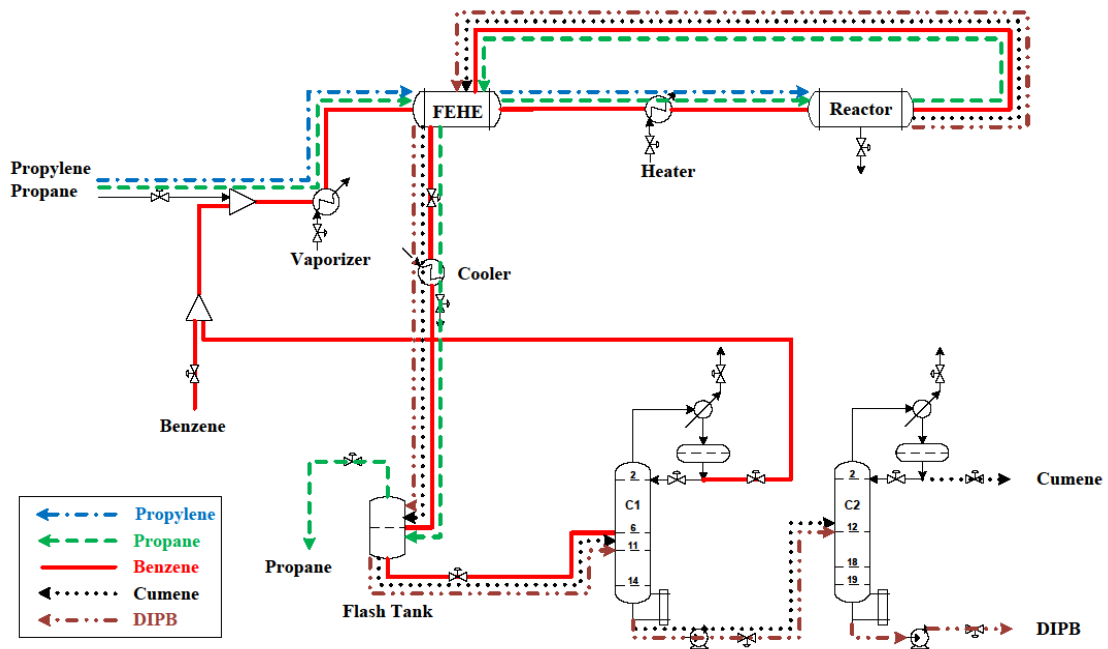


Figure 5.2 Material pathways of cumene process

2.4 Material quantifiers

The material quantifiers are useful to design control loops for component balance as discussed in Step 3.

The propylene quantifier, the place indicating its significant amounts, is the flow rate of the fresh feed mixed C3. The benzene quantifier is the total benzene stream, i.e. the combined flow of recycle stream and make-up of fresh feed benzene. The cumene quantifier is reflux drum level of cumene column C2 and the quantifier of DIPB is C2 bottom level. The propane quantifier is the pressure of flash tank.

Next, the handlers are identified with ease difficulties since the handler must affect the quantifier directly and fast. The pair of quantifier and handler must possess high gain and minimal lag. Five CDOFs in Table 5.2, namely, fresh mixed C3 feed, fresh benzene feed, C2 distillate flow (cumene product), C2 bottom flow (DIPB by-product) are selected to the handlers. The material quantifiers and their handlers are depicted in Figure 5.3 and Table 5.2.

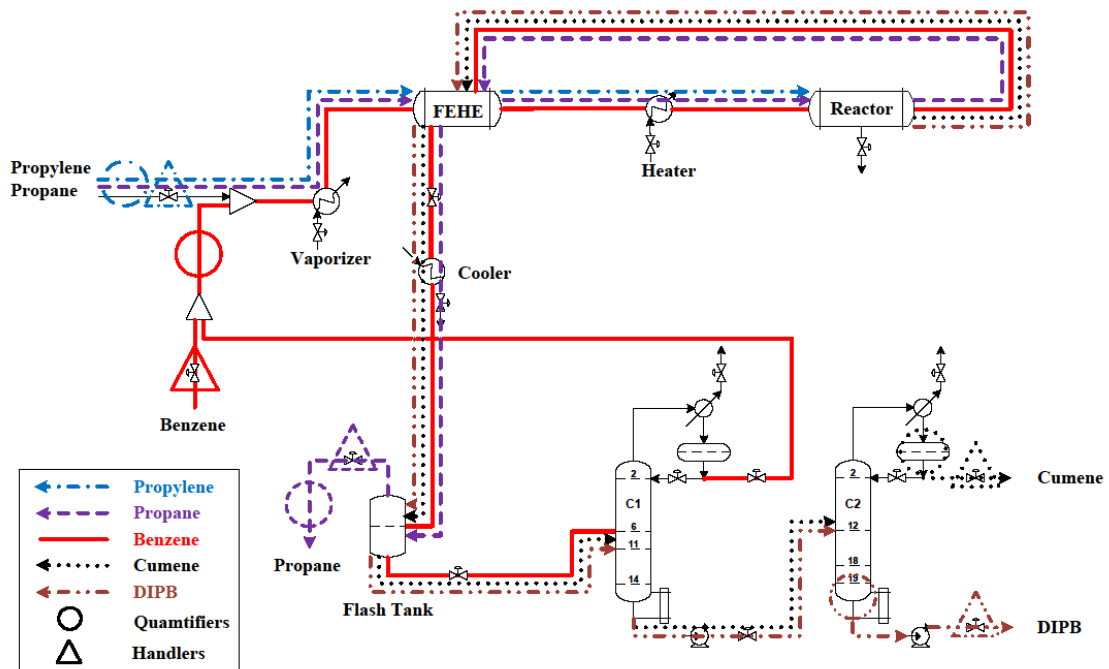


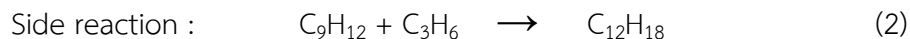
Figure 5.3 Material pathways and material quantifiers

Table 5.2 Quantifiers and handlers of components

Component	Quantifier	Handler
C_3H_8	Gas stream of the flash tank	Purge flow rate
C_3H_6	Fresh feed of mixed C3	Fresh mixed C3 feed
C_6H_6	Combined of recycle and C_6H_6 fresh feed	Fresh feed C_6H_6 flow rate
C_9H_{12}	C2 reflux drum level	C2 distillate flow rate
$C_{12}H_{18}$	C2 reboiler level	C2 bottoms flow rate

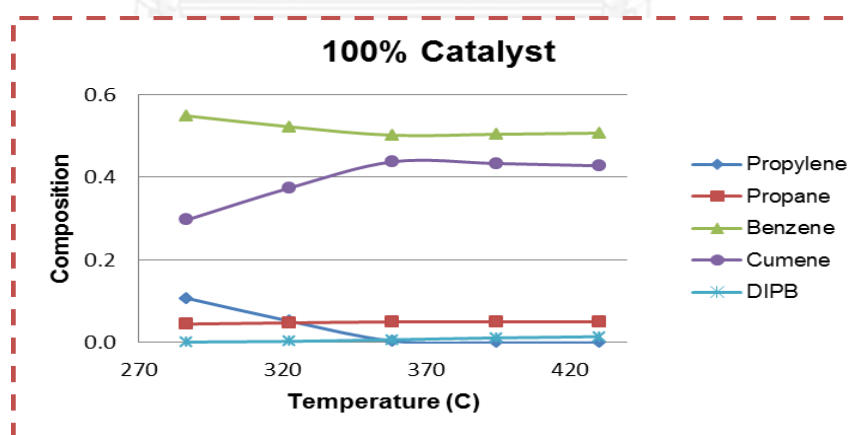
2.5 Reaction section

The reaction is an exothermic reaction. The reactor is a cooled tubular reactor. There are 1500 tubes, 0.0763 m in diameter and 6 m in length. They are filled with a solid catalyst with a void fraction of 0.5 and a solid density of 2000 kg/m^3 . An overall heat transfer coefficient is 0.065 $\text{kW/m}^2 \text{K}$.

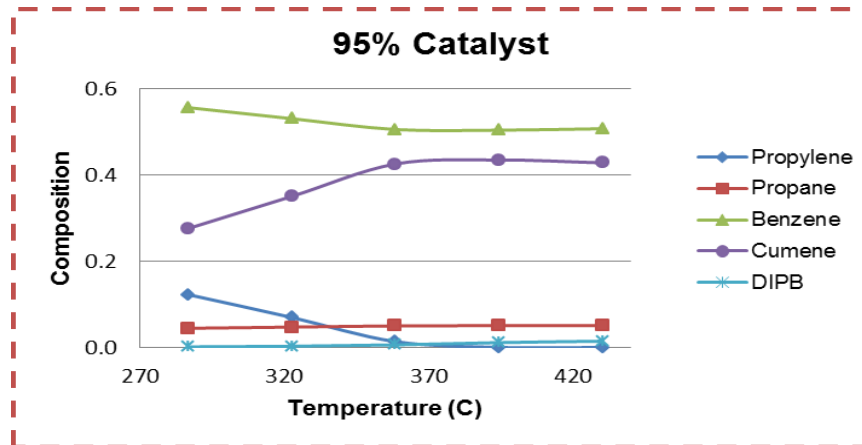


The activation energy of the undesirable reaction is larger than that of the desirable reaction. This translates to low reactor temperatures improving selectivity. Also selectivity can be improved by maintaining the reactor concentration of cumene and propylene low. This is why the process designer used a large excess of benzene, and the unreacted benzene is recovered and recycled.

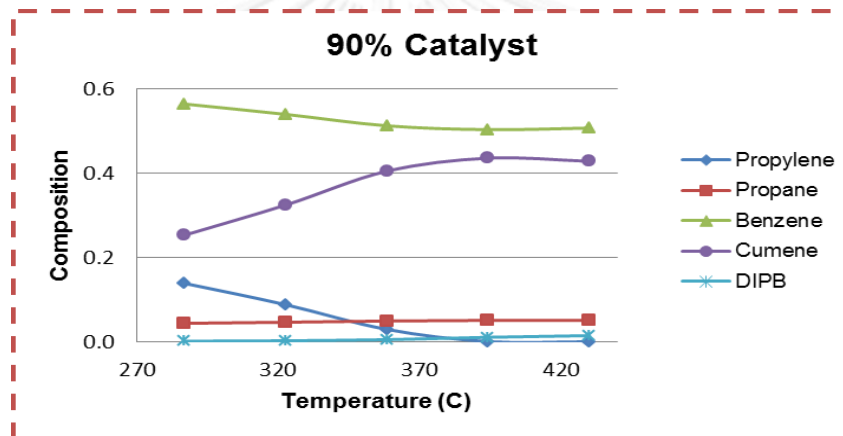
The dominant controlled variables affecting reaction yield are reactor temperature, concentrations of propylene and benzene. The only dominant variable that can be adjusted is reactor temperature confirmed using steady-state simulation by perturbing the reactor inlet temperature. The effects of catalyst deactivations are also study (See Figure 5.4). To maintain the cumene composition in reactor effluent, the reactor temperature should be increased by adjusting reactor cooling duty. However, the higher temperature will increase the production of the undesirable product.



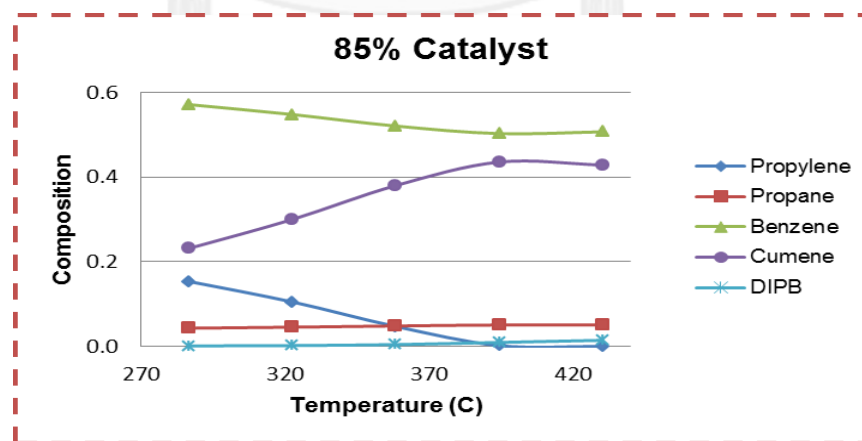
(a)



(b)



(c)



(d)

Figure 5.4 Steady state simulation results in reactor section analysis

2.6 Separation section analysis

The proper directions of material disturbances are analyzed and specified in this section. To begin with, the flash tank separates the inert into liquid and gas stream at 1.75 bar and 90 °C. The inert disturbances (surplus and deficit disturbances of the inert: $DC_3H_8^+$, $DC_3H_8^-$) should be entirely shifted to the top of flash tank to avoid inert drift in the process.

Benzene column C1 separates excess benzene from product and recycles benzene distillate back to the feed station. The surplus and deficit disturbance of the benzene ($DC_6H_6^+$, $DC_6H_6^-$) entered should be shifted to C1 top, since we want to maintain benzene impurity at C1 bottoms. The surplus disturbance of the cumene ($DC_9H_{12}^+$) entered should be shifted to C1 bottoms and the deficit disturbance of the cumene ($DC_9H_{12}^-$) entered should be shifted to C1 top to maintain cumene purity.

Next, the cumene column C2 separate cumene (C_9H_{12}) and DIPB ($C_{12}H_{18}$). The surplus disturbance of cumene ($DC_9H_{12}^+$) should be shifted to C2 top. Finally, the surplus and deficit disturbance of the DIPB ($C_{12}H_{18}^+$, $C_{12}H_{18}^-$) should be shifted to C2 bottoms. Figure 5.5 and Table 5.3 have shown the desired disturbance paths.

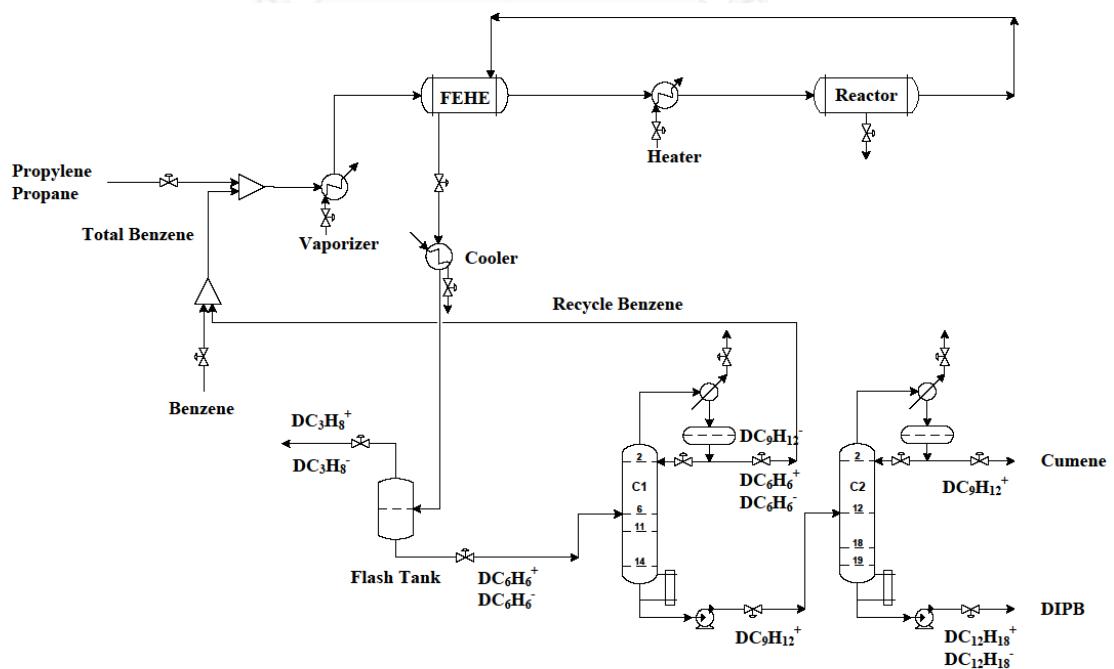


Figure 5.5 The directions of material disturbances predetermined.

Table 5.3 Surplus and deficit disturbances shifting direction

Separation Unit	Top	Bottoms
Flash tank	$DC_3H_8^\pm$	$DC_6H_6^\pm$
C1	$DC_6H_6^\pm, DC_9H_{12}^-$	$DC_9H_{12}^+$
C2	$DC_9H_{12}^+$	$DC_{12}H_{18}^\pm$

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 test is made in a steady-state simulation mode. Selecting the temperature control tray location of C1, the tray sensitivities to important disturbances are performed. The largest changes in temperature profile of the benzene column C1 is tray 9th and The largest changes in temperature profile of the cumene column C2 is tray 14th as shown in Figure 5.6 – 5.9.

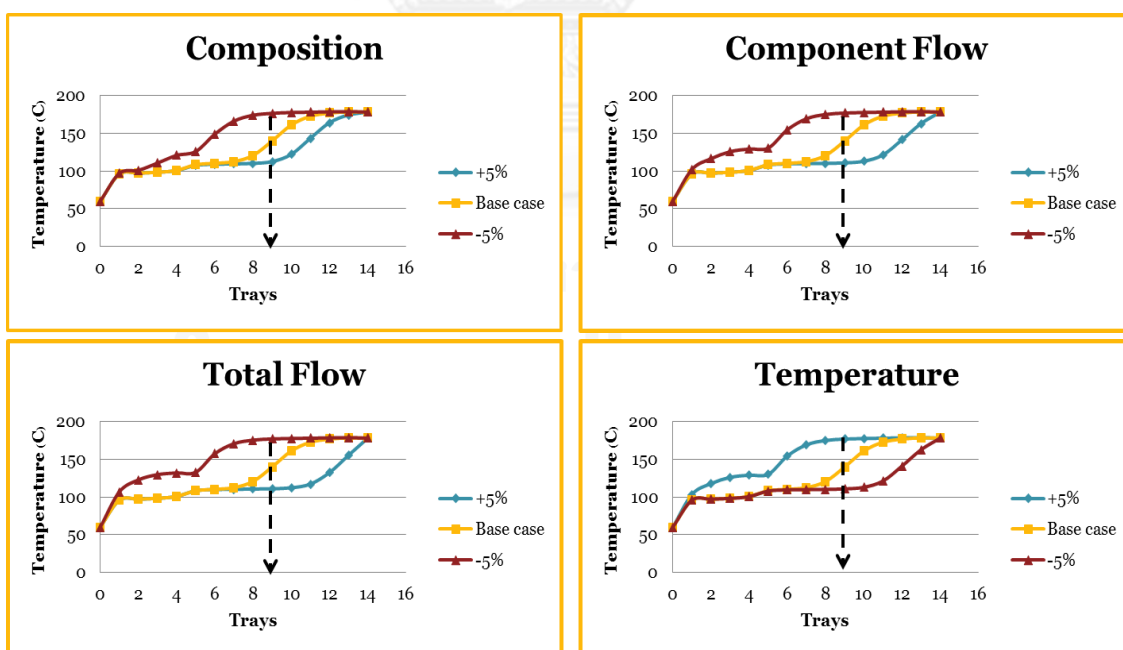


Figure 5.6 Selecting temperature control tray location of C1 by keeping the reboiler heat duty (Q_r) and reflux.

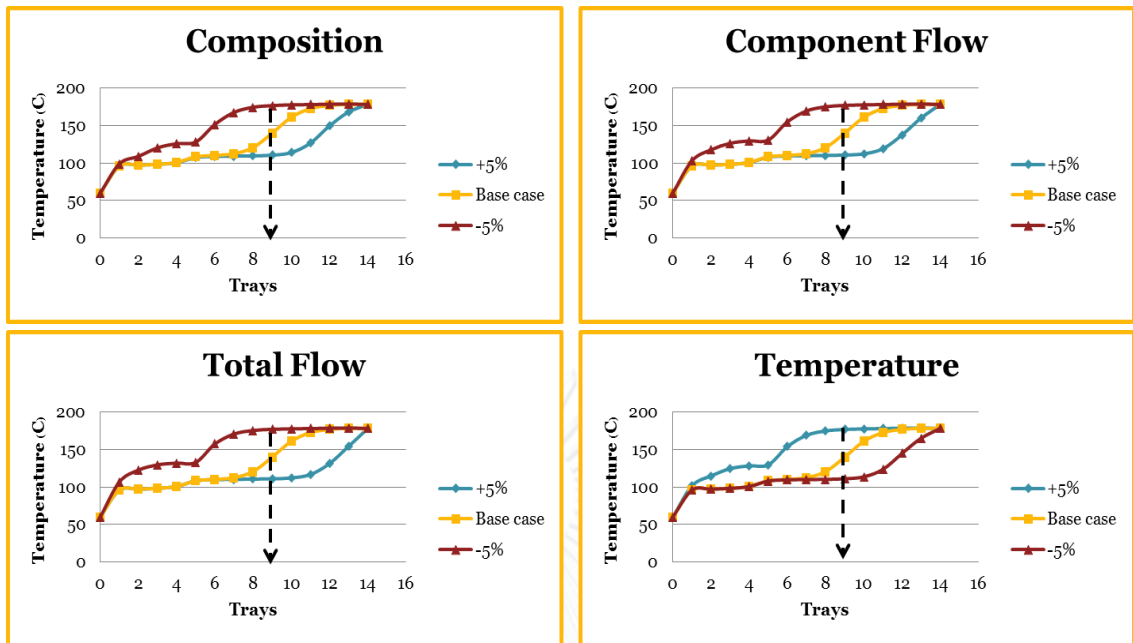


Figure 5.7 Selecting temperature control tray location of C1 by keeping the reboiler heat duty (Q_r) and reflux ratio.

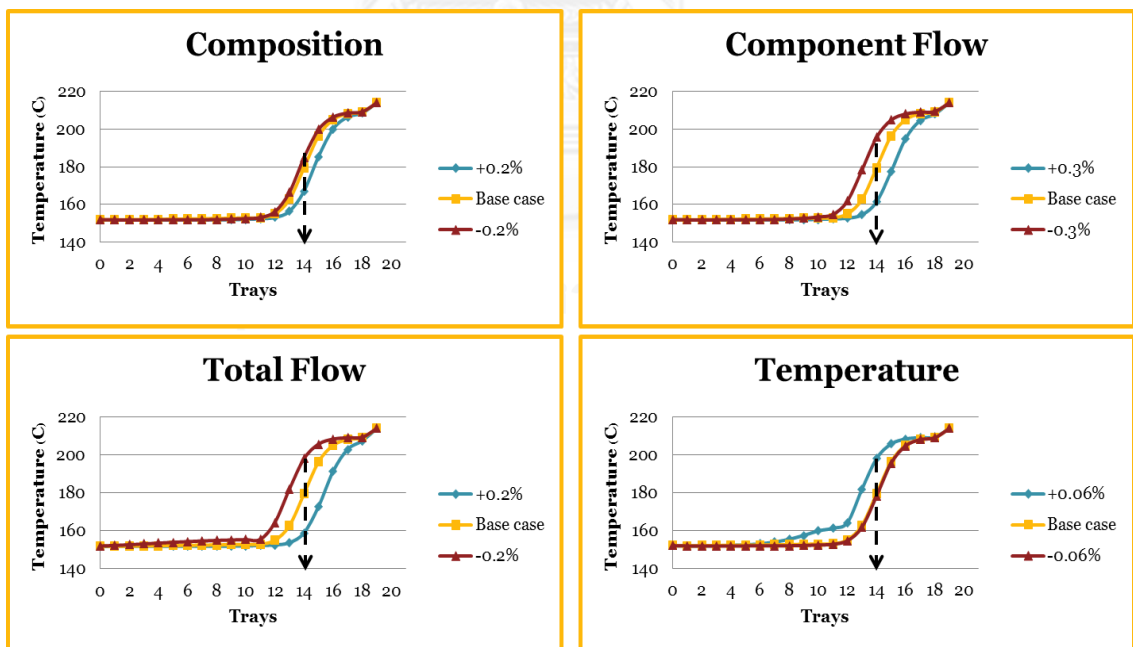


Figure 5.8 Selecting temperature control tray location of C2 by keeping the reboiler heat duty (Q_r) and reflux.

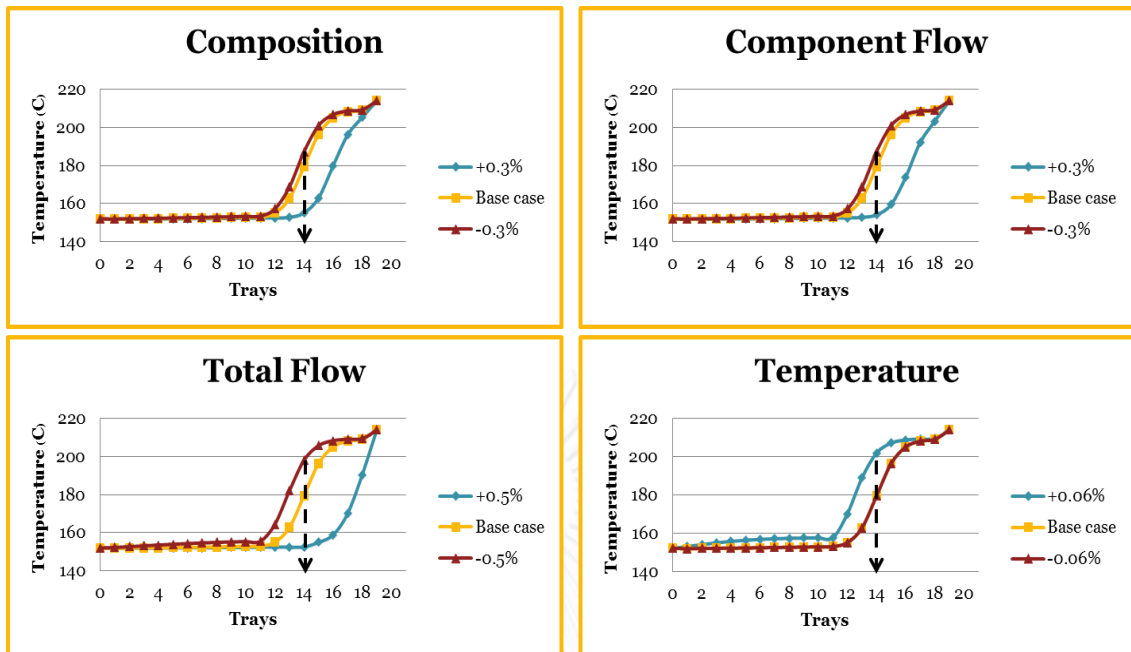


Figure 5.9 Selecting temperature control tray location of C2 by keeping the reboiler heat duty (Q_r) and reflux ratio.

