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PLANTWIDE CONTROL STRUCTURE DESIGN FOR ACETONE PROCESS VIA
DEHYDROGENATION OF 2-PROPANOL

Miss Saowarat Thongkam

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

Department of Chemical Engineering

Faculty of Engineering

Chulalongkorn University

Academic Year 2011

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โรงงานอุตสาหกรรมเคมี โดยส่วนใหญ่ ประกอบไปด้วยหน่วยปฏิบัติการมากมาย
เพื่อให้กระบวนการผลิตดำเนินอย่างปลอดภัยและมีเสถียรภาพ กระบวนการผลิตที่มีการหมุนเวียน
มวลสารและพลังงานกลับมาใช้ทำให้กระบวนการนั้นมีความซับซ้อนมากขึ้นเนื่องจากปฏิสัมพันธ์
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ส่งผลต่อคุณภาพของผลิตภัณฑ์ด้วย อย่างไรก็ตามความต้องการของตลาด สังคม และ
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ควบคุมแบบแพลนที่ไวด์จึงมีความสำคัญอย่างยิ่ง อะซิโตนเป็นสารเคมีหนึ่งที่ยอมรับใช้เป็นตัวทำ
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งานวิจัยนี้ได้ออกแบบโครงสร้างการควบคุมโดย ใช้วิธีการวงค์ศรี (2012) โดยการ
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ออกแบบวิธีนี้สามารถจัดการตัวแปรรบกวนได้อย่างมีประสิทธิภาพ

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Most chemical plants consist of a number of processing units to ensure its safety and stability of process operations. Processes involved recycling of material and energy are much more complex due to intensive interactions among units. These lead to an extremely complex dynamic behavior resulting in consistency of undesired products. However, the requirements of market, social and environment demand constant product quality in order to manage cost, energy and raw materials efficiently. To achieve all objectives, therefore, plantwide control plays an important role in the improvement of the modern chemical processes. Acetone is a common chemical product which has been widely used as a solvent and as a reactant for many chemical processes. One of the syntheses of acetone is dehydrogenation of 2-propanol.

In this research, a control structure of the acetone process is designed by using the heuristics procedure of Wongsri (2012). The procedure takes the fixture plant into consideration to provide a reasonable control structure which is straightforward to understand. The control structure is then designed at steady state and dynamic conditions through a commercial process dynamics simulator. Consequently, the control structure is well handled with both material and thermal disturbances.

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

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CONTENTS

	Page
Abstract (Thai)	iv
Abstract (English)	v
Acknowledgements	vi
Contents	vii
List of Tables	ix
List of Figures	xi
CHAPTER I INTRODUCTION	1
1.1 Background	1
1.2 Research Objectives	2
1.3 Scope of Research	3
1.4 Contribution of Research	3
1.5 Research Procedures	3
1.6 Conceptual Framework	4
CHAPTER II LITERATURE REVIEW	6
CHAPTER III THEORY OF PLANTWIDE CONTROL	10
3.1 Fundamental Concept of Pinch Technology	10
3.2 Heat Exchanger Networks Synthesis and Design	13
3.3 Plantwide Control Issues	23
3.4 Plantwide Control Problem	26
3.5 Fundamental Procedures for Plantwide Control	33
3.6 Step of Plantwide Control Design Procedure	37
3.7 Plantwide Energy Management.....	42

	Page
CHAPTER IV ACETONE PROCESS	47
4.1 Introduction	47
4.2 Process Studied	48
4.3 Heat Exchanger Networks for Acetone Process	54
4.4 New control structures design procedure, Wongsri 2012	59
CHAPTER V CONTROL STRUCTURE DESIGN AND DYNAMIC SIMULATION	62
5.1 Plantwide Control Strategies	62
5.2 Plantwide Control Structures for Acetone Process	80
5.3 Dynamic Simulation Results	88
5.4 Evaluation of Dynamic Performance	108
5.5 Evaluation of Cost	110
CHAPTER VI CONCLUSION AND RECOMMENDATIONS	123
6.1 Conclusion	123
6.2 Recommendation	123
REFERENCES	124
APPENDICES	126
APPENDIX A	127
APPENDIX B	132
VITAE	143