2.7 Mode of operation: On-supply

Figure 5.10 shows control structure design of the on-supply structure. The primary pathway is a path that affected to the production rate of the process. Throughput manipulator (TPM) is fixed at the fresh feed stream of mixed C3. The inventory of the on-supply structure should be controlled in the direction to flow that it is controlled at the exit of each unit operation.

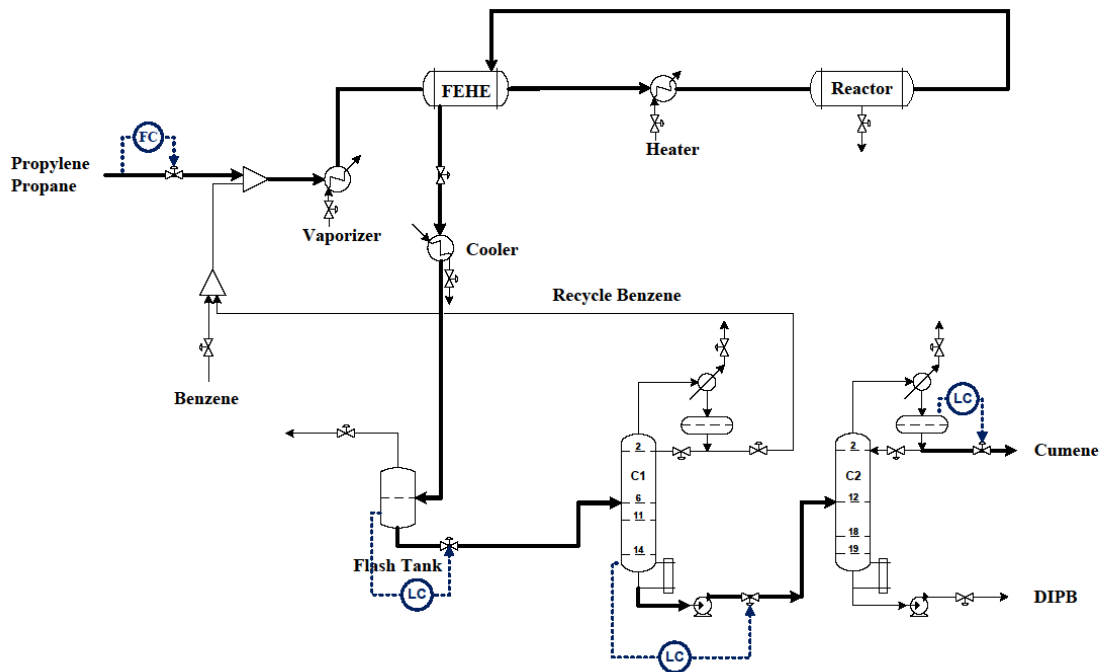


Figure 5.10 On supply design structure

2.8 Production rate control

The production rate control is set at the fresh feed flow of mixed C3 control loop as On-supply mode.

Stage 2 Fixture Plant and Disturbance Management

Step 3: Establish fixture plant

Creating a material balances in an entire plant by regulate the amount of each component at its quantifier.

3.1 Keep the materials entered and reentered fixed

The raw materials were very important for demand production. The fresh feed of mixed C3 and total benzene is fixed flow rate. The flow rate of the fresh feed stream fed to the process must be controlled by adjusting their flow rate. Figure 5.11 shown the position of control loops are controlled which includes the fresh feed of mixed C3 and total benzene. They are fixed to maintain the flow rate into the process. The flow rate of the fresh feed of mixed C3 stream is controlled by

manipulating flow rate of mixed C3 at valve to maintain the flow rate. The benzene fresh feed and the benzene recycles, entered and reentered benzene, are regulated by measuring their combined flow (benzene quantifier) and adjusting benzene fresh feed (benzene handler).

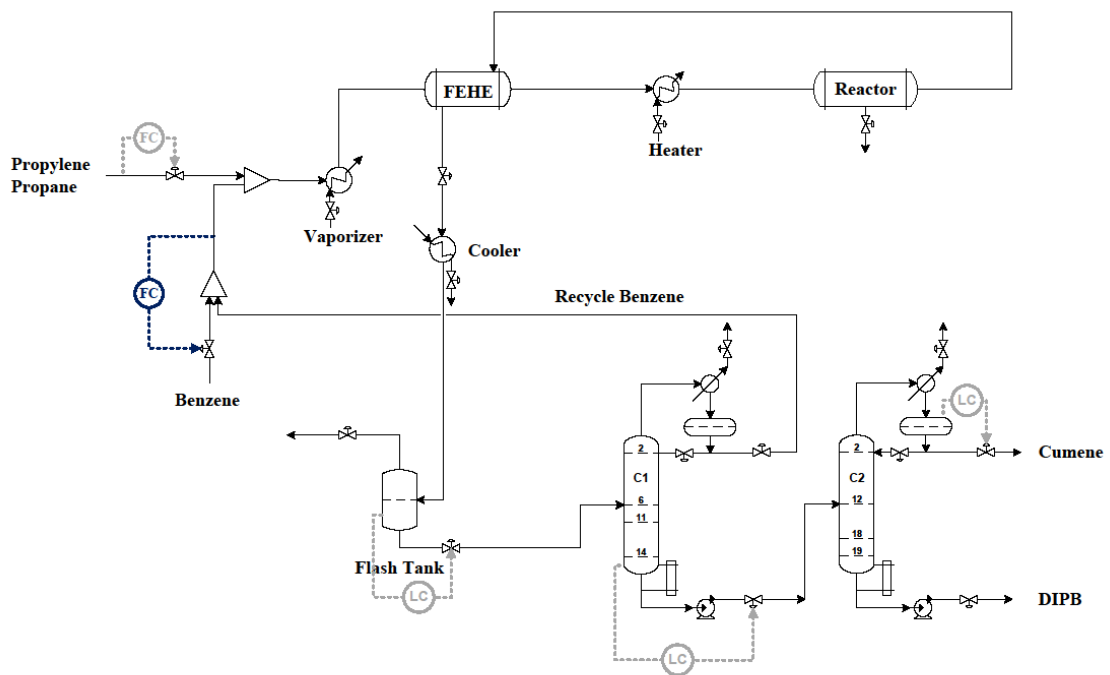


Figure 5.11 Keep the materials entered of cumene process

3.2 Adjust the flow of exit material streams (products, byproducts, and inert) according to their accumulations

There are three exit material streams, namely cumene, DIPB and propane, are regulated at their quantifiers. The amount of cumene at its quantifier is controlled by adjusting its handler, C2 distillate flow. DIPB is regulated by adjusting its handler, C2 bottoms flow. Propane is regulated by adjusting its handler, the gas stream flow rate. This step is shown in Figure 5.12.

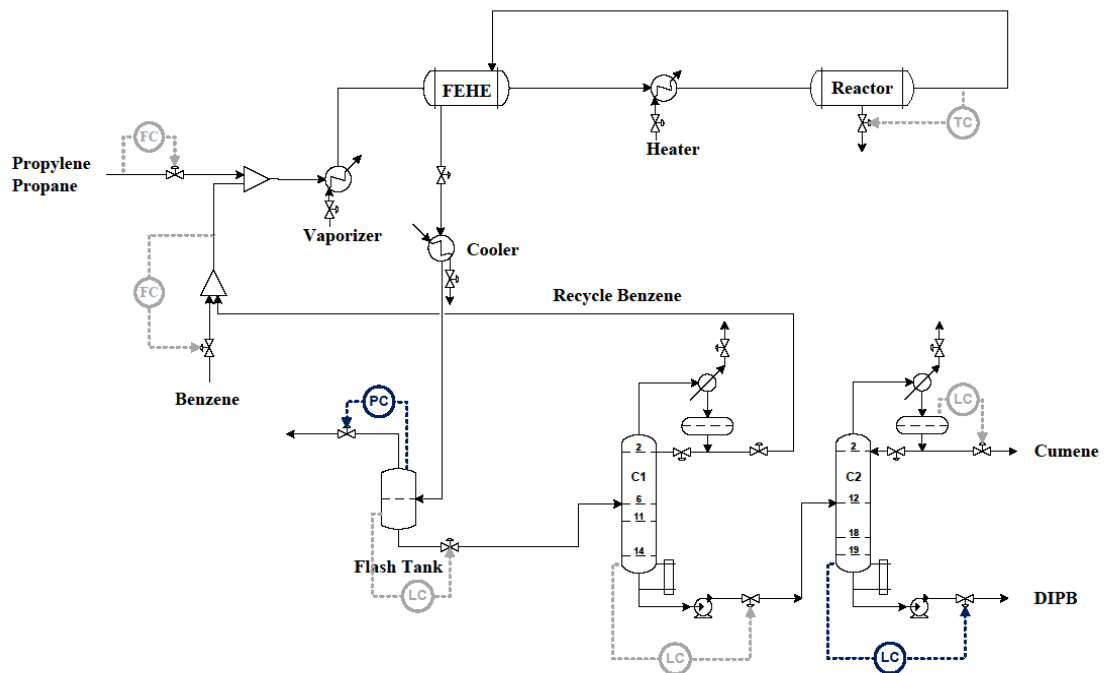


Figure 5.12 Adjust the flow of exit material streams

3.3 Handling the material that is not leaving the process

There is no component not leaving the process so we will not consider this step.

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

There is no the rest of the component in the process. All components are considered in 3.1 and 3.2 so we will not consider this step.

3.5 Maintain the production rate

To maintain the production rate, the cumene in reactor effluence is monitored and control by adjusting the reactor temperature. This step is shown in Figure 5.13.

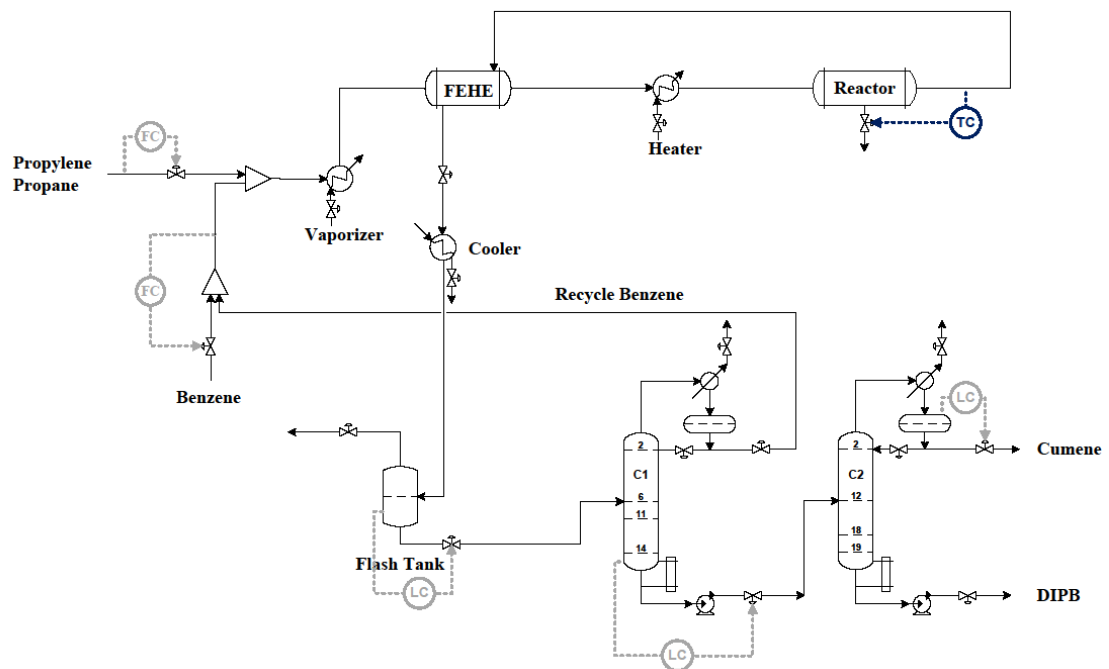


Figure 5.13 Maintain the production rate

Step 4: Disturbance management for quality control

4.1 Heat disturbance management

According to the analysis made in Step 2.2, the temperatures of the stream going out of the vaporizer and cooler, the stream entering the reactor and the stream leaving the reactor must be maintained by rejecting the heat disturbances to the environment.

4.1.1 The thermal disturbance entering the vaporizer is compensated by the vaporizer heating duty. The temperature of the vapor leaving the vaporizer is controlled by adjusting the duty. The temperature of the reactor feed must be maintained at 358 °C by the heater. Also the temperature of flash tank feed must be at 85 °C as shown in Figure 5.14.

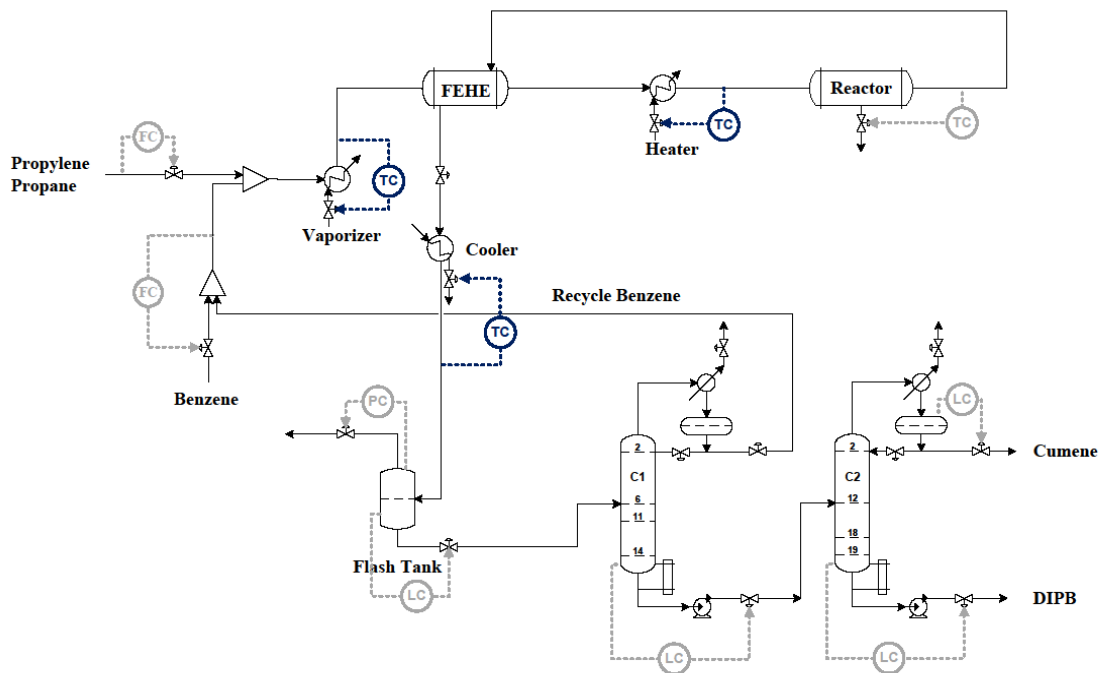


Figure 5.14 Direct the heat disturbances that are not directly related to quality

4.1.2 The temperature of reactor effluent is controlled by manipulating the heat removal in reactor. The column temperature at tray 9th of benzene column C1 and tray 14th of cumene column C2 are handled by manipulating the column reboiler duties as shown in Figure 5.15.

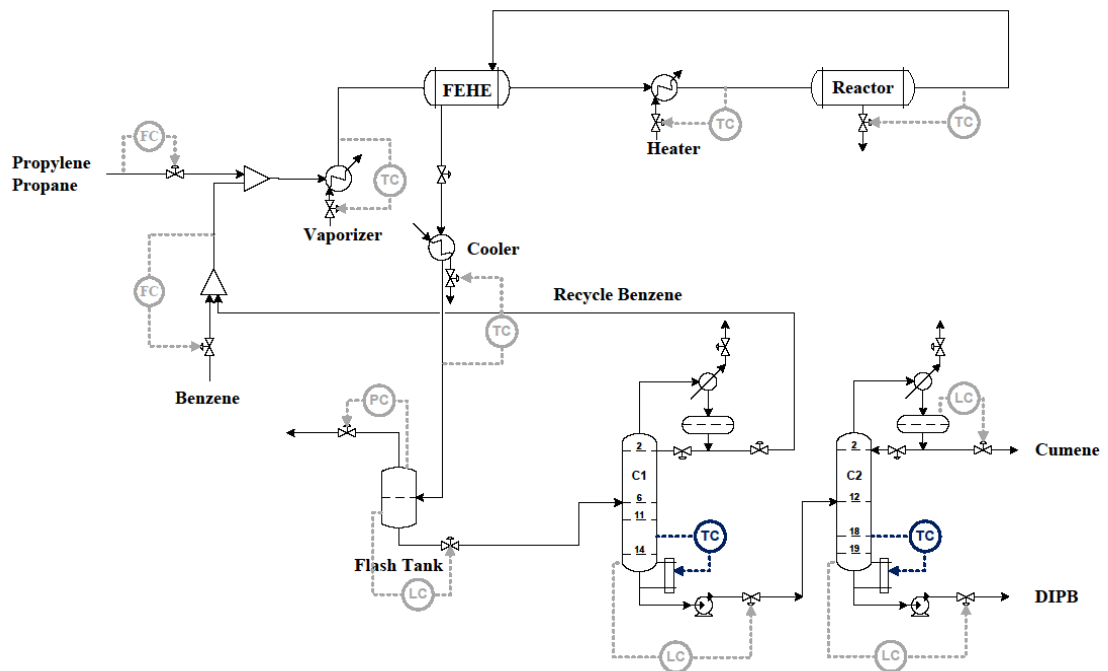
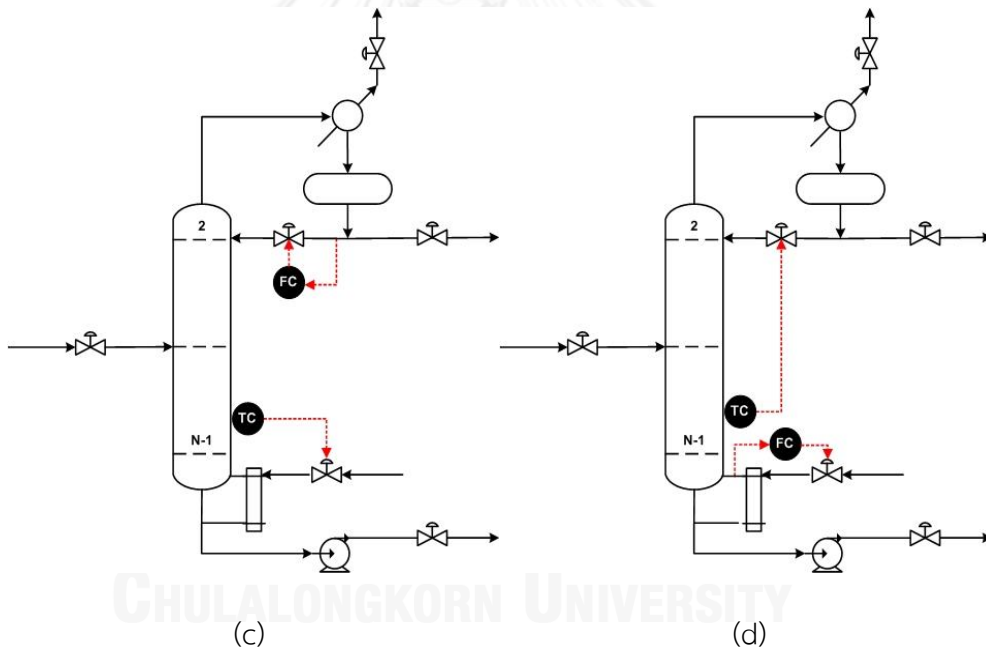
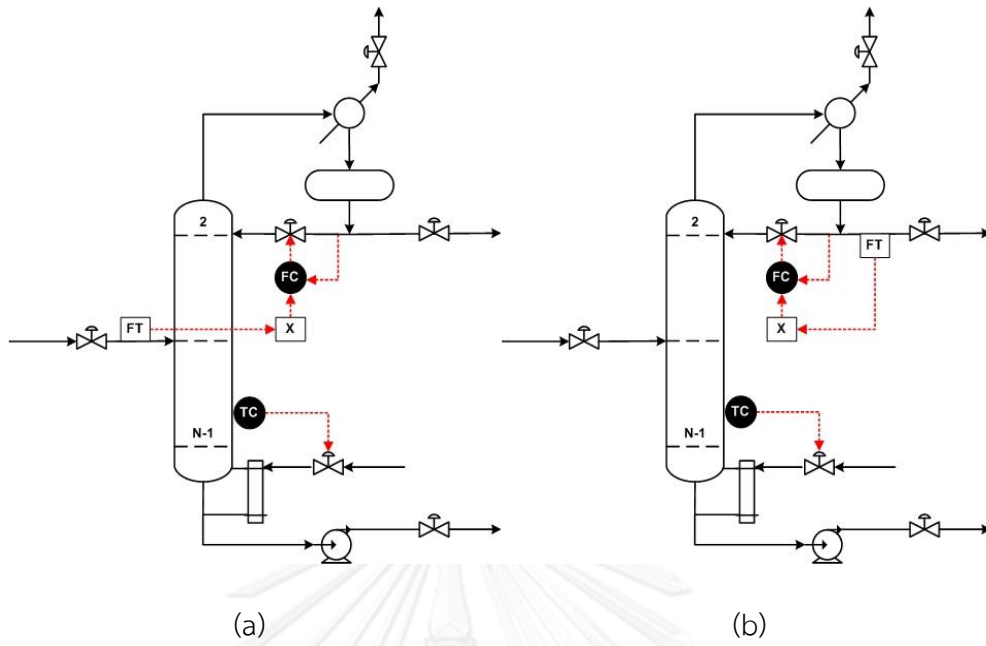


Figure 5.15 The heat disturbance that related to quality in order to maintain the product constraints

4.2 Material disturbance management

The direct of material disturbances should reject to the environment via the nearest exit points to avoid disturbance recycle into the process.

Testing the several disturbances is made to identify control structure to achieve the desired material disturbance shifting directions made in Section 2.6. Five single temperature control structures, namely, R, RR, R/F, R/(R+D) and V are proposed to regulate the material disturbances as shown in Figure 5.16.



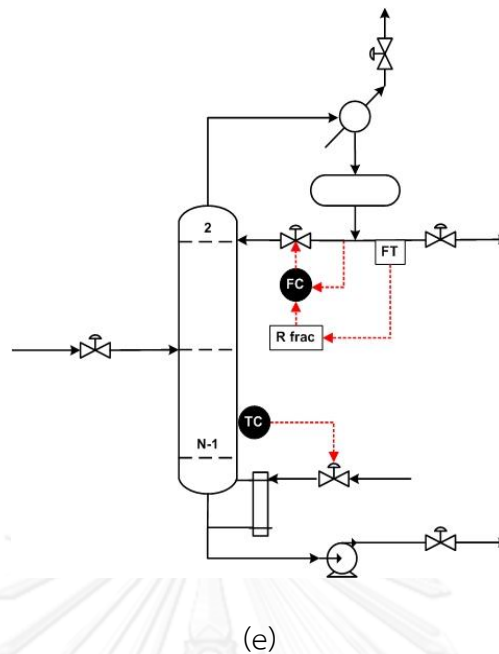


Figure 5.16 The control structure for handle disturbances in separation section

Several disturbance tests are made to identify control structure to achieve the desired material disturbance shifting directions made in Section 2.6. Five single temperature control structures, namely R, R/D, R/F, R/(R+D) and V are proposed.

In order to find which structures yield the design shifting, we run dynamic simulation tests for changes in feed component (light and heavy keys) flow and feed composition (light and heavy keys) that they are introduced to both columns. In addition the effects of feed flow rate and feed temperature changes on column product purities are considered. The responses are shown in Figure 5.17-5.26.

Column C1

For change in benzene feed flow, All structures can maintain impurity of benzene in the bottom stream since we want to maintain purity of product in this stream. As for benzene composition in distillate, V structure is the best performance structure to maintain benzene composition in distillate stream. In addition, reboiler heat duty of R structure can maintain the nearest steady state value while R/F, RR and R/(R+D) are minor structures.

For change in cumene feed flow, since we want to shift the plus and minus disturbance of cumene to the bottom for maintaining cumene composition in distillate. For this reason, V structure is not suitable to be used in the benzene column C1. As for reboiler heat duty of R, RR and R/(R+D) structures, they can maintain reboiler heat duty nearest the steady state value.

For change in benzene composition in feed, R, R/F, RR and R/(R+D) structures are the best structure in term of maintain cumene composition in distillate stream but RR and R/(R+D) structures are the best structure to maintain cumene component flow in distillate stream at their steady state value.

For change in temperature feed, the composition of cumene in distillate (x_{D1}) result shows that R, R/F, RR and R/(R+D) are the best structure to keep impurity of cumene in distillate stream.

For change in total feed, R, R/F, RR and R/(R+D) are the best performance to regulate impurity of cumene in distillate stream. While R structure can maintain impurity of cumene in D1 worse than R/F, RR and R/(R+D) structures.

For all disturbance tests in the benzene column C1, structures are chosen for use in benzene column C1 as R/F, RR and R/(R+D) structures. Since the initial response of RR and R/(R+D) structures are smoother than R/F structure so RR and R/(R+D) structures are the best candidates for C1 disturbance management but RR and R/(R+D) structures give all same results. So we choose RR structure for use in this design.

Figure 5.17 Column dynamic results for $\pm 10\%$ changes of benzene component feed flow.

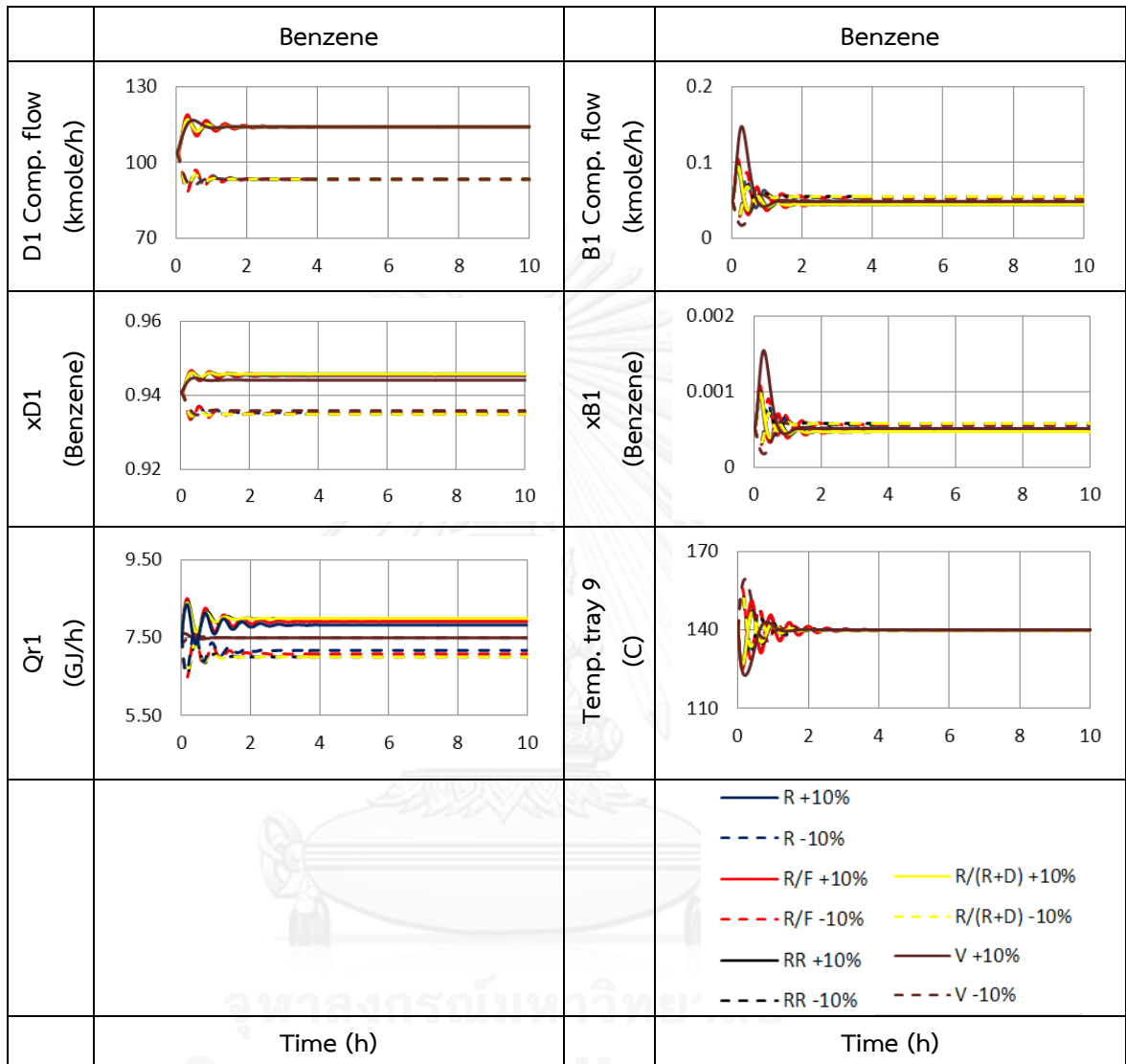


Figure 5.18 Column dynamic results for $\pm 10\%$ changes of Cumene component feed flow.

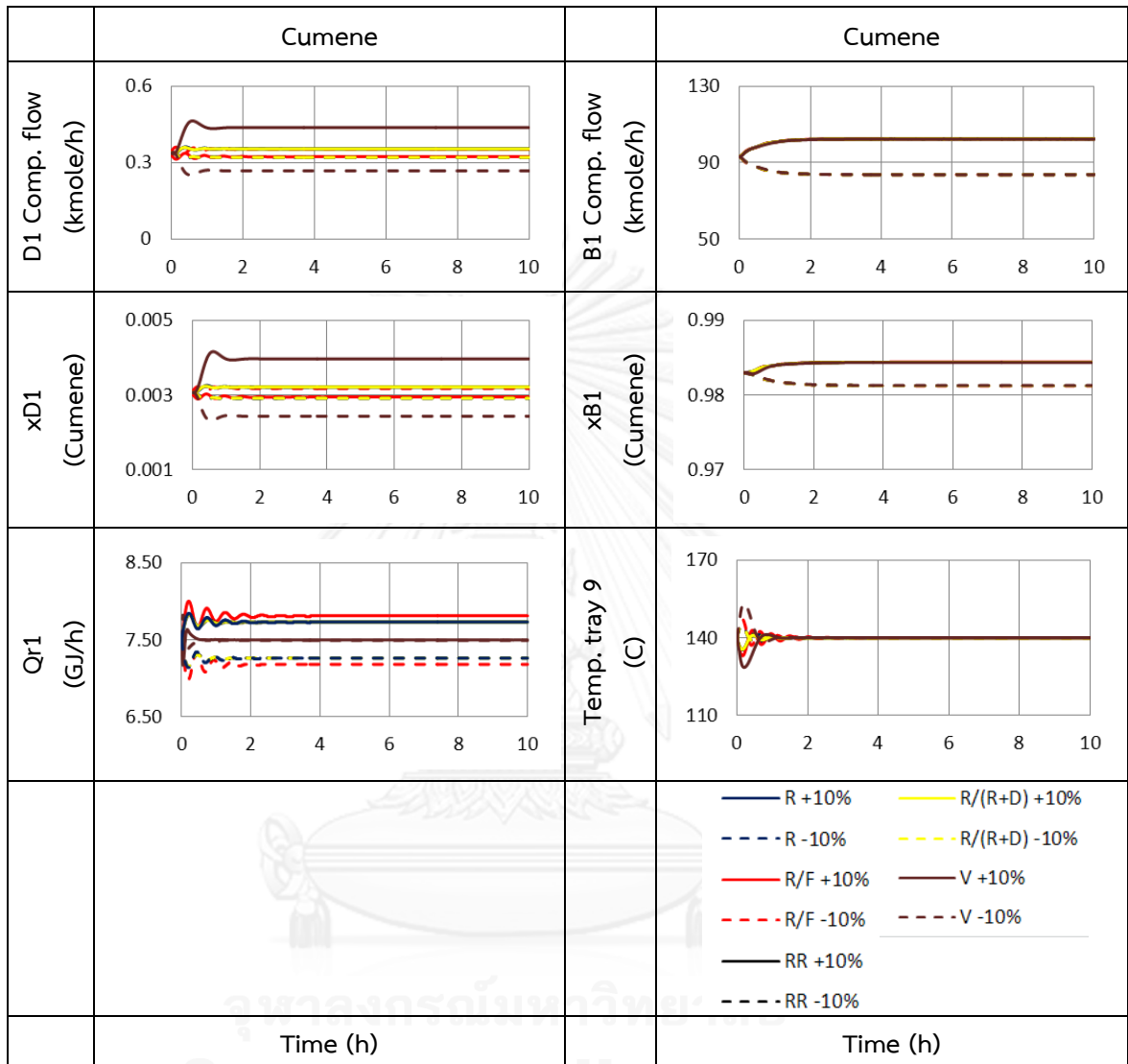


Figure 5.19 Column C1 dynamic results for ± 5 mole % benzene changes in column feed

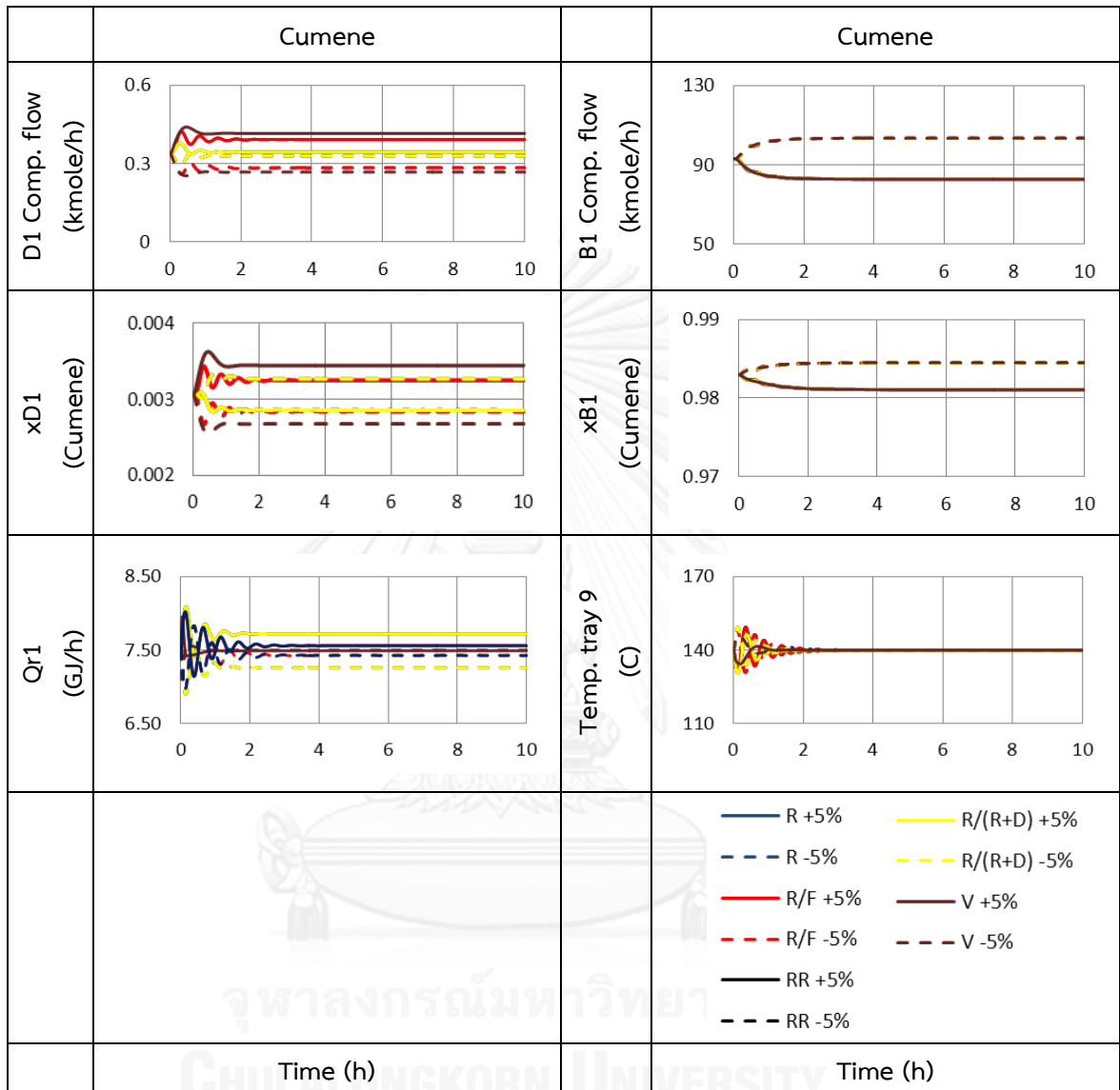


Figure 5.20 Column C1 dynamic results for $\pm 10\%$ temperature changes in column feed

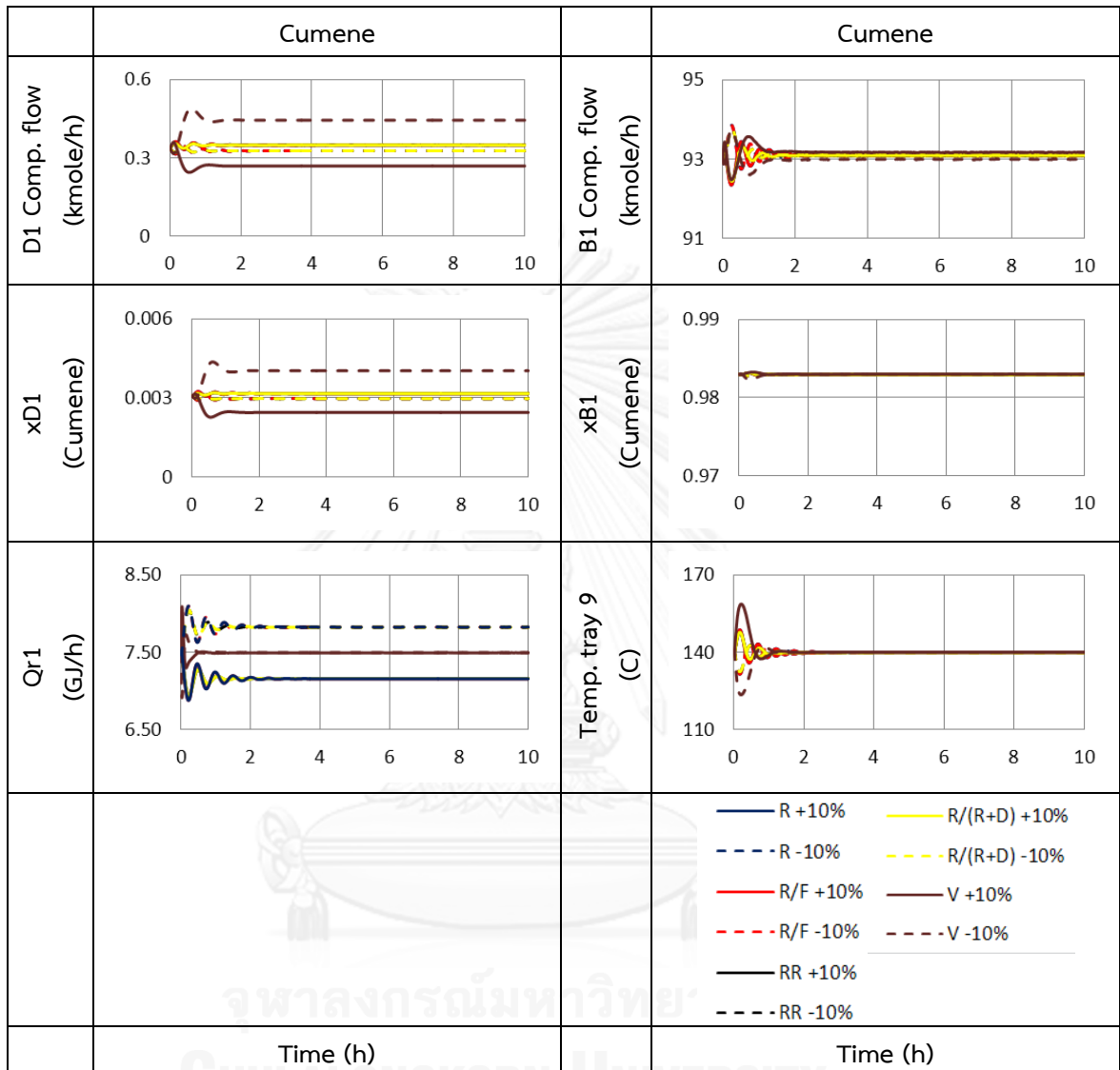
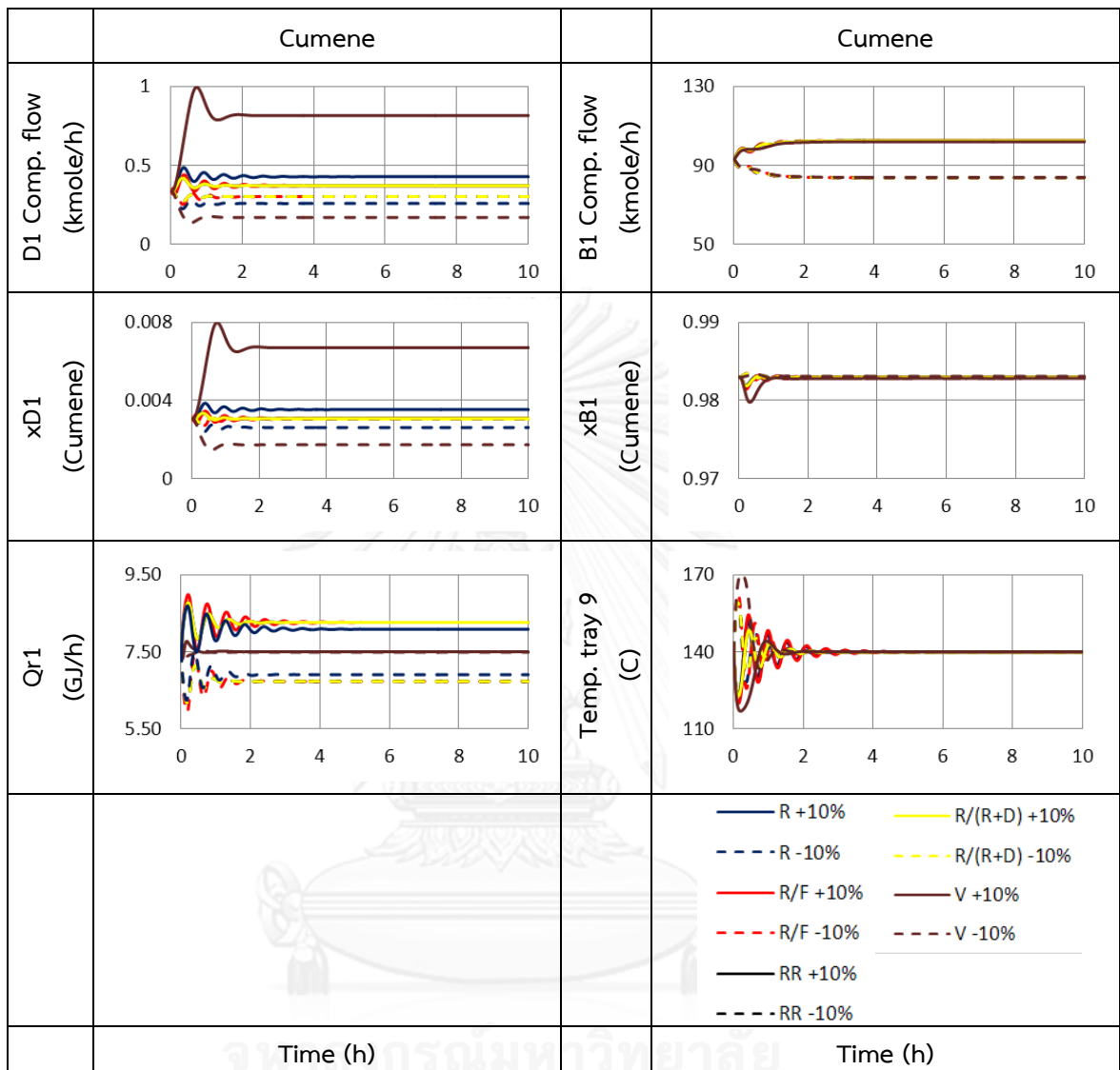


Figure 5.21 Column C1 dynamic results for $\pm 10\%$ total flow changes in column feed

Column C2

For change in cumene feed flow, All structures give the plus disturbance shifting to the distillate stream whereas no structures can shift the minus disturbance to the bottom stream due to limit in the column design and the availability of cumene in bottom. However, R and R/F structures give the best performance to maintain reboiler duty at the specified value.

For change in DIPB feed flow, we want to shift the plus and minus disturbance of DIPB to the bottom for maintaining purity of cumene in distillate. All structures can shift plus and minus disturbance to the bottom. However, R, RR and R/(R+D) structures obviously used less reboiler duty.

For change in cumene composition in feed, all structures are the best performance to keep purity of cumene in bottom. However, R and R/F structure can maintain reboiler duty nearest the steady state value.

For change in temperature feed, V structure cannot keep impurity of DIPB in the product stream while R, R/F, RR and R/(R+D) structures can maintain impurity of DIPB in the product stream.

For change in total feed, V and R structure cannot maintain impurity of DIPB in the product stream. So this disturbance test, we choose R/F, RR and R/(R+D) structures.

For all disturbance tests in the cumene column C2, we have the 3 candidates for C2 column, R/F, RR and R/(R+D) structures. The RR structure is selected because it gives the fast response in all case.

Figure 5.22 Column dynamic results for $\pm 10\%$ changes of cumene component feed flow.

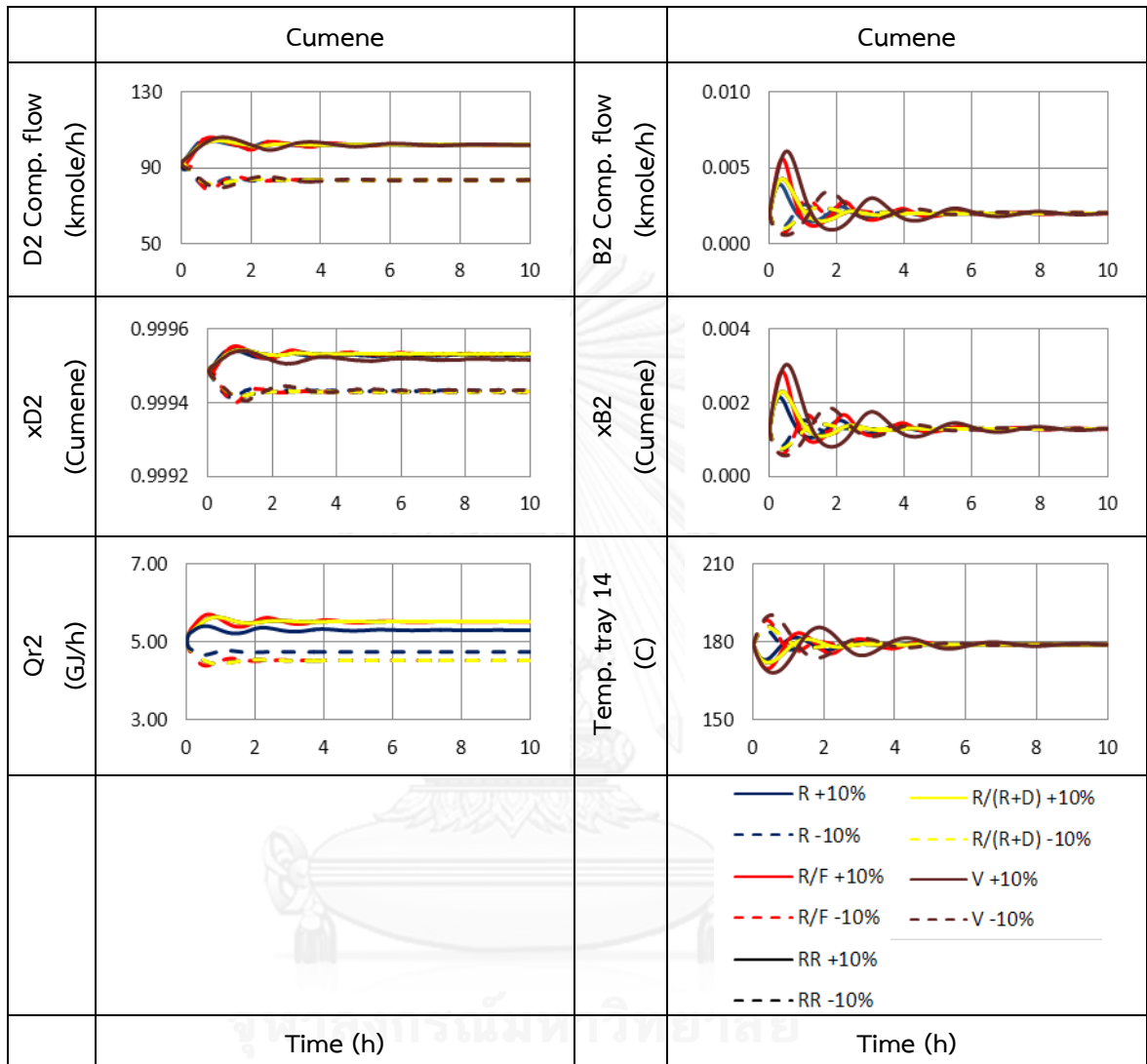


Figure 5.23 Column dynamic results for $\pm 10\%$ changes of DIPB component feed flow.

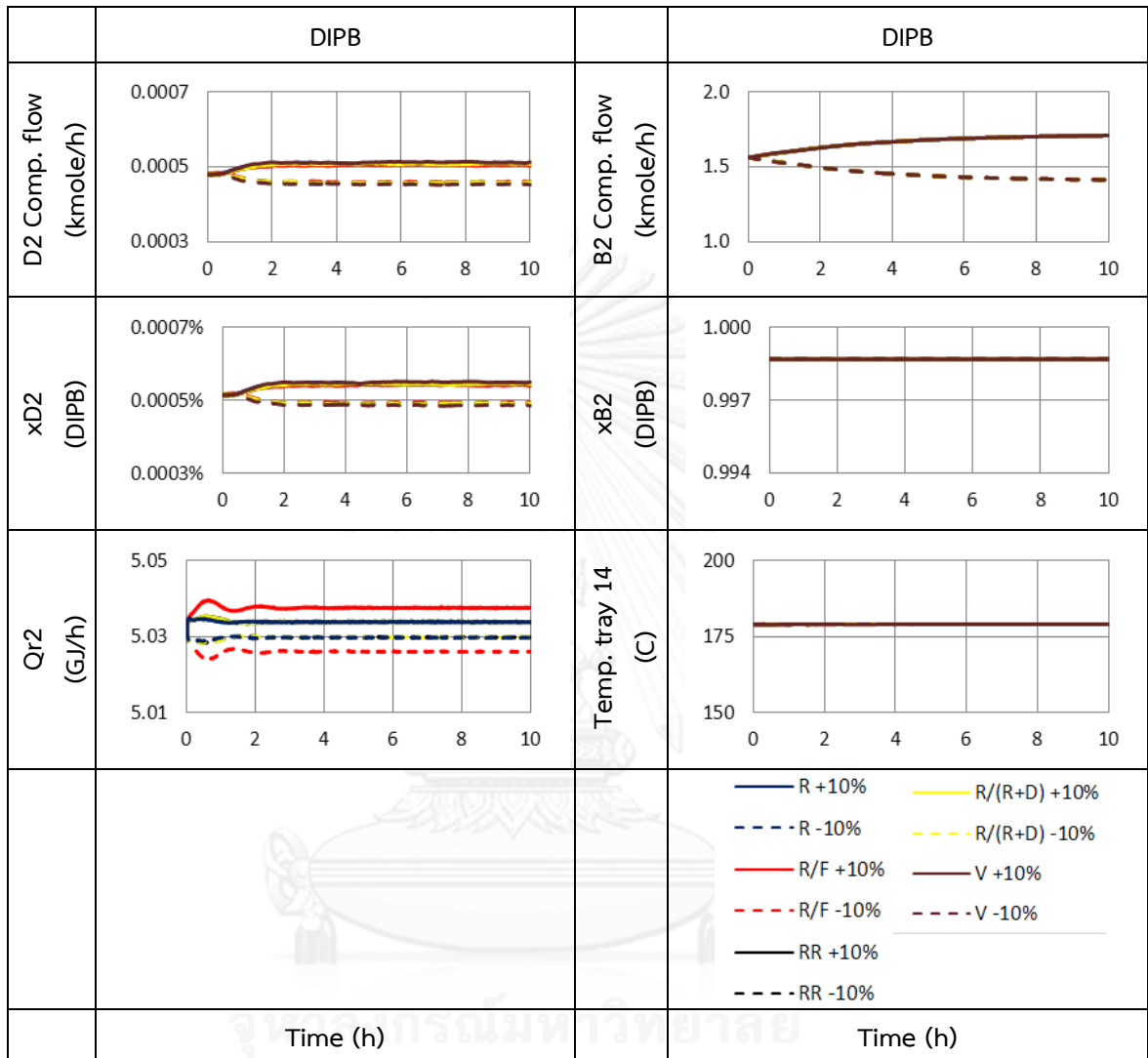


Figure 5.24 Column C2 dynamic results for ± 2 mole % cumene changes in column feed

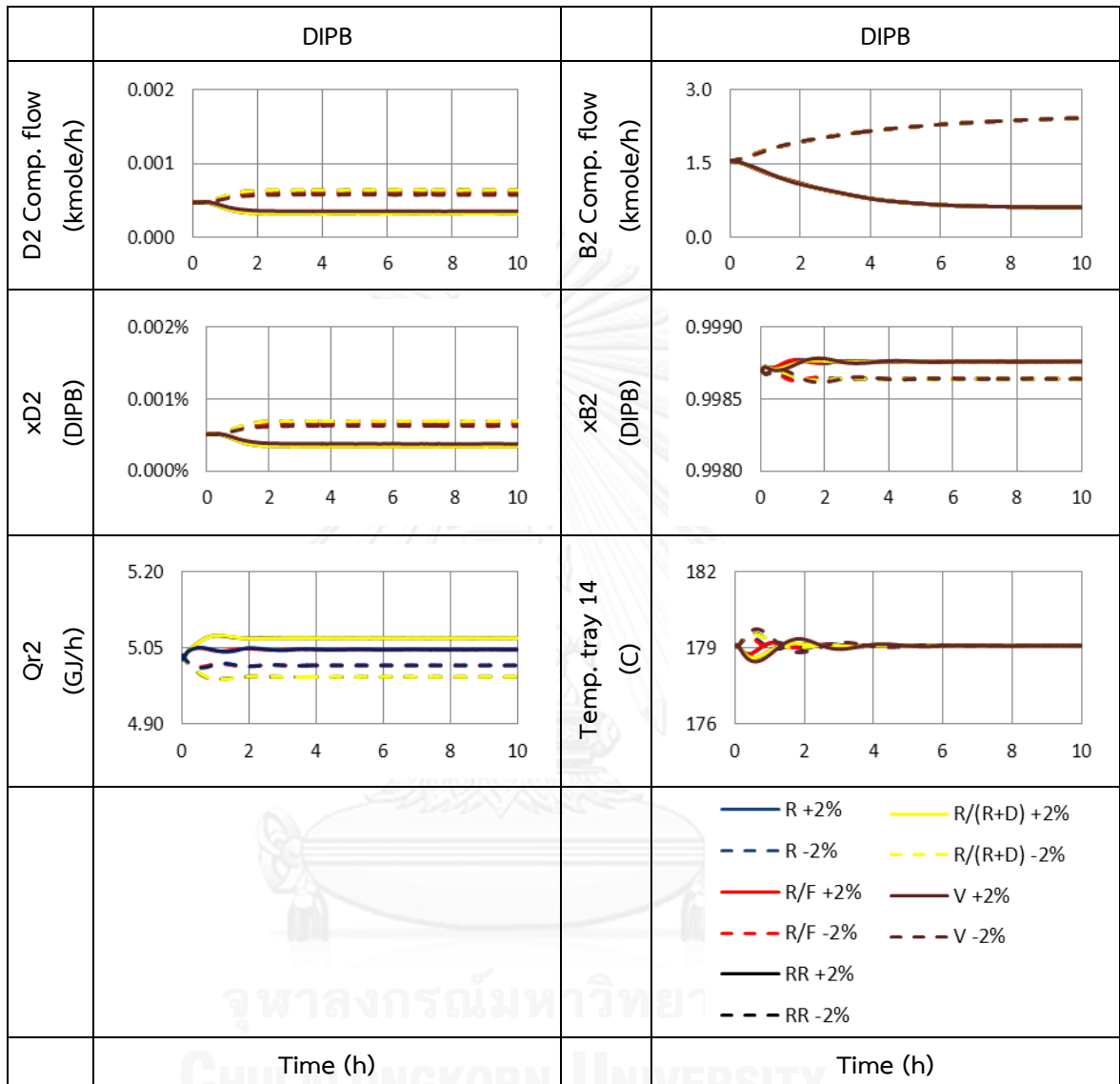


Figure 5.25 Column C2 dynamic results for $\pm 10\%$ temperature changes in column feed

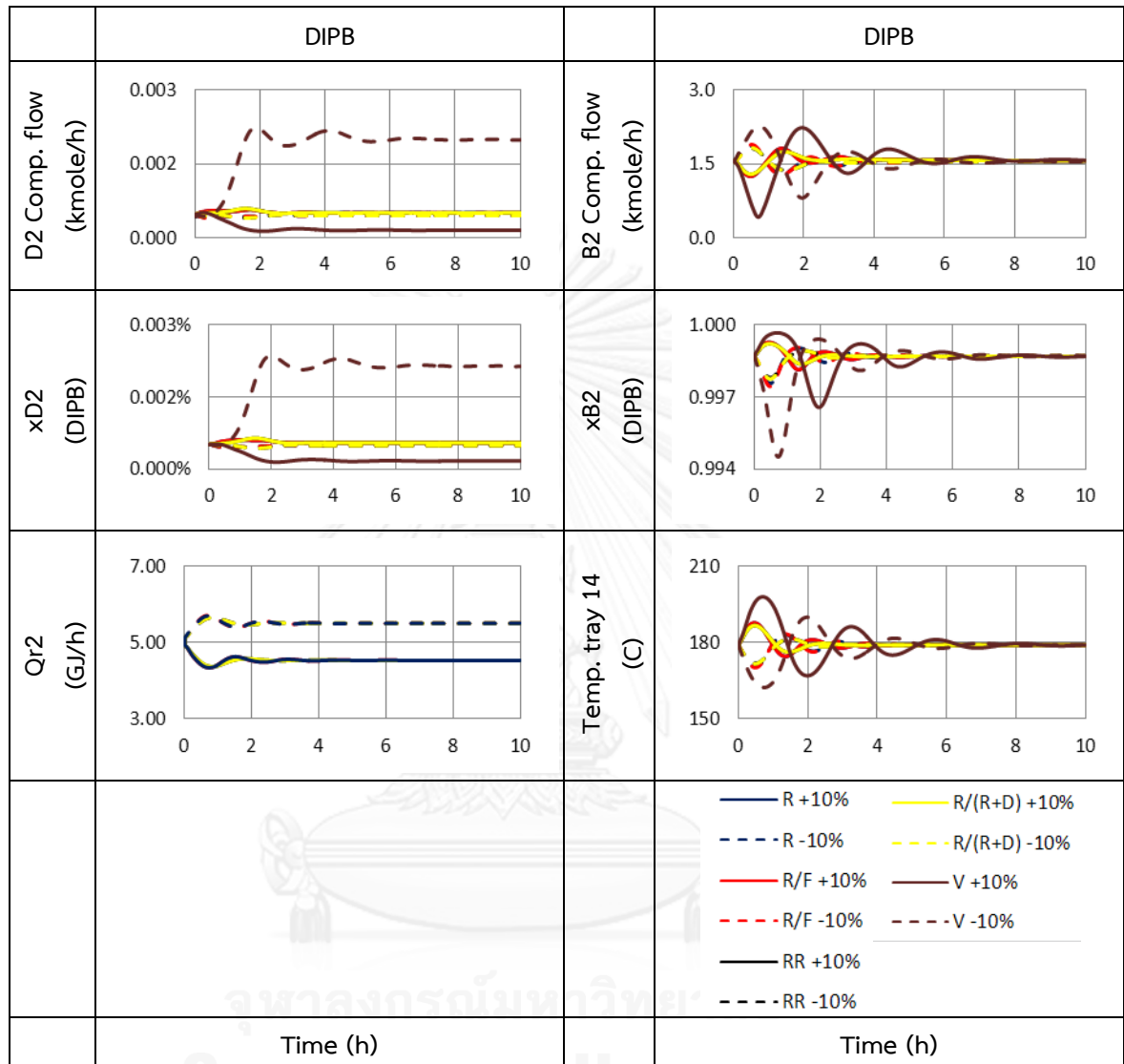
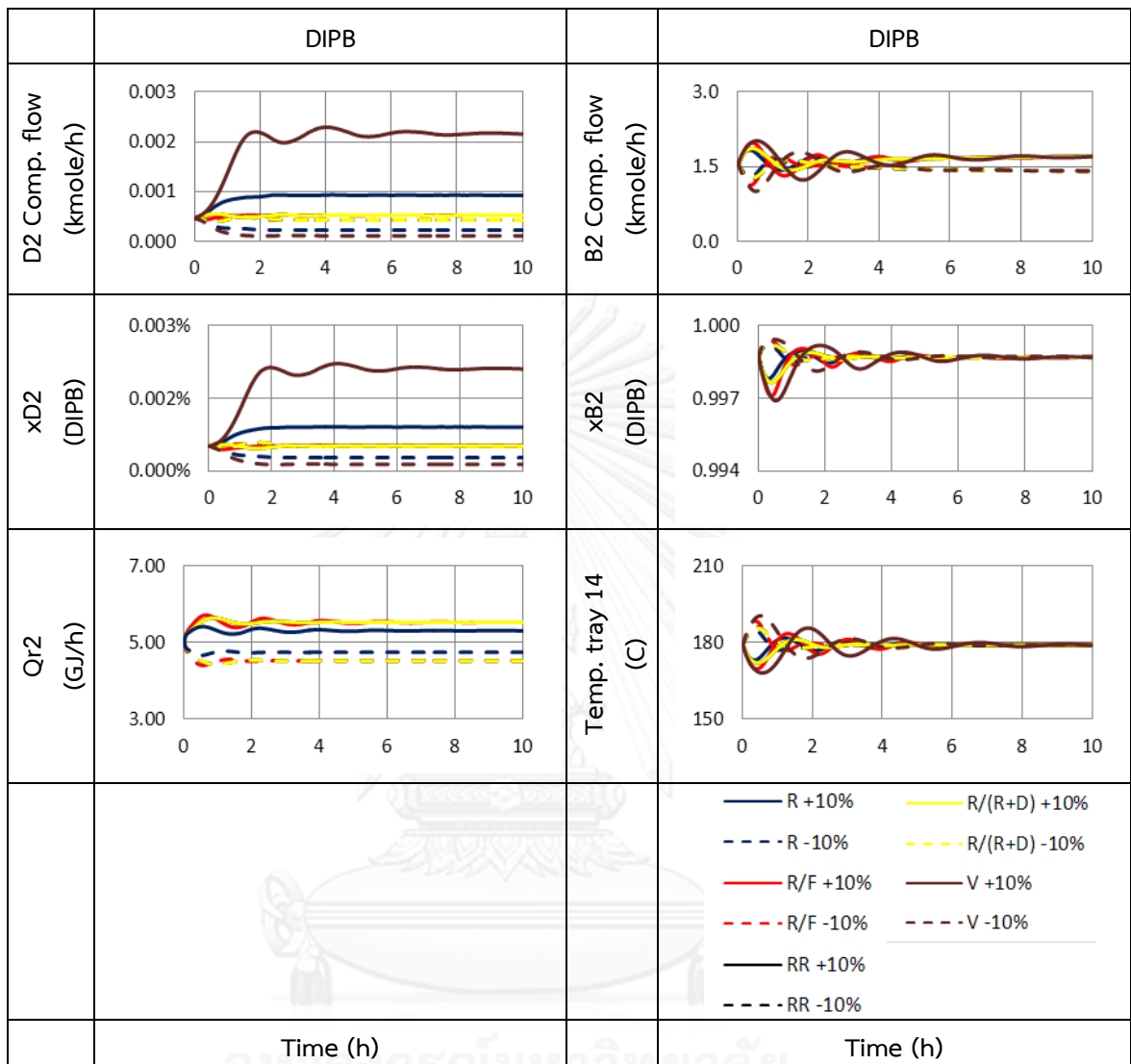


Figure 5.26 Column C2 dynamic results for $\pm 10\%$ total flow changes in column feed

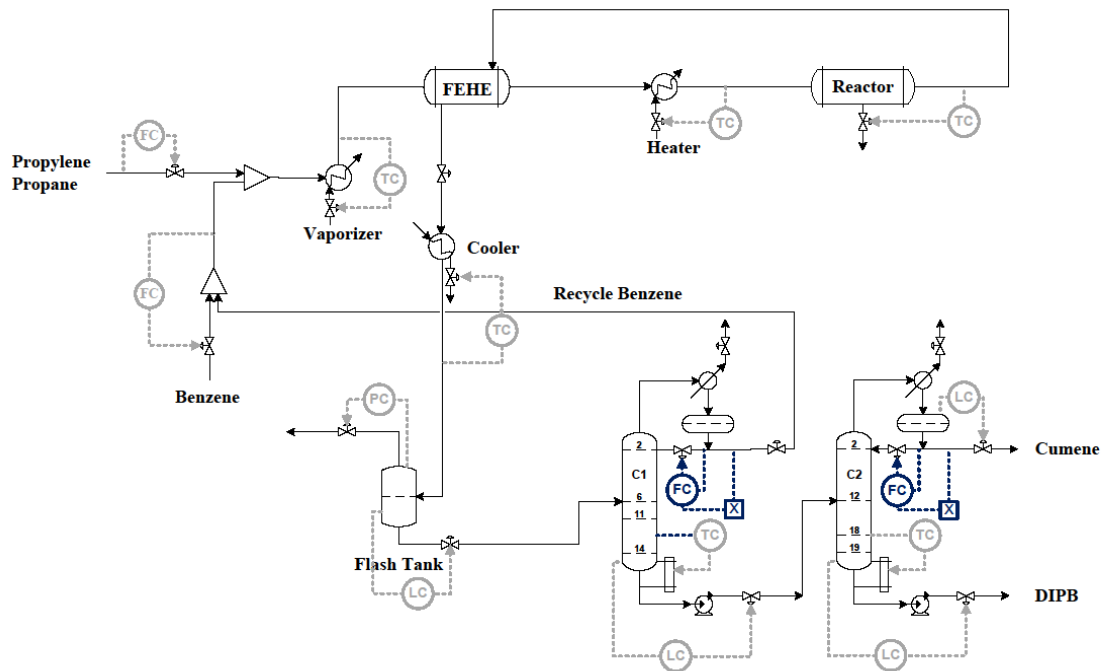


Figure 5.27 Material disturbance structure

Stage 3 Unit Level Designs

Control loop design at this stage is solely based on individual unit operations.

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 inventory

The units left to be considered in this step are a pressure reduced valve unit on an FEHE exit stream, column C1 for its liquid and vapor inventory and column C2 for its vapor inventory. The pressure of FEHE exit stream is regulated by its pressure. C1 condenser level is regulated by C1 distillate flow. C1 pressure is handled by C1 condenser cooling duty. C2 pressure is controlled by C2 condenser cooling duty. Please note that C2 liquid inventories are utilized in Step 3.2. The control loops obtained in this step are shown in Figure 5.28.

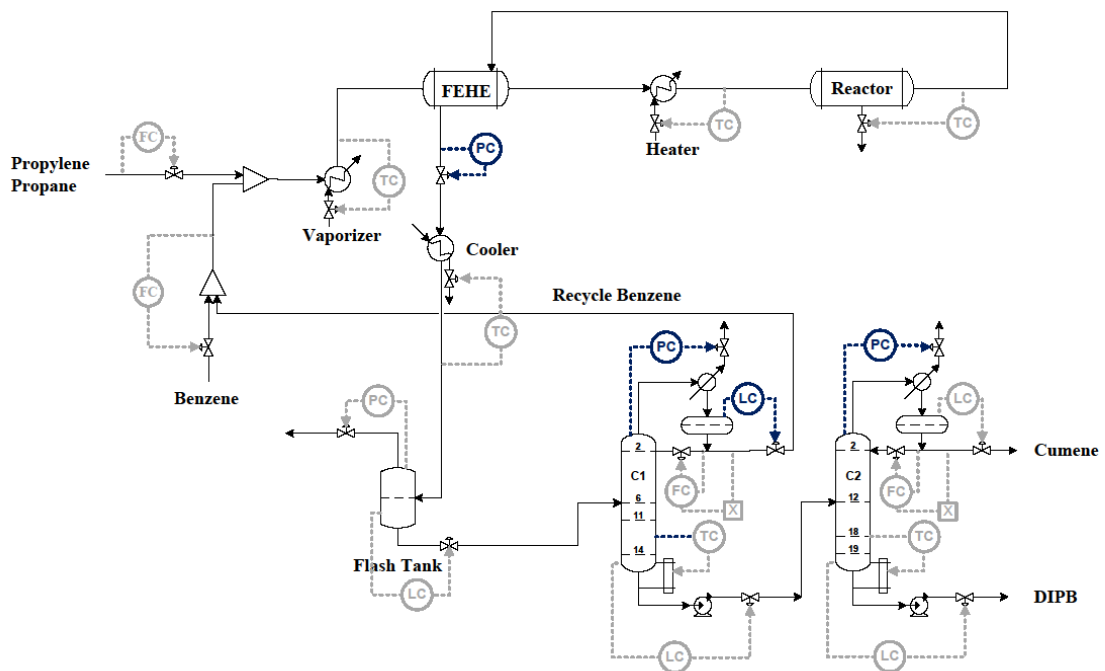


Figure 5.28 The control loops for the remaining control variables

5.2 Adding simple enhanced controls, e.g. cascade, feed forward controls

The mixed C3 feed and total benzene flow must be ratioed to 0.49 as required. The ratio controller is added by adjusting the setpoint of the total benzene controller.

The utilization of propylene at reactor should be regulated to ensure that its fraction in reactor effluent is regulated throughout the operation period despite catalyst deactivation. The propylene composition is measured and sent to a cascade controller to adjust the setpoint of reactor temperature loop. The entire control loops designed above to this point setup control structure 1 (CS1).

The other consideration to be made is the design specification which is to attain high-purity cumene in the distillate and minimize the loss of cumene in the bottoms. To be ensured that high purity cumene product is attained, the benzene concentration in C1 bottoms must be maintained at 0.05 mol%. The benzene concentration in B1 is controlled by adding a cascade control on C1 bottom temperature loop. The high purity cumene is assured by monitor the DIPB amount in cumene product and adjust C2 reboiler loop. This two enhanced loops added constitutes control structure 2 (CS2).

Instead of adjusting C2 reboiler loop of the second added loop, another alternative is to adjust C2 reflux flow. In this option, the output of DIPB controller is sent to the setpoint of reflux ratio control loop. This establishes control structure 3 (CS3). This step is shown in Figure 5.29-5.31.

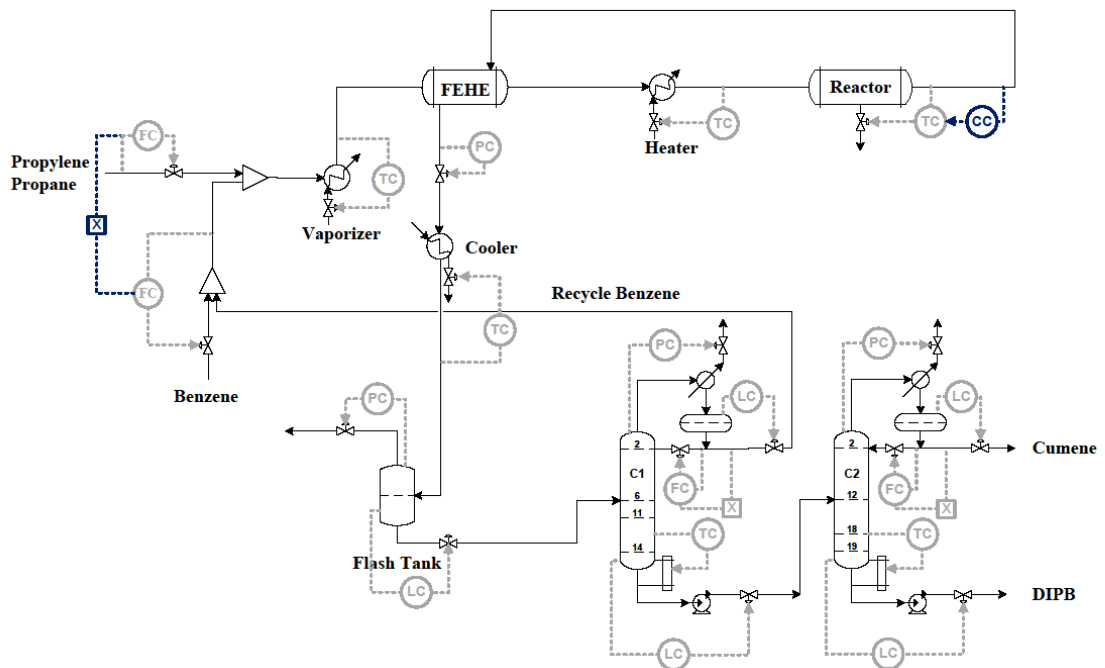


Figure 5.29 Enhanced control structure 1 (CS1)

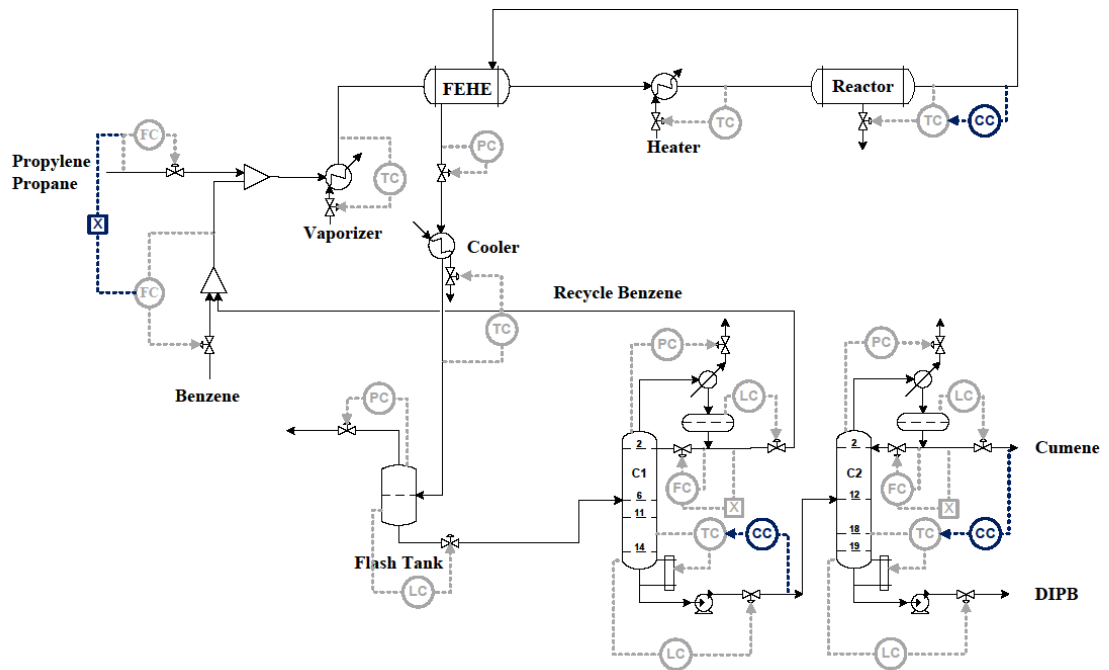


Figure 5.30 Enhanced control structure 2 (CS2)

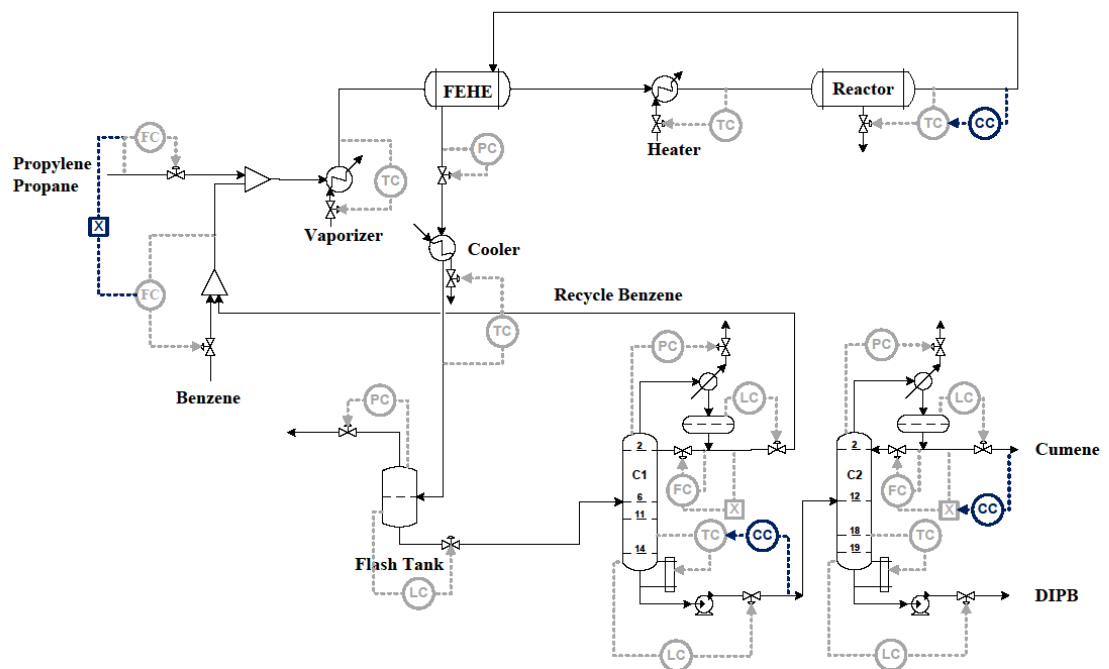


Figure 5.31 Enhanced control structure 3 (CS3)

Stage 4 Energy Management and Optimization

The supplementary design activities involve heat exchanger network design and control, and plant operation and design optimization.

Step 6: Energy management via heat exchanger networks

In this step is not considered because there is no alternative heat integrated processes available in the cumene process.

Step 7: Optimize economics or improve control performance

The design in this step is omitted due to the scope of study.

Stage 5 Design Validation

The validation of the design control structures using rigorous nonlinear simulation is inevitable; whatever may be the design procedure.

Step 8: Validate the designed control structures by rigorous dynamic simulation via HYSYS process simulation software

The measures would be costs, raw material and energy consumptions, control performances of the total plant or some selected loops, etc. Expected disturbances must be listed to perform the disturbance test on the plant with designed control structures.

Figure 5.33-5.35 shows the plantwide control structure developed for cumene process by using Wongsri's design procedure. The PID controllers are used in temperature loops. The PI controllers are used in flow rate and pressure loops and P controllers are used in level loops. The various loops are listed below with their controlled and manipulated variables.

1. The fresh feed of mixed C3 stream is flow controlled at the throughput handle.
2. The total benzene, fresh feed benzene stream combine with benzene recycle stream from the benzene distillation column C1, is ratioed with the fresh feed of

mixed C3 stream. The total benzene stream is flow controlled by manipulating flow rate at the fresh feed benzene.

3. The temperature of vaporizer is controlled by manipulating heat input.
4. The inlet temperature of tubular reactor is controlled by manipulating heat input in the heater.
5. The exit temperature of tubular reactor is controlled by manipulating heat removal in the reactor.
6. The pressure in the exit stream of FEHE is controlled by manipulating % opening of control valve. This valve drops the pressure from 23 bar in the reactor to 2 bar in the flash tank.
7. The temperature of the exit stream at condenser is controlled by heat removal.
8. Level of flash separator is controlled by manipulating the flow rate at the exit stream.
9. Pressure in the flash tank is controlled by manipulating the flow rate of gas stream at the top of tank.
10. Pressure in the benzene column and cumene column are controlled by manipulating heat removal at condenser of reflux drum.
11. Level in the benzene column and cumene column are controlled by manipulating flow rates at the bottom of columns.
12. Level of reflux drum in the benzene column and cumene column are controlled by manipulating flow rate in the distillate stream.
13. Reflux ratio of all columns is controlled by manipulating the reflux flow rate.
14. The temperature control of benzene column C1 at tray 9th is controlled by manipulating heat input at the reboiler.

15. The temperature control of cumene column C2 at tray 14th is controlled by manipulating heat input at the reboiler.

A quantitative comparison of the performances of plantwide control structure is our focus. Rigorous dynamic simulations are performed in Aspen HYSYS to test the designed plantwide control structures, CS1, CS2, and CS3 for selected disturbances. The control structure designed by Luyben (2010) (CS0) is also tested in comparison. The four control structures are shown in Figure 5.32-5.35.

The selected disturbances include changes of fresh feed flow rate of mixed C3 by 10%, propylene composition in feed by 2%, and catalyst deactivation by 5%.

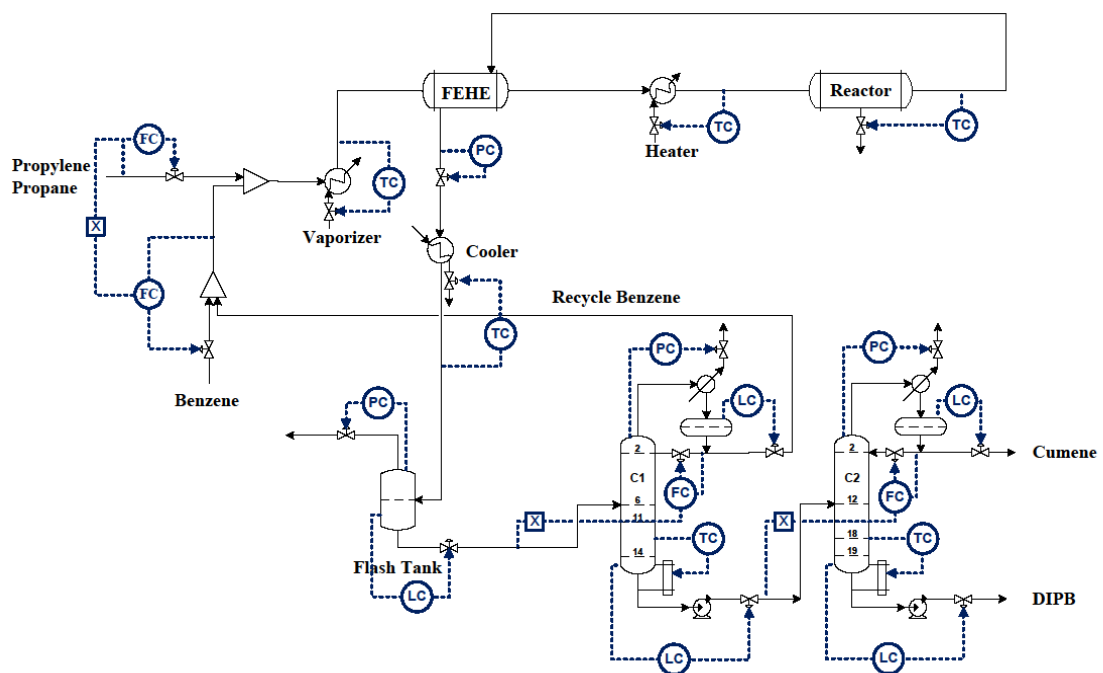


Figure 5.32 The base case control structure (CS0)

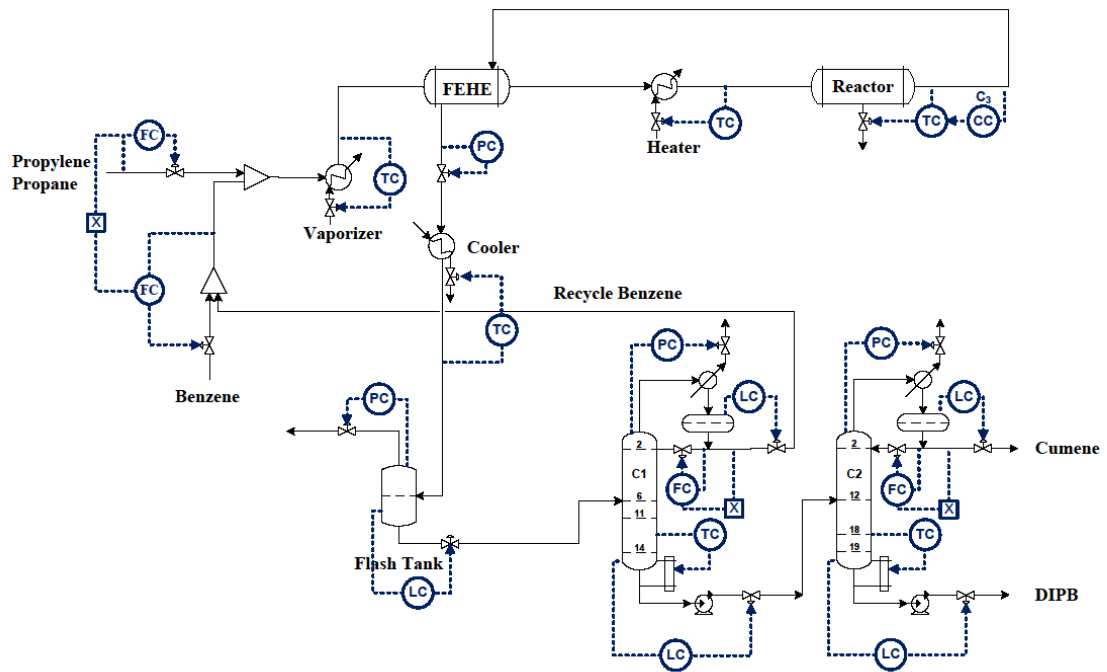


Figure 5.33 The new control structure 1 (CS1)

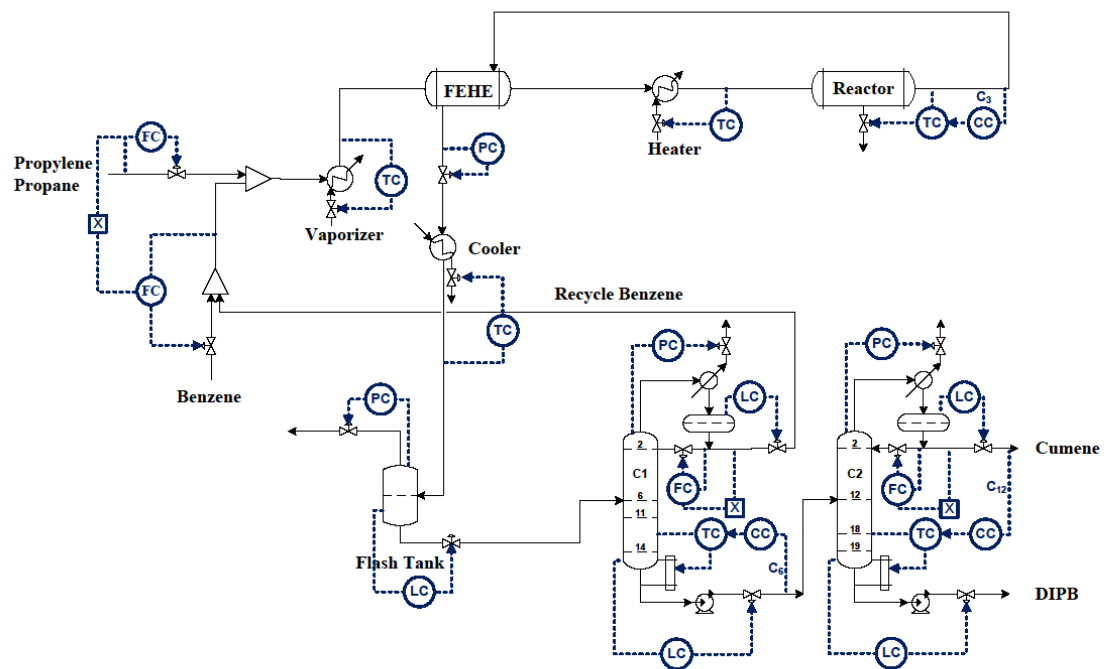


Figure 5.34 The new control structure 2 (CS2)

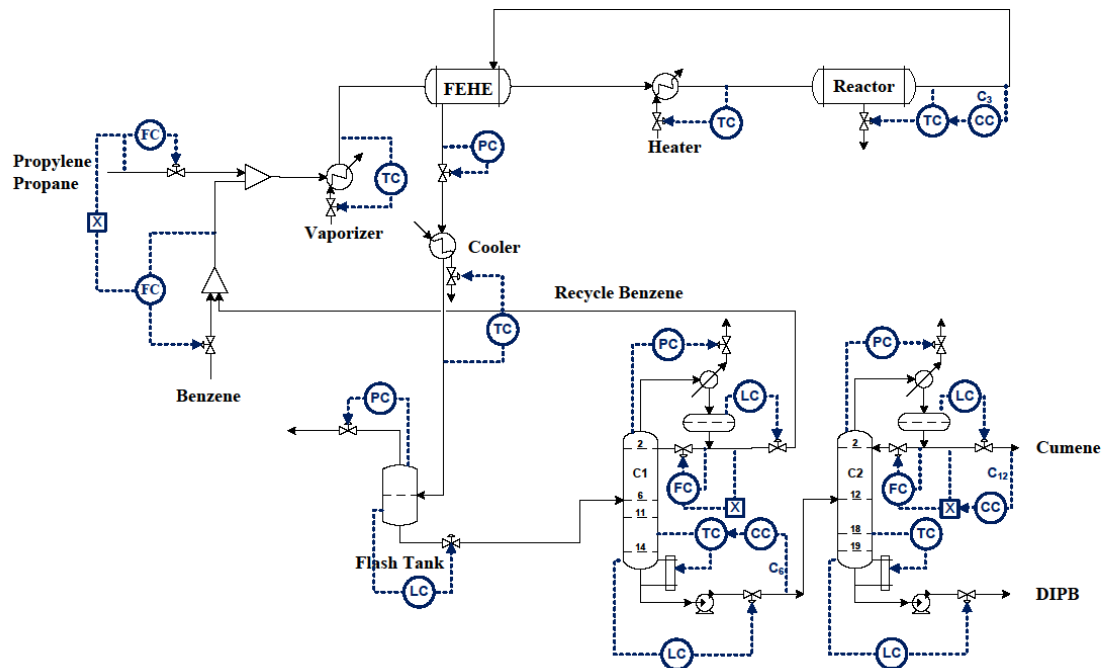


Figure 5.35 The new control structure 3 (CS3)

5.3 Dynamic simulation results

The effectiveness of these structures are demonstrated next for the selected disturbances. 19 loops for each structure are chosen for observation and evaluation. The controller tuning parameters are shown in Table B.1-B.4. Level and pressure controller parameters use generic values given in Luyben (Luyben 1998). Flow loops and temperature loops with 1 min dead times are auto tuned.

The performance of these structures is shown in Figure 5.36, 5.37, and 5.38 for three disturbances (fresh feed flow rate of mixed C3, composition of the fresh mixed C3 feed, and catalyst deactivation).

5.3.1 The fresh feed flow rate of mixed C3 disturbances

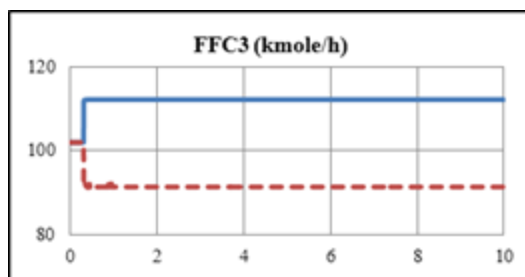


Figure 5.36 Dynamic results for $\pm 10\%$ fresh feed flow rate of mixed C3 disturbances

Figure 5.36 shows the set point at the fresh feed of mixed C3 flow controller is changed at time = 0.3 h. The solid lines are the fresh feed flow rate of mixed C3 by 10% increase. The dashed lines are the fresh feed flow rate of mixed C3 by 10% decrease.

Total benzene flow (TotB) responses are similar for 4 control structures. The gas stream flow rates increase as mixed C3 increase and vice versa. In the case of mixed C3 increase, there is more benzene loss about 15.0980 kmol/h for CS0 compared to 10.5342 kmol/h of our 3 structures.

The temperature of reactor effluent (T_{out}) stays about the setpoint for CS0. For the new designs, it increases as mixed C3 increase and vice versa to maintain propylene composition in the reactor outlet stream. The Luyben's structure (CS0) with no regulation on propylene composition cannot convert surplus mixed C3 to cumene.

Benzene composition in C1 bottoms ($x_{B1(B)}$): Our CS1 structure with no enhanced loops on distillation train exhibits less over shoot compare to CS0. Our CS2 and CS3 perform remarkably well due to the presence of enhanced loops. The setpoint of C1 tray loop (Temp1) is adjusted slightly in the cases of CS2 and CS3.

The production rates (D2) in our 3 cases are higher than the base case, since more mixed C3 is converted at the reactor so our cumene in the product is higher than the base case. The production rate (D2) for the new designs rise from 93.0798

kgmole/h to 102.3567 kgmole/h compared to 100.6124 kgmole/h for CS0 (Luyben's design).

The by-product (B2), DIPB responses for our structures are contrary to CS0, since more product and of-cause by-product are produced in our cases.

The C2 tray temperature control is better in our cases, especially in the case of CS3.

Stable regulatory control is achieved with the product quality of the cumene product ($x_{D2(C)}$) being maintained above the desired 99.9 mol % specification for all structures. With the enhanced loops, CS2 and CS3 achieve surprisingly smooth transient responses.

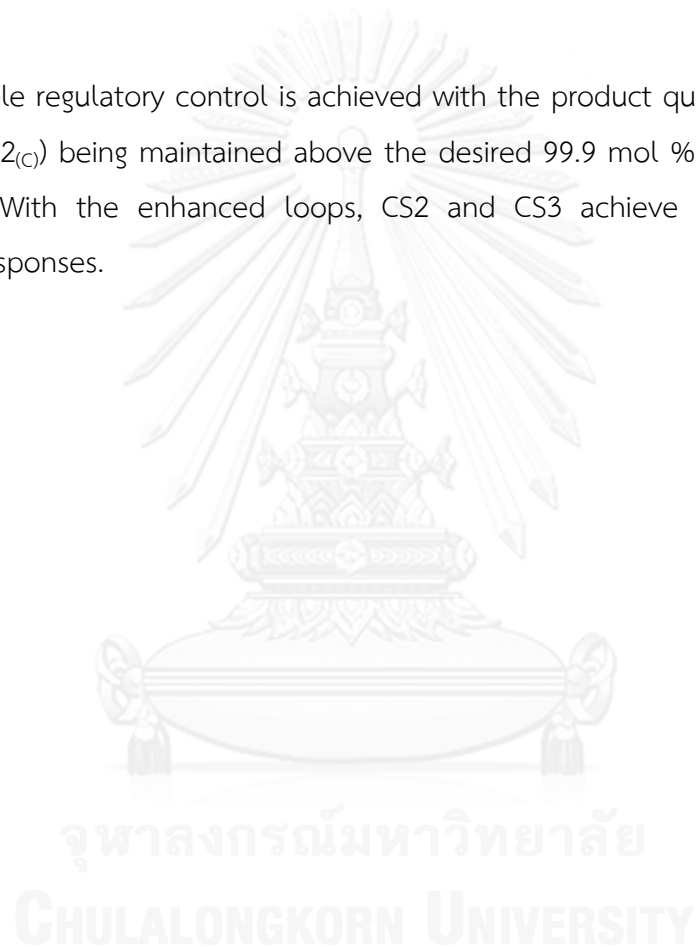


Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3.

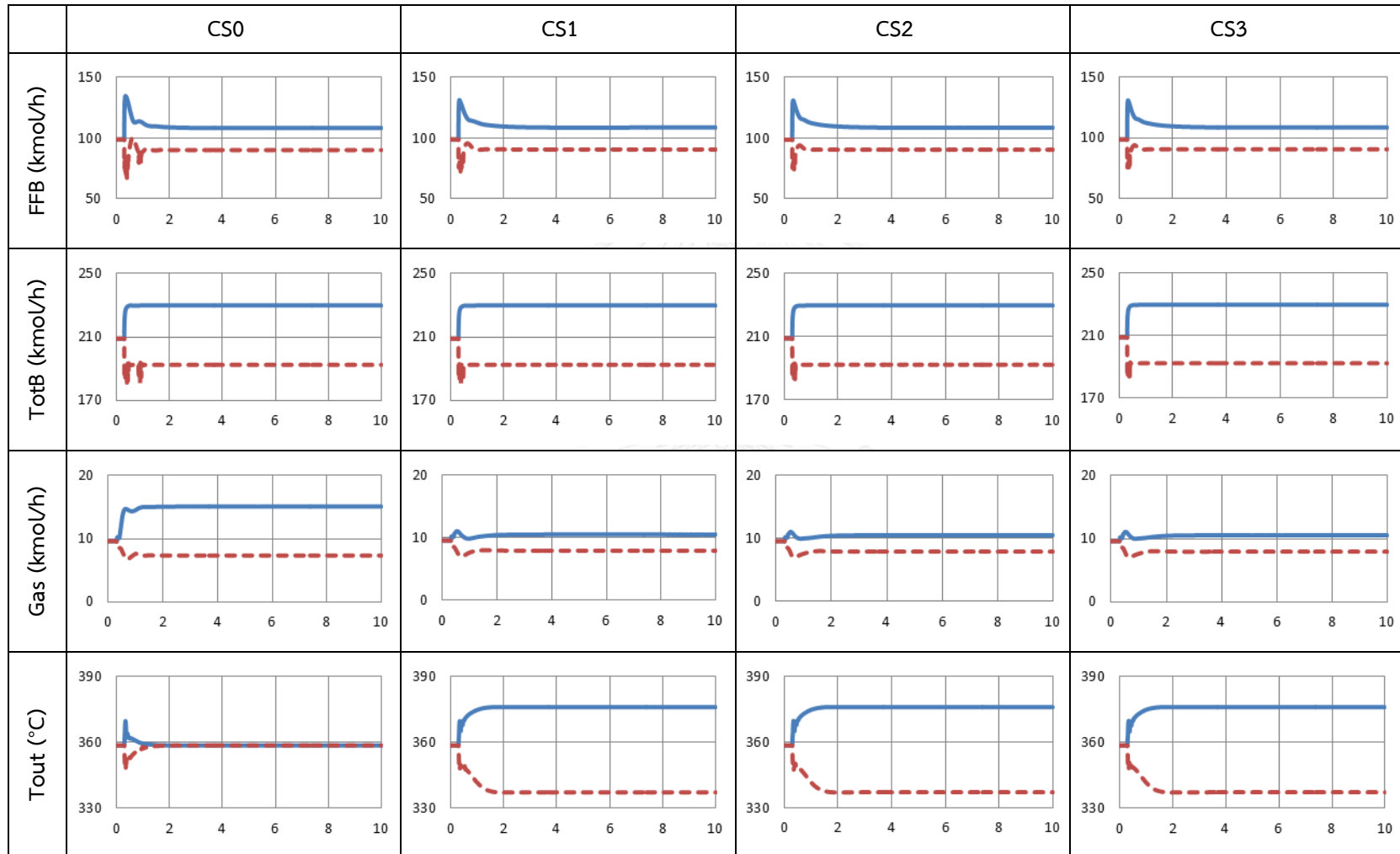


Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3. (cont.)

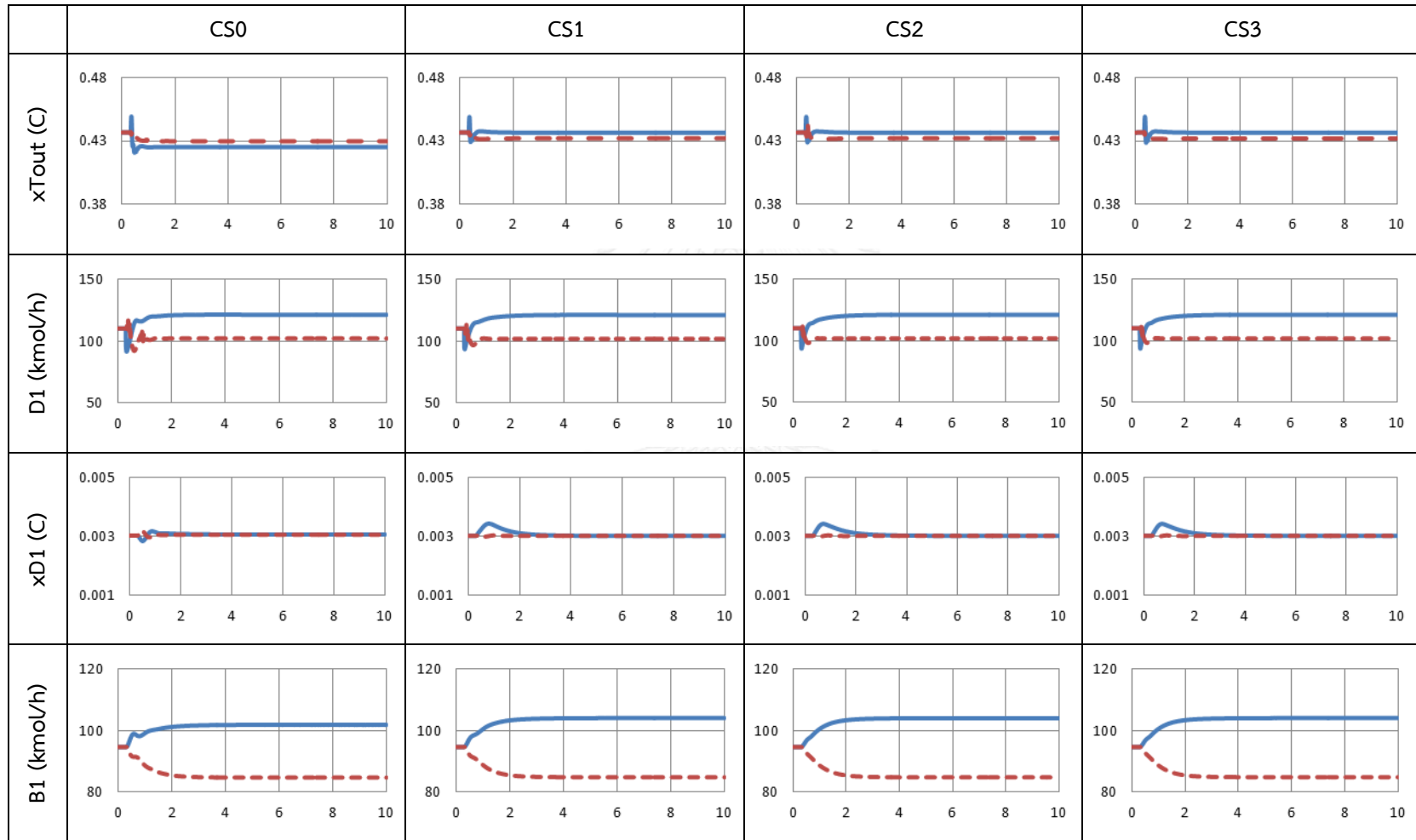


Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3. (cont.)

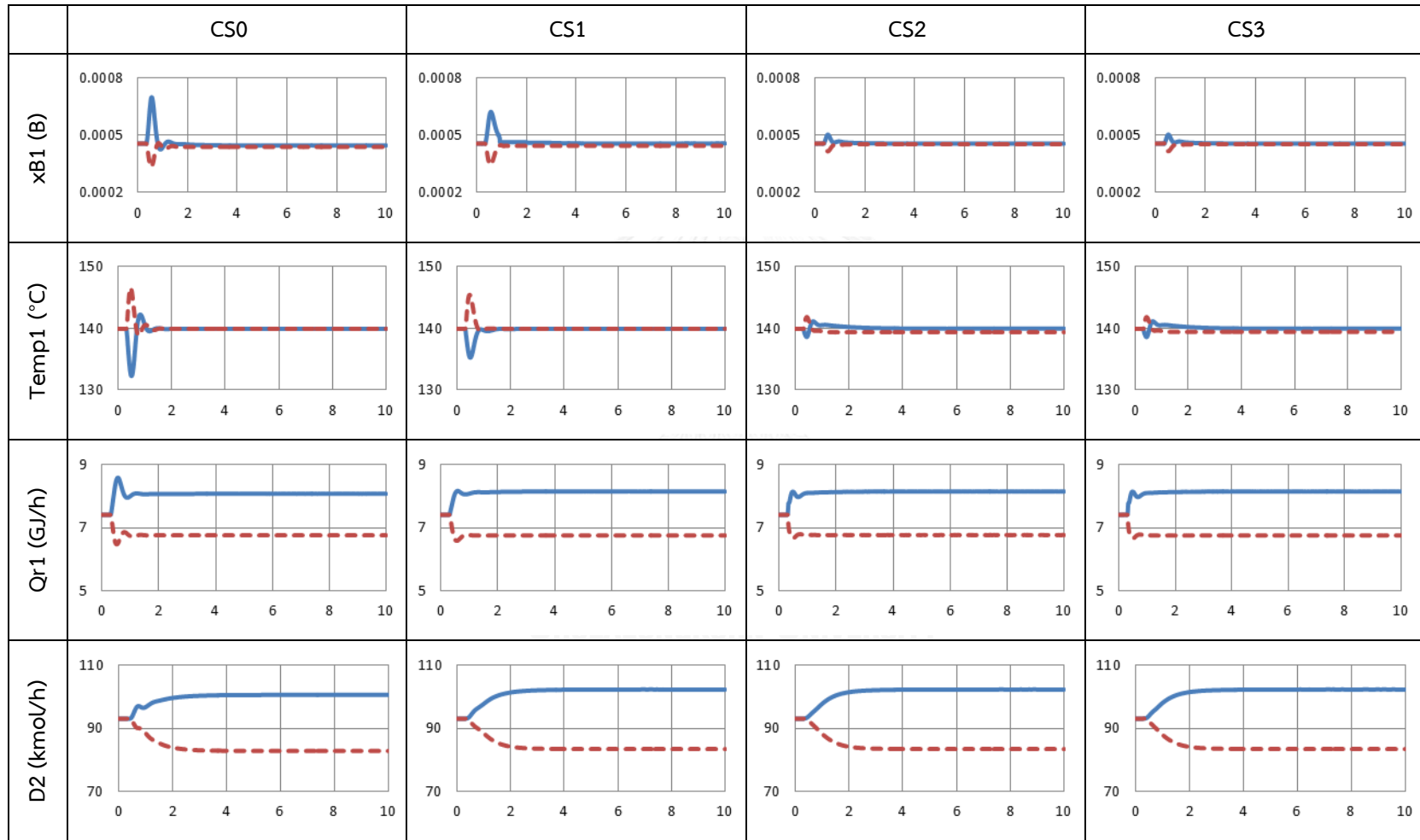


Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3. (cont.)

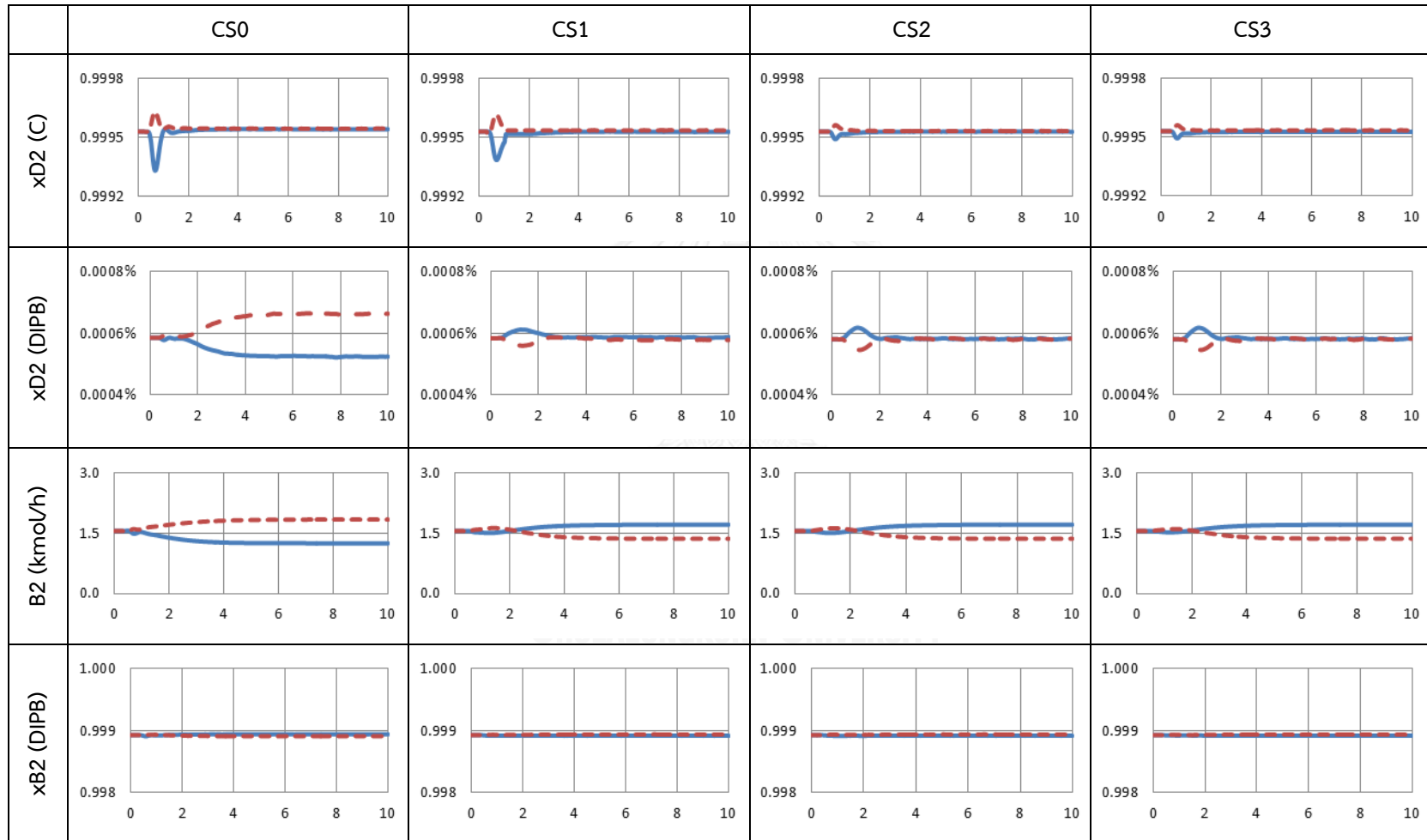
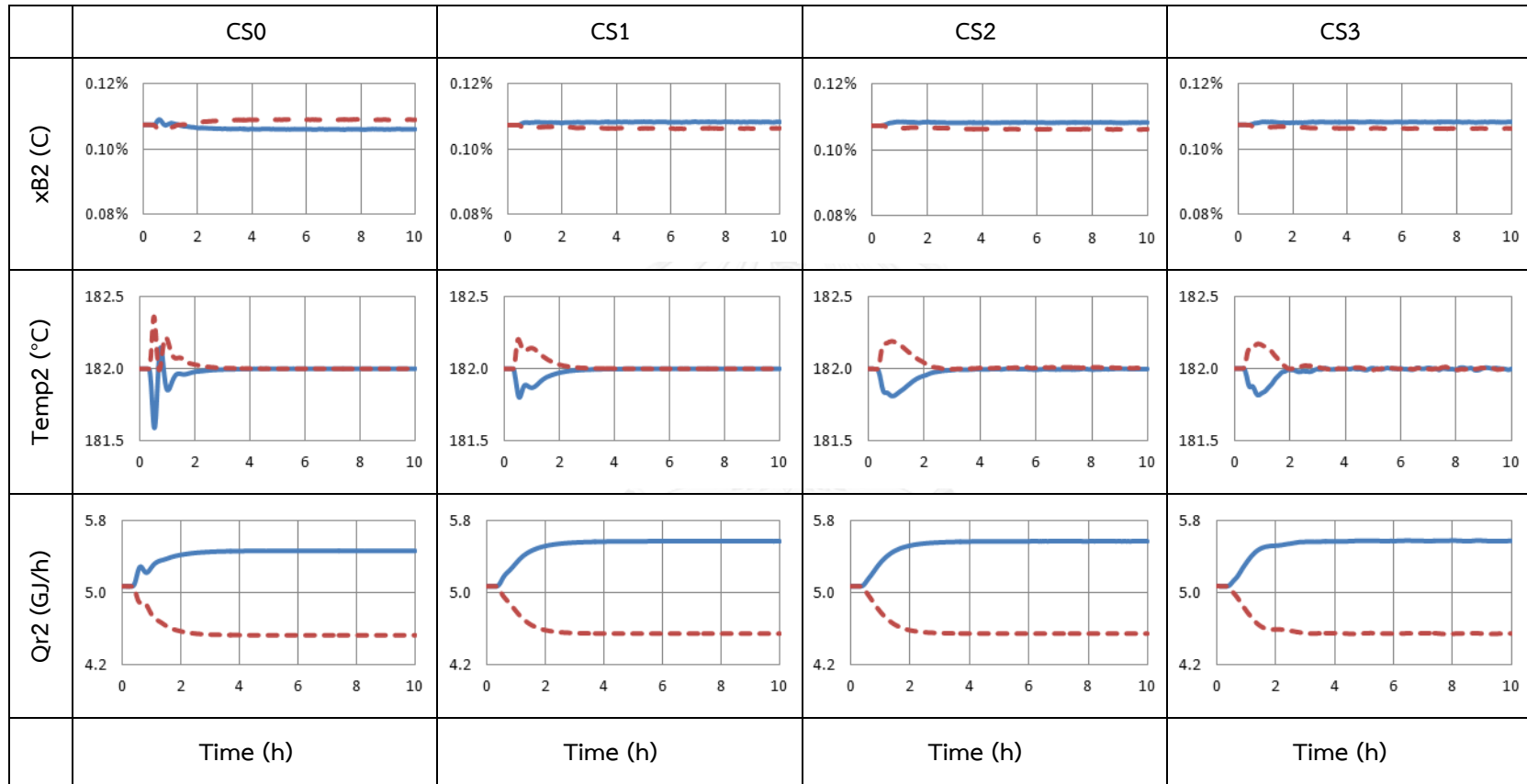


Table 5.4 $\pm 10\%$ changes in the mixed C3 fresh feed flow rate disturbance for CS0, CS1, CS2, and CS3. (cont.)



5.3.2 The composition of propylene feed disturbances

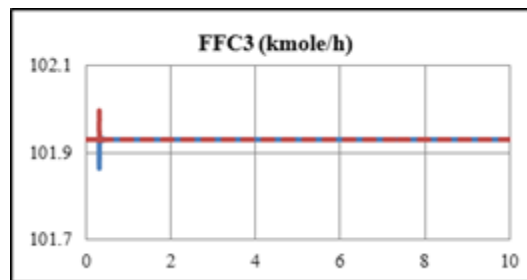


Figure 5.37 Dynamic results for $\pm 2\%$ propylene composition feed disturbances

Table 5.5 shows responses of disturbances in the composition of the fresh mixed C3 feed. The solid lines are the propylene composition change from 95 mol% to 93 mol% and propane from 5 mol% to 7 mol%. The dashed lines are the propylene composition change from 95 mol% to 97 mol%. When less propylene is fed into the process, the flow rate of fresh benzene is reduced. For this reason, amount of excess benzene from the reaction is increased so distillate flow rate of benzene column C1 is increased too. Moreover, more gas flow rate in the top of flash tank is purged as fuel. From this situation, since control structure of benzene column C1 of CS0 is reflux to feed ratio (R/F). When the constant molar feed flow is fed into column C1, reflux flow rate is constant too so impurity of cumene in the distillate stream is increased. In contrast, control structure of benzene column C1 of CS1, CS2, and CS3 structures are reflux ratio (R/D) so reflux flow rate depends on distillate flow rate. The amount of benzene in condenser is increased so distillate flow rate and reflux flow rate are increased too. For this reason, impurity of cumene in the distillate stream is decreased.

The performance of CS1 structure, the initial response of temp1 has a smooth operation than CS0 structure so Qr1 has change of heat duty less than CS0 structure. For this reason, distillate flow rate (D1) and fresh feed benzene flow rate (FFB) are swing less than CS0 structure too. As for CS2, CS3 structures, they have cascade controller at the tubular reactor, cascade controller at the bottom stream of C1 column (B1) for quality control of benzene, and cascade controller at the product stream of C2 column (D2) for quality control of cumene so CS2, CS3 structures can maintain purity of product (cumene) better than CS0, CS1 structures.

Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3.

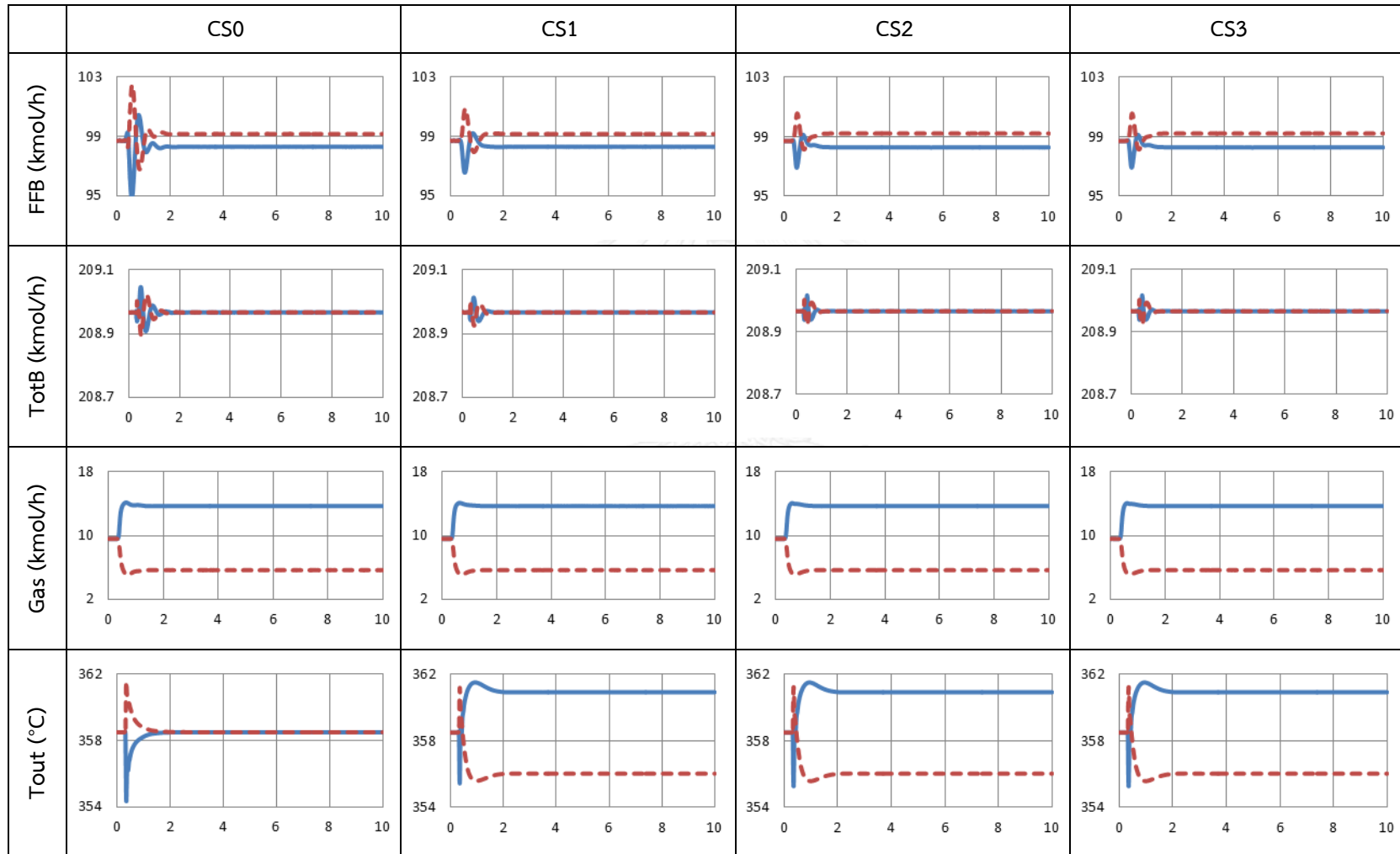


Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3. (cont.)

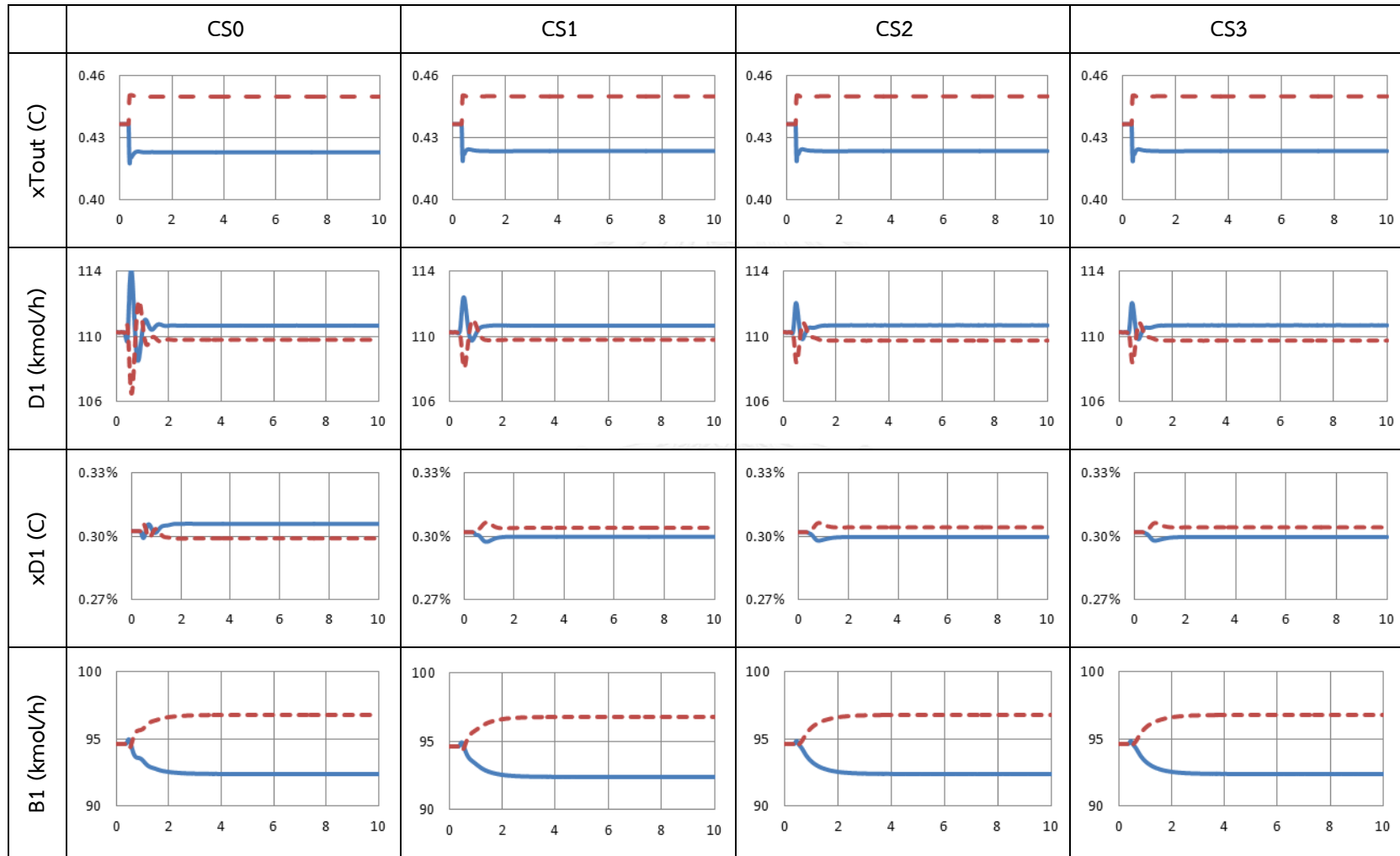


Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3. (cont.)

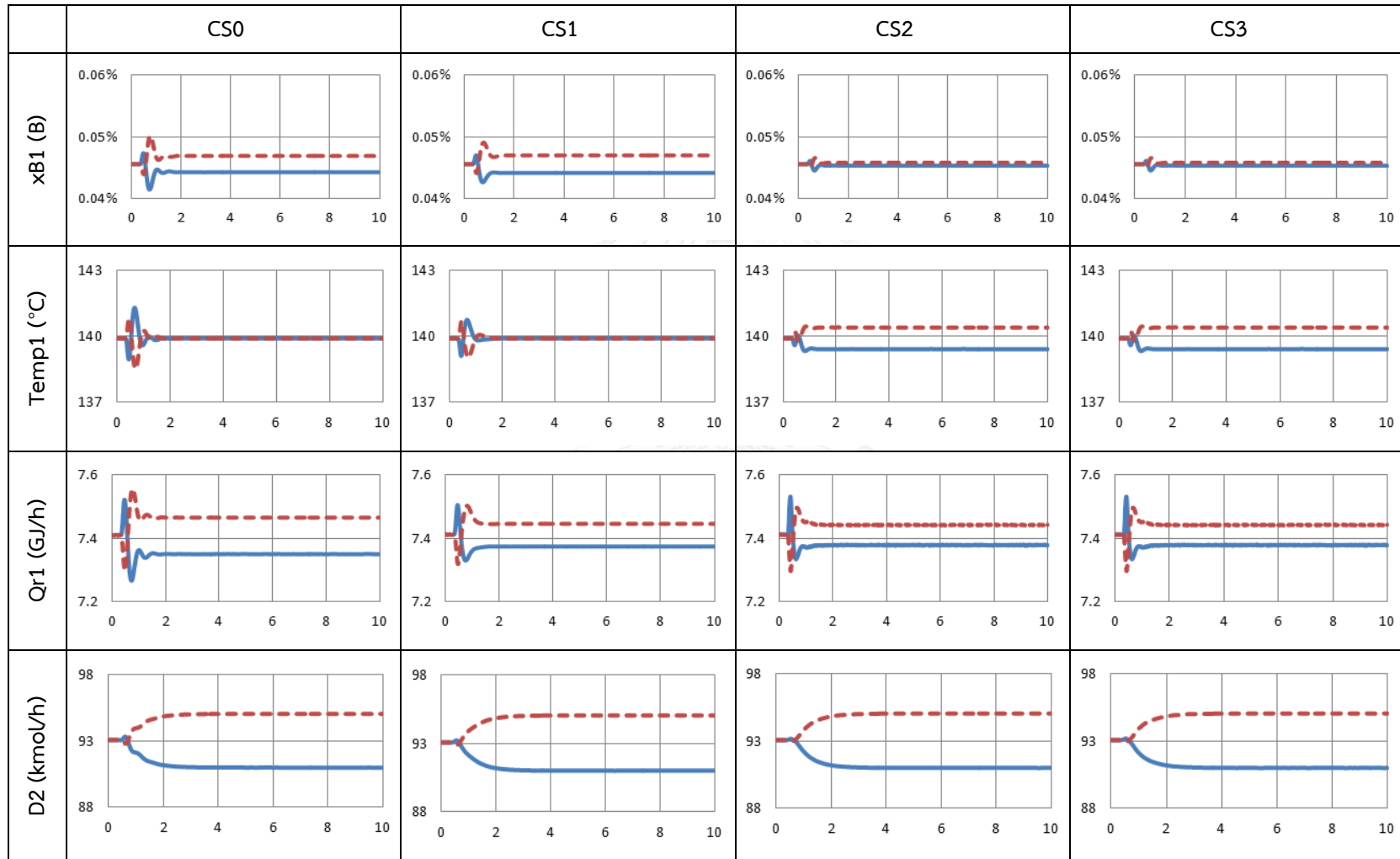


Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3. (cont.)

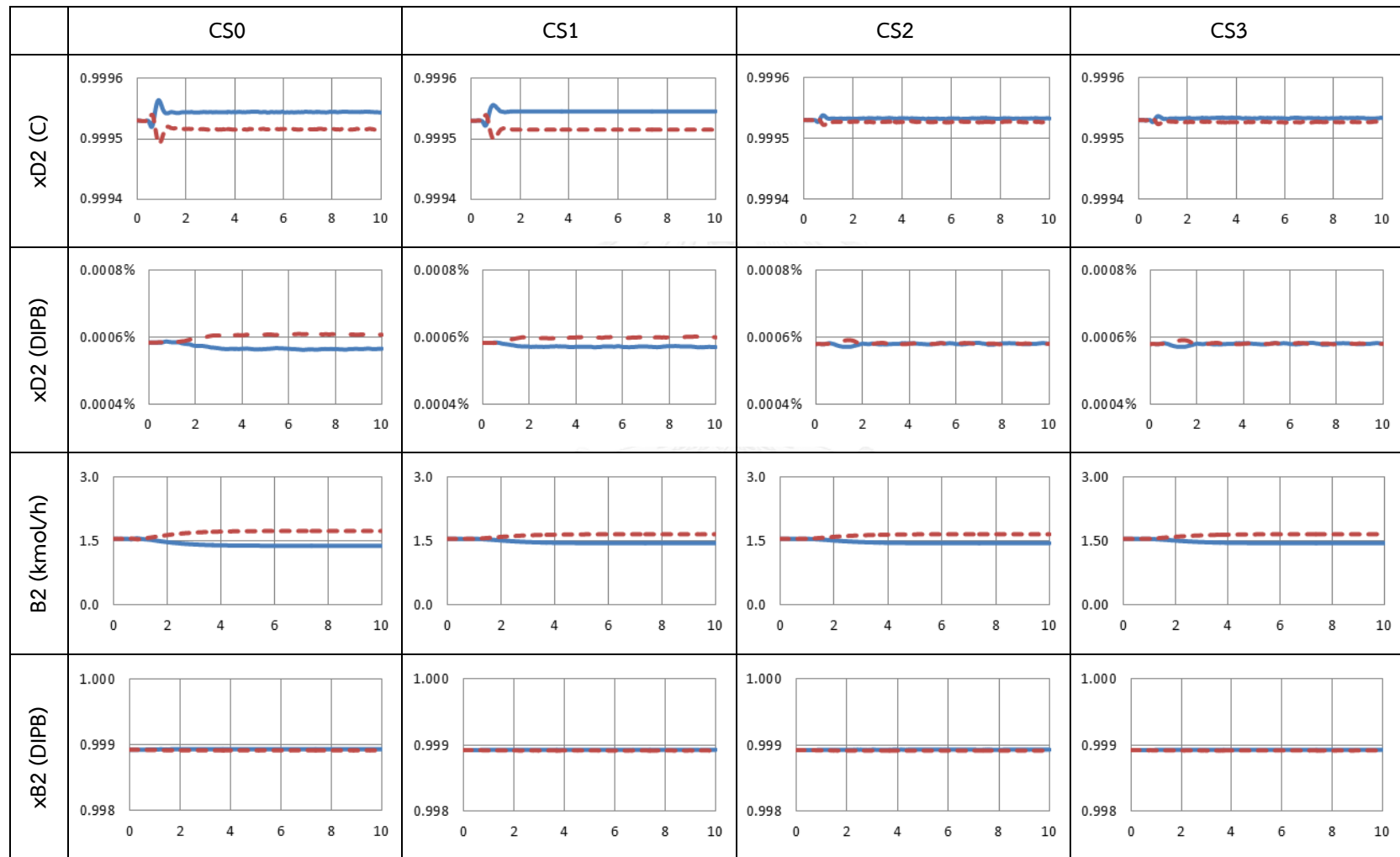
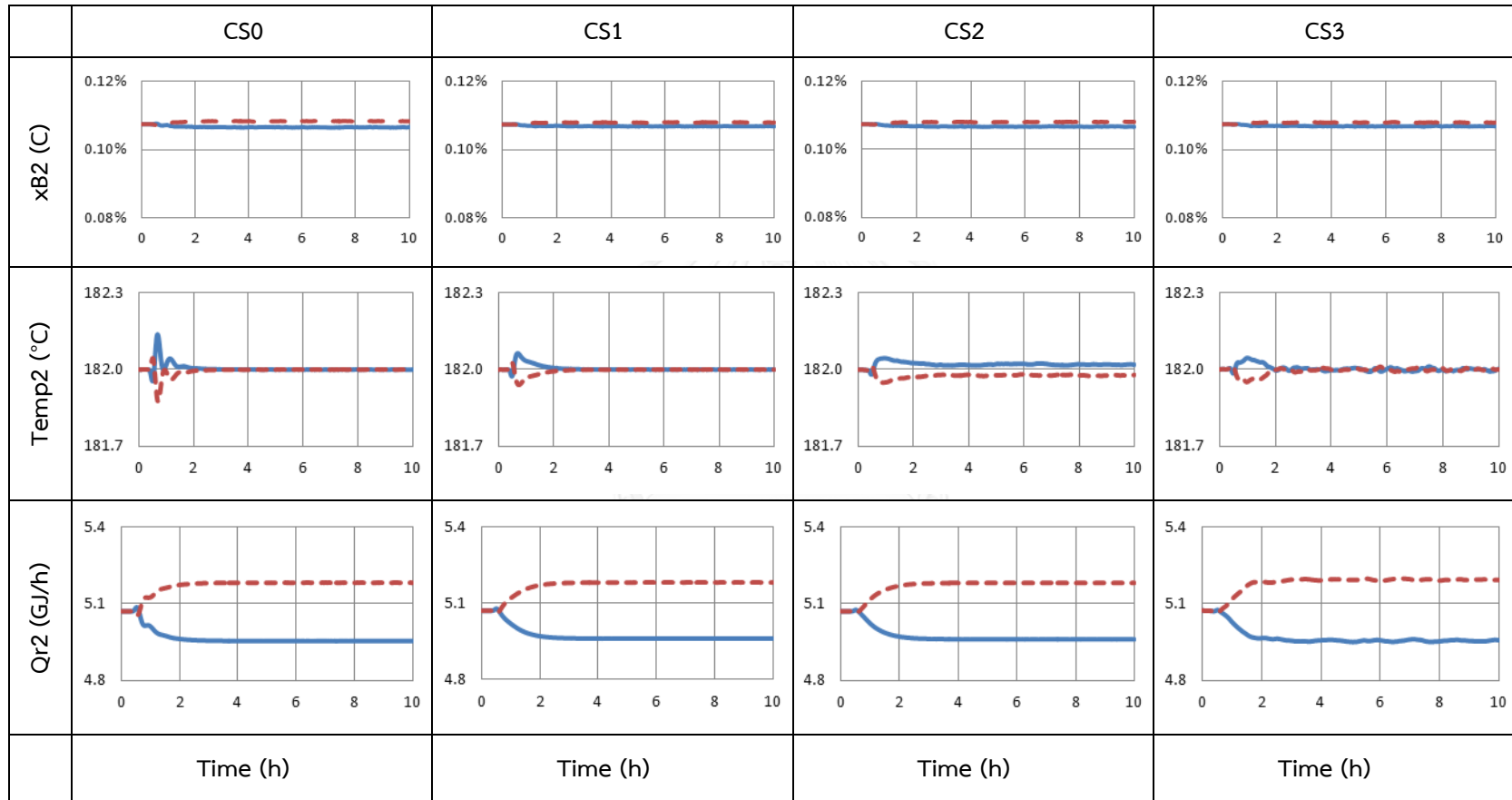


Table 5.5 $\pm 2\%$ changes in the composition of propylene feed disturbance for CS0, CS1, CS2, and CS3. (cont.)



5.3.3 The catalyst deactivation disturbances

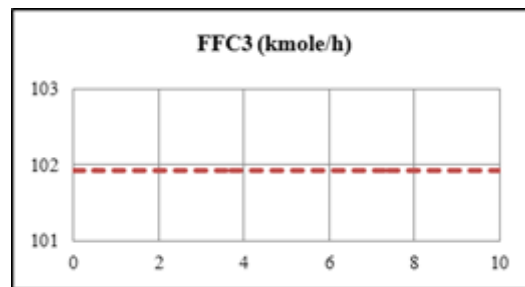


Figure 5.38 Dynamic results for 95% catalyst deactivation disturbances

The final disturbance is a change in the catalyst activity of the reactor. Table 5.6 gives responses for a change from 100% to 95%. The proposed of this is to demonstrate the necessity of the reactor composition control as expected, decreasing catalyst activity produces less product. While the new structure with the reactor composition control loop maintain the product composition and the production rate close to the case where the catalyst is 100% in activity. There is little change in the cumene production D2 for an increase in reactor temperature, but there is a significant decrease for a decrease in reactor temperature (T_{out}). This occurs because the lower conversion of propylene in the reactor produces a large increase in the gas.

As for CS1, CS2, and CS3 structures, they have improved by measuring propylene composition at the outlet stream of the reactor and cascade control with temperature controller at the reactor so the temperature of the reactor is changed by the propylene composition. For this reason, CS1, CS2, and CS3 can maintain impurity of cumene in D1 (x_{D1}), impurity of benzene in B1 (x_{B1}), production rate of cumene (D2), and purity of cumene (x_{D2}) near their set point better than CS0 structure. As for CS2, CS3 structures, they can maintain purity of product (cumene) better than CS0, CS1 structures from the same reasons in the composition of propylene feed disturbances.

Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3.

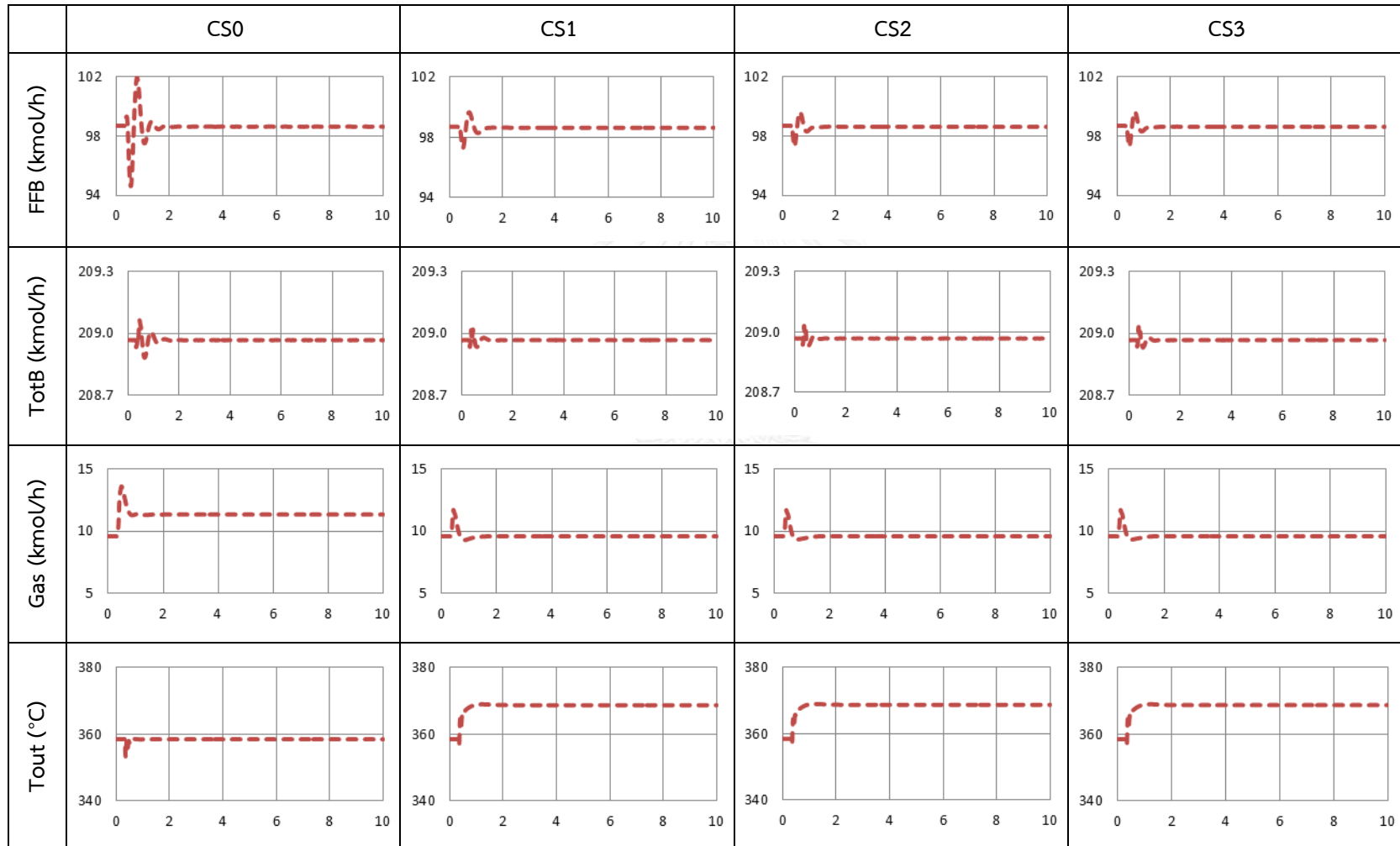


Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3. (cont.)

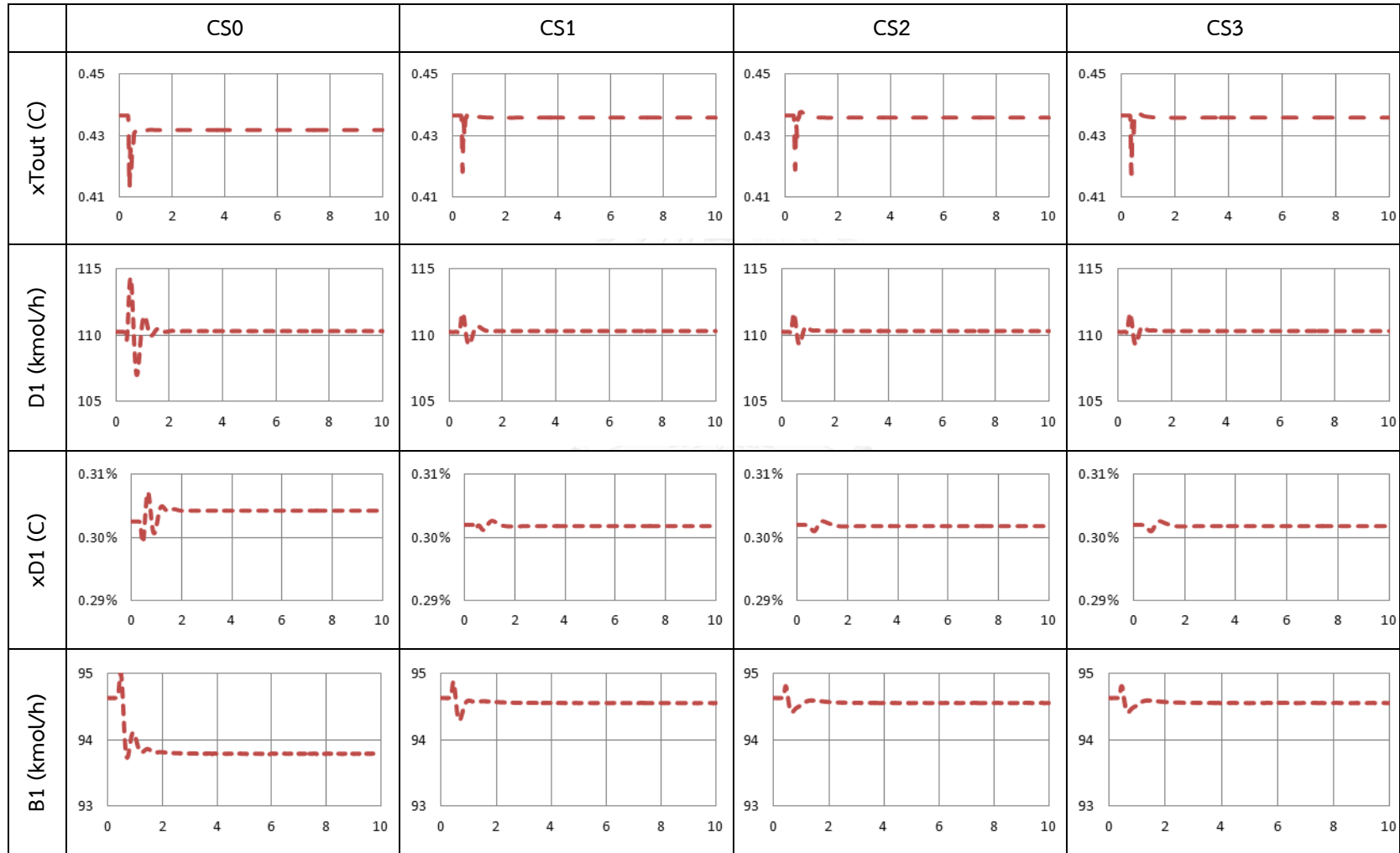


Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3. (cont.)

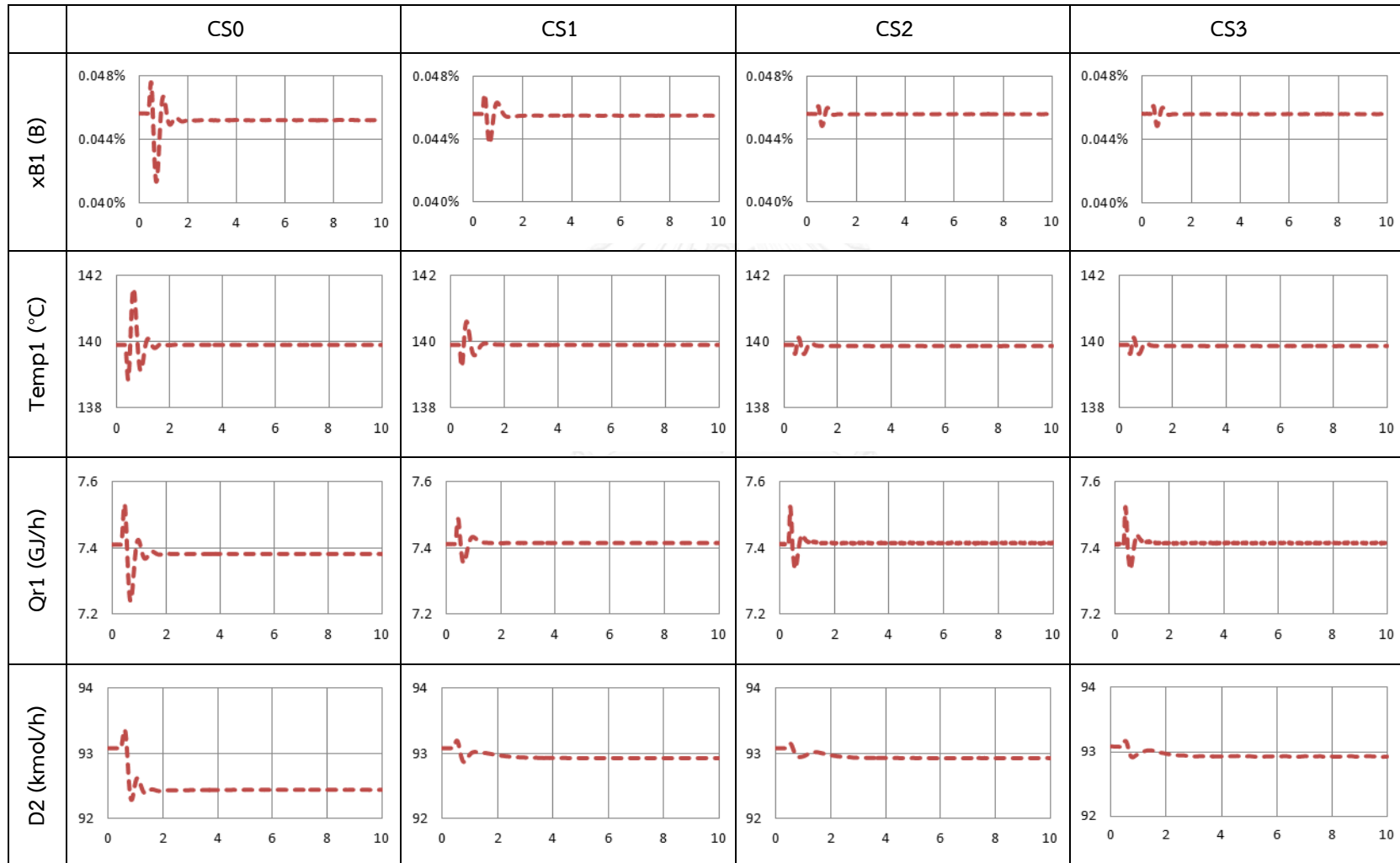


Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3. (cont.)

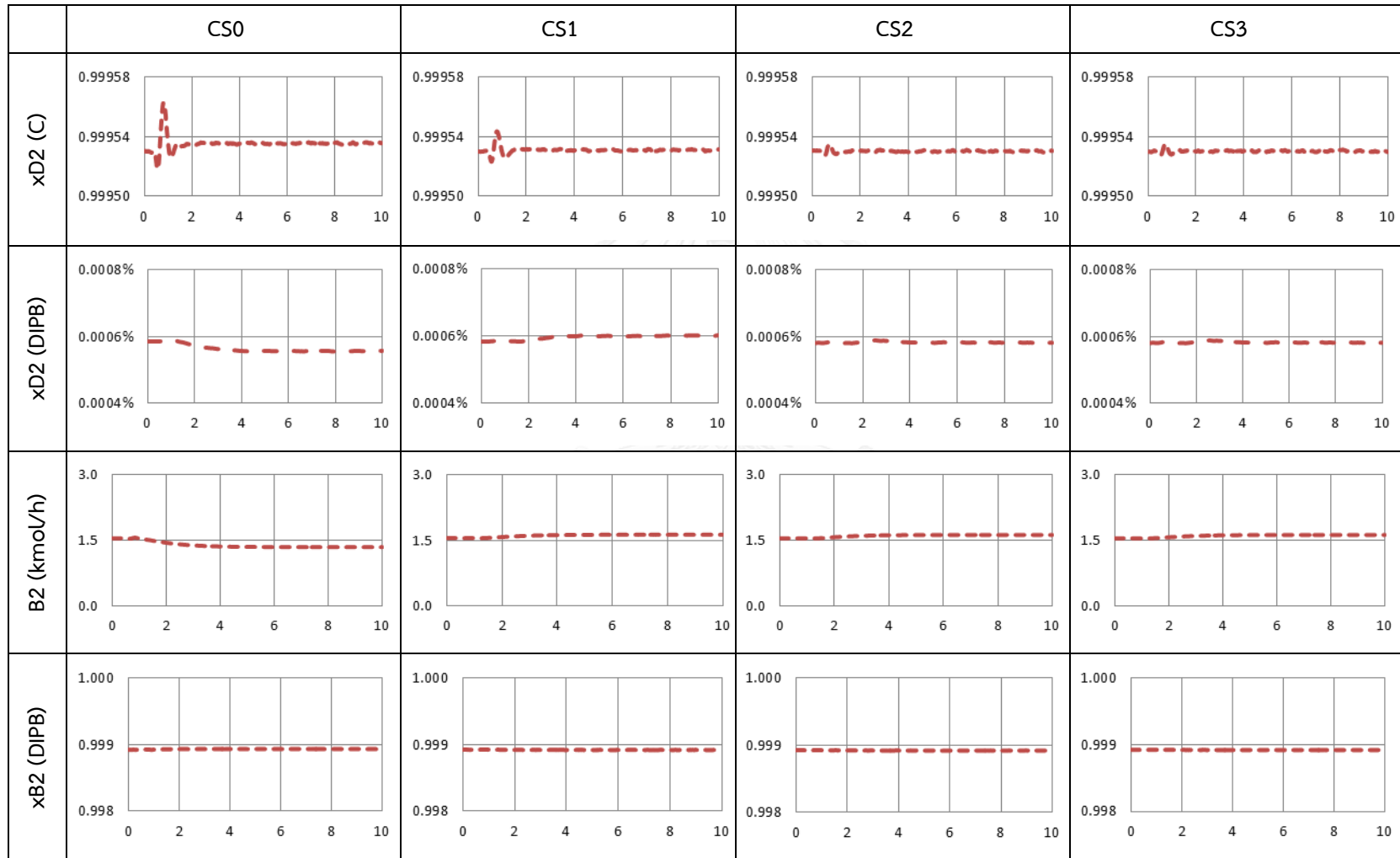


Table 5.6 -5% changes in the catalyst deactivation disturbance for CS0, CS1, CS2, and CS3. (cont.)

	CS0	CS1	CS2	CS3
xB2 (C)				
Temp2 (°C)				
Qr2 (GJ/h)				
	Time (h)	Time (h)	Time (h)	Time (h)

5.4 Control Structure Performance Evaluation

In this work, integral absolute error (IAE) is used to evaluate the control structure performance for the base case (CS0) and new designed control structures (CS1, CS2, and CS3). IAE values are usually used in an academic research and uses different criteria to minimize the value of error from the setpoint. Integral absolute error is widely used and the formulation as written below:

$$IAE = \int |e(t)| dt$$

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

For change in disturbances consists of mixed C3 fresh feed flowrate change, propylene composition feed change and catalyst deactivation. The IAE results for regulates each disturbance and maintain quality of product are shown in Table 5.7-5.9.

Table 5.7 Summation of the IAE results for handle mixed C3 fresh feed flowrate disturbance

Control Structures	Control loops		
	Temperature	Pressure	Composition
CS0	14.5455	10.1159	0.1760
CS1	14.1072	8.3134	0.0467
CS2	12.9397	8.0799	0.0460
CS3	12.9465	7.9184	0.0461

Table 5.8 Summation of the IAE results for handle propylene composition feed disturbance

Control Structures	Control loops		
	Temperature	Pressure	Composition
CS0	1.0309	5.4605	0.2619
CS1	0.7124	4.9221	0.2573
CS2	0.4222	4.8793	0.2568
CS3	0.4371	4.8621	0.2568

Table 5.9 Summation of the IAE results for handle catalyst deactivation disturbance

Control Structures	Control loops		
	Temperature	Pressure	Composition
CS0	0.6372	2.0713	0.0476
CS1	0.3128	1.3834	0.0080
CS2	0.1501	1.3884	0.0077
CS3	0.1663	1.3806	0.0077

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The problem of plantwide control is to design a control system for an entire complex and integrated process that satisfies the plant's operation objectives. The presence of recycle streams and energy integration in chemical processes creates unique features for plantwide control problems because of the potential source for disturbance propagation and results in changing of the plant's dynamic behavior.

The new design procedure of Wongsri (2012) has been applied in this research to design the plantwide control structure of cumene process. The new plantwide control structures designed (CS1, CS2, CS3) by procedure of Wongsri (2012) compared with the base-case control structure designed (CS0) by procedure of Luyben (2010). Wongsri's design procedure can be regulating the material disturbances and the energy disturbances better than the control structure design of Luyben (2010) since Wongsri's procedure has the stage of fixture plant and disturbance management design that the heat and material disturbances must be rejected to the nearest exits or directed to less significant streams. Moreover, the responses of all cases by Wongsri's design procedure can perform more smoothly than ones of Luyben's structure. As for CS2 and CS3 structures, they have cascade controller at the tubular reactor, cascade controller at the bottom stream of C1 column (B1), and cascade controller at the product stream of C2 column (D2) so CS2 and CS3 structures can maintain purity of product (cumene) better than CS0 and CS1 structures.

6.2 Recommendations

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

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APPENDIX

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CHULALONGKORN UNIVERSITY

APPENDIX A

EQUIPMENTS DATA AND PROCESS STREAMS

The equipment of each unit operations should be sized for dynamic simulation and sizing data are shown in Table A.1

Table A.1 Equipment sizing data of benzene process

Equipment	Specifications	
Tubular reactor	Diameter (m)	0.0763
	Length (m)	6
	Number of tubes	1500
	Void fraction	0.5
	Solid density (kg/m ³)	2000
	Heat duty (kJ/hr)	9.24E+06
Vaporizer	Volume (m ³)	4.59
	Heat duty (kJ/hr)	1.56E+07
FEHE	Heat transfer area (m ²)	460
	Tubes diameter (m)	0.0762
	Tubes length (m)	6
	Tube volume (m ³)	8.76
	Shell volume (m ³)	8.76
Flash tank	Volume (m ³)	4.15
	Diameter (m)	1.522
	Height (m)	2.282

Table A.1 Equipment sizing data of benzene process (cont.)

Equipment	Specifications	
Benzene column (C1)	Number of trays	15
	Feed tray	6
	Condenser Pressure (bar)	1.75
	Reboiler Pressure (bar)	1.83
	Diameter (m)	1.524
	Condenser volume (m ³)	2
	Reboiler volume (m ³)	22.3
	Reflux ratio	0.44
	Condenser duty (kJ/hr)	5.66E+06
	Reboiler duty (kJ/hr)	7.46E+06
Cumene column (C2)	Number of trays	20
	Feed tray	12
	Condenser Pressure (bar)	1.00
	Reboiler Pressure (bar)	1.09
	Diameter (m)	1.372
	Condenser volume (m ³)	2.5
	Reboiler volume (m ³)	16.45
	Reflux ratio	0.63
	Condenser duty (kJ/hr)	5.71 E+06
	Reboiler duty (kJ/hr)	5.03 E+06

Table A.2 Stream table of cumene process in steady state mode operation.

	1	2	3	4	5	6
Vapor Fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Temperature (°C)	25.00	25.00	25.00	25.00	38.13	40.45
Pressure (bar)	30.00	26.00	3.00	1.00	1.00	26.00
Molar Flow (kmol/hr)	101.9	101.9	98.78	98.78	209	209
Mass Flow (kg/hr)	4300	4300	7716	7716	16130	16130
Comp. Propylene	0.9500	0.9500	0.0000	0.0000	0.0022	0.0022
Comp. Propane	0.0500	0.0500	0.0000	0.0000	0.0274	0.0274
Comp. Benzene	0.0000	0.0000	1.0000	1.0000	0.9688	0.9688
Comp. Cumene	0.0000	0.0000	0.0000	0.0000	0.0016	0.0016
Comp. DIPB	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table A.2 Stream table of cumene process in steady state mode operation (cont.).

	7	8	9	10	11	12
Vapor Fraction	0.0000	0.9357	1.0000	1.0000	1.0000	0.7224
Temperature (°C)	35.84	210.00	330.00	358.00	358.50	274.20
Pressure (bar)	26.00	25.00	25.00	25.00	24.00	23.00
Molar Flow (kmol/hr)	310.9	310.9	310.9	310.9	214.5	214.5
Mass Flow (kg/hr)	20430	20430	20430	20430	20430	20430
Comp. Propylene	0.3129	0.3129	0.3129	0.3129	0.0041	0.0041
Comp. Propane	0.0348	0.0348	0.0348	0.0348	0.0504	0.0504
Comp. Benzene	0.6512	0.6512	0.6512	0.6512	0.5017	0.5017
Comp. Cumene	0.0011	0.0011	0.0011	0.0011	0.4365	0.4365
Comp. DIPB	0.0000	0.0000	0.0000	0.0000	0.0072	0.0072

Table A.2 Stream table of cumene process in steady state mode operation (cont.).

	13	14	15	16	17	18
Vapor Fraction	1.0000	0.0447	1.0000	1.0000	0.0000	0.0000
Temperature (°C)	234.70	85.00	85.00	85.00	85.00	85.08
Pressure (bar)	2.00	1.75	1.75	1.00	1.75	2.75
Molar Flow (kmol/hr)	214.5	214.5	9.598	9.598	204.9	204.9
Mass Flow (kg/hr)	20430	20430	572.8	572.8	19860	19860
Comp. Propylene	0.0041	0.0041	0.0443	0.0443	0.0022	0.0022
Comp. Propane	0.0504	0.0504	0.5306	0.5306	0.0279	0.0279
Comp. Benzene	0.5017	0.5017	0.3964	0.3964	0.5067	0.5067
Comp. Cumene	0.4365	0.4365	0.0287	0.0287	0.4556	0.4556
Comp. DIPB	0.0072	0.0072	0.0000	0.0000	0.0076	0.0076

Table A.2 Stream table of cumene process in steady state mode operation (cont.).

	19	20	21	22	23	24
Vapor Fraction	0.0000	0.0000	0.0000	0.0359	0.0000	0.0000
Temperature (°C)	85.09	49.46	49.55	44.17	178.90	179.00
Pressure (bar)	1.81	1.75	2.75	1.00	1.90	2.90
Molar Flow (kmol/hr)	204.9	110.3	110.3	110.3	94.63	94.63
Mass Flow (kg/hr)	19860	8419	8419	8419	11440	11440
Comp. Propylene	0.0022	0.0041	0.0041	0.0041	0.0000	0.0000
Comp. Propane	0.0279	0.0519	0.0519	0.0519	0.0000	0.0000
Comp. Benzene	0.5067	0.9409	0.9409	0.9409	0.0005	0.0005
Comp. Cumene	0.4556	0.0031	0.0031	0.0031	0.9832	0.9832
Comp. DIPB	0.0076	0.0000	0.0000	0.0000	0.0163	0.0163

Table A.2 Stream table of cumene process in steady state mode operation (cont.).

	25	26	27	28	29	30	31
Vapor Fraction	0.1819	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Temperature (°C)	154.60	151.70	151.80	151.70	209.3	209.4	209.3
Pressure (bar)	1.06	1.00	2.00	1.00	1.00	2.00	1.00
Molar Flow (kmol/hr)	94.63	93.09	93.09	93.09	1.548	1.548	1.548
Mass Flow (kg/hr)	11440	11190	11190	11190	251.1	251.1	251.1
Comp. Propylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp. Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp. Benzene	0.0005	0.0005	0.0005	0.0005	0.0000	0.0000	0.0000
Comp. Cumene	0.9832	0.9995	0.9995	0.9995	0.0010	0.0010	0.0010
Comp. DIPB	0.0163	0.0000	0.0000	0.0000	0.9990	0.9990	0.9990



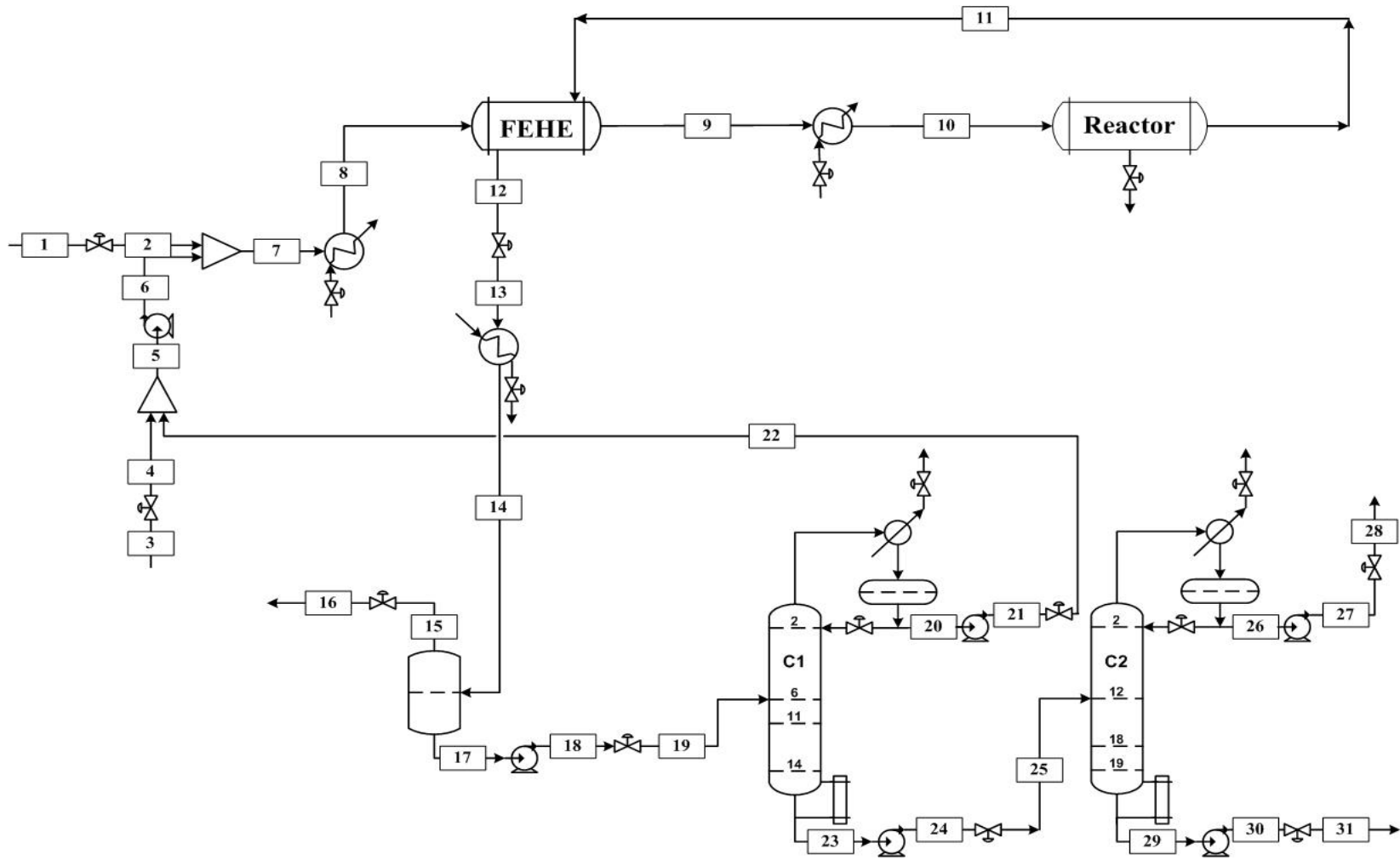


Figure A.1 Cumene process flow sheet for steady state simulation

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 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.

Table B.1 Tuning parameters for cumene process of CS0

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
FC1	Fresh feed flowrate of mixed C3	Stream flowrate	PI	Reverse	5-200 kgmole/hr	0.194	0.008	-
FC2	Total benzene flowrate	Stream flowrate	PI	Reverse	100-300 kgmole/hr	0.5	0.026	-
R/F1	Reflux to feed ratio at C1	Reflux flow	PI	Reverse	-	0.432	0.035	-
R/F2	Reflux to feed ratio at C2	Reflux flow	PI	Reverse	-	0.432	0.035	-
LC1	Level of flash tank	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC2	Level of reflux drum at C1	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC3	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC4	Level of reflux drum at C2	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC5	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
PC1	Pressure at the exit stream of FEHE	Valve	PI	Direct	10-30 bar	7.92	0.028	-
PC2	Pressure at the top of flash tank	Valve	PI	Direct	0.75-2.75 bar	6.16	0.018	-
PC3	Pressure column at C1	Qc1	PI	Direct	0.75-2.75 bar	1.8	10.0	-
PC4	Pressure column at C2	Qc2	PI	Direct	0-2 bar	2.0	10.0	-
TC1	Outlet vaporizer temperature	Heating duty	PID	Reverse	100-300 °C	6.06	0.198	0.044
TC2	Outlet heater temperature	Heating duty	PID	Reverse	300-400 °C	4.92	0.235	0.052
TC3	Outlet reactor temperature	Cooling duty	PID	Direct	250-450 °C	10.0	11.0	1.0

Table B.1 Tuning parameters for cumene process of CS0 (cont.)

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
TC4	Outlet cooler temperature	Cooling duty	PID	Direct	5-150 °C	0.6	11.0	1.0
TC5	Tray 9 th temperature at C1	Qr1	PID	Reverse	40-240 °C	11.2	1.54	0.343
TC6	Tray 14 th temperature at C2	Qr2	PID	Reverse	100-250 °C	8.41	1.72	0.382

Table B.2 Tuning parameters for cumene process of CS1

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
FC1	Fresh feed flowrate of mixed C3	Stream flowrate	PI	Reverse	5-200 kgmole/hr	0.194	0.008	-
FC2	Total benzene flowrate	Stream flowrate	PI	Reverse	100-300 kgmole/hr	0.5	0.026	-
R/D1	Reflux to distillate ratio at C1	Reflux flow	PI	Reverse	-	0.175	0.036	-
R/D2	Reflux to distillate ratio at C2	Reflux flow	PI	Reverse	-	0.175	0.036	-
LC1	Level of flash tank	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC2	Level of reflux drum at C1	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC3	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC4	Level of reflux drum at C2	Distillate flowrate	P	Direct	0-100 %	2.0	-	-

Table B.2 Tuning parameters for cumene process of CS1 (cont.)

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
LC5	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
PC1	Pressure at the exit stream of FEHE	Valve	PI	Direct	10-30 bar	7.92	0.028	-
PC2	Pressure at the top of flash tank	Valve	PI	Direct	0.75-2.75 bar	6.16	0.018	-
PC3	Pressure column at C1	Qc1	PI	Direct	0.75-2.75 bar	1.8	10.0	-
PC4	Pressure column at C2	Qc2	PI	Direct	0-2 bar	2.0	10.0	-
TC1	Outlet vaporizer temperature	Heating duty	PID	Reverse	100-300 °C	6.06	0.198	0.044
TC2	Outlet heater temperature	Heating duty	PID	Reverse	300-400 °C	4.92	0.235	0.052
TC3	Outlet reactor temperature	Cooling duty	PID	Direct	250-450 °C	10.0	11.0	1.0
TC4	Outlet cooler temperature	Cooling duty	PID	Direct	5-150 °C	0.6	11.0	1.0
TC5	Tray 9 th temperature at C1	Qr1	PID	Reverse	40-240 °C	11.2	1.54	0.343
TC6	Tray 14 th temperature at C2	Qr2	PID	Reverse	100-250 °C	8.41	1.72	0.382
CC1	Propylene composition at reactor	Setpoint at TC3	PI	Direct	0-0.01	0.202	2.42	-

Table B.3 Tuning parameters for cumene process of CS2

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
FC1	Fresh feed flowrate of mixed C3	Stream flowrate	PI	Reverse	5-200 kgmole/hr	0.194	0.008	-
FC2	Total benzene flowrate	Stream flowrate	PI	Reverse	100-300 kgmole/hr	0.5	0.026	-
R/D1	Reflux to distillate ratio at C1	Reflux flow	PI	Reverse	-	0.175	0.036	-
R/D2	Reflux to distillate ratio at C2	Reflux flow	PI	Reverse	-	0.175	0.036	-
LC1	Level of flash tank	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC2	Level of reflux drum at C1	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC3	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC4	Level of reflux drum at C2	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC5	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
PC1	Pressure at the exit stream of FEHE	Valve	PI	Direct	10-30 bar	7.92	0.028	-
PC2	Pressure at the top of flash tank	Valve	PI	Direct	0.75-2.75 bar	6.16	0.018	-
PC3	Pressure column at C1	Qc1	PI	Direct	0.75-2.75 bar	1.8	10.0	-
PC4	Pressure column at C2	Qc2	PI	Direct	0-2 bar	2.0	10.0	-
TC1	Outlet vaporizer temperature	Heating duty	PID	Reverse	100-300 °C	6.06	0.198	0.044
TC2	Outlet heater temperature	Heating duty	PID	Reverse	300-400 °C	4.92	0.235	0.052
TC3	Outlet reactor temperature	Cooling duty	PID	Direct	250-450 °C	10.0	11.0	1.0

Table B.3 Tuning parameters for cumene process of CS2 (cont.)

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
TC4	Outlet cooler temperature	Cooling duty	PID	Direct	5-150 °C	0.6	11.0	1.0
TC5	Tray 9 th temperature at C1	Qr1	PID	Reverse	40-240 °C	11.2	1.54	0.343
TC6	Tray 14 th temperature at C2	Qr2	PID	Reverse	100-250 °C	8.41	1.72	0.382
CC1	Propylene composition at reactor	Setpoint at TC3	PI	Direct	0-0.01	0.202	2.42	-
CC2	Benzene composition at B1	Setpoint at TC5	PI	Direct	0-0.001	8.39	0.048	-
CC3	DIPB composition at D2	Setpoint at TC6	PI	Reverse	0-0.001	28.2	4.74	-

Table B.4 Tuning parameters for cumene process of CS3

Controller s	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
FC1	Fresh feed flowrate of mixed C3	Stream flowrate	PI	Reverse	5-200 kgmole/hr	0.194	0.008	-
FC2	Total benzene flowrate	Stream flowrate	PI	Reverse	100-300 kgmole/hr	0.5	0.026	-
R/D1	Reflux to distillate ratio at C1	Reflux flow	PI	Reverse	-	0.175	0.036	-
R/D2	Reflux to distillate ratio at C2	Reflux flow	PI	Reverse	-	0.175	0.036	-

Table B.4 Tuning parameters for cumene process of CS3 (cont.)

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
LC1	Level of flash tank	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC2	Level of reflux drum at C1	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC3	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
LC4	Level of reflux drum at C2	Distillate flowrate	P	Direct	0-100 %	2.0	-	-
LC5	Level of reboiler at C1	Bottom flowrate	P	Direct	0-100 %	2.0	-	-
PC1	Pressure at the exit stream of FEHE	Valve	PI	Direct	10-30 bar	7.92	0.028	-
PC2	Pressure at the top of flash tank	Valve	PI	Direct	0.75-2.75 bar	6.16	0.018	-
PC3	Pressure column at C1	Qc1	PI	Direct	0.75-2.75 bar	1.8	10.0	-
PC4	Pressure column at C2	Qc2	PI	Direct	0-2 bar	2.0	10.0	-
TC1	Outlet vaporizer temperature	Heating duty	PID	Reverse	100-300 °C	6.06	0.198	0.044
TC2	Outlet heater temperature	Heating duty	PID	Reverse	300-400 °C	4.92	0.235	0.052
TC3	Outlet reactor temperature	Cooling duty	PID	Direct	250-450 °C	10.0	11.0	1.0
TC4	Outlet cooler temperature	Cooling duty	PID	Direct	5-150 °C	0.6	11.0	1.0
TC5	Tray 9 th temperature at C1	Qr1	PID	Reverse	40-240 °C	11.2	1.54	0.343
TC6	Tray 14 th temperature at C2	Qr2	PID	Reverse	100-250 °C	8.41	1.72	0.382

Table B.4 Tuning parameters for cumene process of CS3 (cont.)

Controller	Controlled variables	Manipulate Variables	Controller Types	Action	PV Range	Tuning parameter		
						K_C	τ_I	τ_D
CC1	Propylene composition at reactor	Setpoint at TC3	PI	Direct	0-0.01	0.202	2.42	-
CC2	Benzene composition at B1	Setpoint at TC5	PI	Direct	0-0.001	8.39	0.048	-
CC3	DIPB composition at D2	Setpoint at R/D2	PI	Reverse	0-0.001	3.87	12.1	-



APPENDIX C

Research Review of Wongsri

Arrayasinlapathorn and Wongsri (2011) presented plantwide control structures design of methyl acetate process. The plantwide control structure design procedure of Wongsri (2012) is applied to methyl acetate process. Two disturbances are used to evaluate performance of the new control structure, namely, fresh feed composition and production rate. (Arrayasinlapathorn 2011)

Benchavichien and Wongsri (2011) developed the plantwide control structure design of Wongsri (2012) for auto-refrigerated alkylation process. This procedure based on heuristic to find fixture plant which it can handle material and thermal disturbances into the plant. (Benchavichien 2011)

Detjareansri and Wongsri (2009) applied the plantwide control structure design procedure of Wongsri (2009) for alkylation process. This research used HYSYS simulation software to simulate alkylation process in steady state and dynamic modes. Eight new control structure design (CS1 to CS8) are designed followed by Wongsri (2009)'s procedure and compared with the base case (Luyben, 2002). The new control structures have a dynamic performance better than base case since they can reject all disturbances into process and maintain purity of product better than base case. (Detjareansri 2009)

Kanchanawong and Wongsri (2012) presented the application of plantwide control structure design of Wongsri (2012) for modified ethyl benzene process. The main points of this procedure are establishing a fixture plant, material balance and fixed plant, and disturbance management. The new control structures have control performance better than structure of Luyben (2010). (Kanchanawong 2012)

Khamanarm and Wongsri (2011) presented the application of plantwide control structure design procedure of Wongsri (2009) for alkylation process. The new control structures are compared to the structure of Luyben (2002). Two

disturbances are evaluated the performance of new control structure, namely, temperature change in fresh feed, and substances flow rate. (Khamanarm 2011)

Machuay and Wongsri (2011) proposed the application of plantwide control structure design of Wongsri (2009) for styrene process. Four new control structures are simulated in steady state and dynamic mode via HYSYS simulator. The new control structures are evaluated the dynamic performance and compared with the Luyben (2011)'s structure. The control structure 1 (CS1) can regulate disturbances and maintain purity of product better than the other structures. (Machuay 2011)

Phetyodsri and Wongsri (2011) proposed the development of plantwide control structure design for methanol process using Wongsri (2009)'s procedure. They simulated methanol process via Aspen Plus simulation software in steady state and dynamic modes. Three control structures (CS1, CS2, and CS3) are evaluated the dynamic performance and compared with Luyben (2010)'s structure. The performance of all case similar to the Luyben's structure but the new control structures can reduce energy consumption, reject disturbances, and maintain purity of product better than Luyben (2010). (Phetyodsri 2011)

Plonprasert and Wongsri (2009) applied the fixture point theorem and designed the plantwide control structure followed by design procedure of Wongsri (2009). They used 2 set of controlled variables and 3 control structures which used to design and compare. Wongsri's procedure has a good performance of plantwide control structure better than Luyben (2002). (Plonprasert 2009)

Saeleaw and Wongsri (2006) presented design of control structures of energy-integrated HAD plant with minimum auxiliary reboiler. They applied the plantwide control design approach for a complex heat-integrated scheme like Alternative 6 of HAD process. They specified the disturbances and their magnitudes, and then designed the resilient HEN for minimize heat supply and maximize heat demand. (Saeleaw 2006)

Sapsawaipol and Wongsri (2007) presented the resilient heat exchanger network design procedure of Wongsri (1990) and presented procedure for the control structure design of HEN using heuristic approach to solve three HEN problems. (Sapsawaipol 2007)

Srithong and Wongsri (2009) applied the plantwide control structure design of Luyben (1999) and fixture point theorem of Wongsri (2008) for biodiesel production process with alkyl-catalyst. They used Aspen HYSYS simulator to design this plant. (Srithong 2009)

Tapaneeyapong and Wongsri (2012) applied the plantwide control structure design of Wongsri (2012) for tert-amyl methyl ether (TAME) process. This procedure includes 8 steps which emphasis on plantwide level design, namely, establish material balance, disturbance management, and fixed material feed stream into the process. The new control structures are compared the dynamic performance with Luyben's design. (Tapaneeyapong 2012)

Thipsukhum and Wongsri (2011) designed heat exchanger network (HEN) for cumene process and applied the plantwide control structure design of Wongsri (2009) to the cumene process. They used HYSYS simulation software to evaluate the dynamic performance. Two types of disturbance include material and thermal disturbances. (Thipsukhum 2011)

Thongkam and Wongsri (2011) presented the new control structures of acetone process that they are designed followed by Wongsri (2012)'s design procedure. The new control structures can be regulating both material and thermal disturbances better than base case since fixture plant analysis. (Thongkam 2011)

VITA

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