LIST OF TABLES

Table	Page
3.1 Thermal data for pinch analysis (Linnhoff, 1998)	11
3.2 Problem table for data given in Table 3.1	12
3.3 Match Pattern Operators of Class A and B	21
3.4 Match Pattern Operators of Class C and D	22
4.1 Reaction kinetic parameters (Luyben, 2011).....	51
4.2 Process data for heat-integration plant of acetone process	54
4.3 Utility costs (Luyben, 2011).....	55
4.4 Energy consumption and energy cost of acetone process	55
5.1 Potential controlled variables of each unit operation	63
5.2 Manipulated variables and number of control degree of freedom	64
5.3 Case study of flowrate in reactor inlet stream	72
5.4 Case study of composition in reactor inlet stream	73
5.5 Case study of temperature in reactor inlet stream	73
5.6 Case study of total flow in feed C1	74
5.7 Case study of composition in feed C1	75
5.8 Case study of feed temperature C1	75
5.9 Case study of total flow in feed C2	76
5.10 Case study of total flow in feed C2	77
5.11 Case study of total flow in feed C2	77
5.12 Summary control loops of all control structure for acetone process.....	86
5.13 Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process	91
5.14 Dynamic responses of the system to disturbance in fresh feed composition for acetone process.....	98
5.15 Dynamic responses of the system to disturbance in fresh feed temperature for acetone process.....	105
5.16 IAE result for handling the disturbance in fresh feed flowrate	108
5.17 IAE result for handling the disturbance in fresh feed composition	109

Table	Page
5.18 IAE result for handling the disturbance in fresh feed temperature	109
5.19 Energy consumption and cost when fresh feed flowrate changed.....	110
5.20 Energy consumption and costs fresh feed composition changed	111
5.21 Energy consumption and costs fresh feed temperature changed	111
5.22 Dynamic responses of the system to disturbance in fresh feed flowrate for heat-integrated process of acetone	112
5.23 Dynamic responses of the system to disturbance in fresh feed composition for heat-integrated process of acetone.....	116
5.24 Dynamic responses of the system to disturbance in fresh feed temperature for heat-integrated process of acetone.....	119
5.25 IAE result for handling the disturbance in fresh feed flowrate	120
5.26 IAE result for handling the disturbance in fresh feed composition	121
5.27 IAE result for handling the disturbance in fresh feed temperature	121
5.28 Energy consumption and cost when fresh feed flowrate changed.....	121
5.29 Energy consumption and cost fresh feed composition changed	121
5.30 Energy consumption and cost fresh feed temperature changed	121
A.1 Flow summary for the acetone process shown in Figure 4.2.....	128
A.2 Equipment summary for the acetone process	130
B.1 Tyreus-Luyben rule	132
B.2 Type of controllers and tuning parameters of base case	133
B.3 Type of controllers and tuning parameters of CS1	135
B.4 Type of controllers and tuning parameters of CS2	137
B.5 Type of controllers and tuning parameters of CS3	139
B.6 Type of controllers and tuning parameters of CS4	141

LIST OF FIGURES

Figure	Page
3.1 Class A Match Pattern	18
3.2 Class B Match Pattern	18
3.3 Class C Match Pattern	19
3.4 Class A Match Pattern	19
3.5 Control of P/P heat exchangers:	43
4.1 Acetone flowsheet.	49
4.2 Steady-state simulation of acetone process using Aspen HYSYS simulators. ..	53
4.3 Heat-exchanger networks representation in grid diagram.	54
4.4 Acetone process with heat exchanger network flowsheet.	56
4.5 Steady-state simulation of acetone process with heat exchanger.	58
5.1 Control loops to fix the raw materials entered and reentered in the process. ...	65
5.2 Control loops to balance the accumulation of products, by-products, and inert.	66
5.3 Control loop to balance the amount of acetone and IPA.	67
5.4 Control loops not related to quality of product.	68
5.5 Control loops related to quality of product	69
5.6 IPA pathway through the process.	70
5.7 Water pathway through the process.	70
5.8 Acetone pathway through the process.	71
5.9 Hydrogen pathway through the process.	71
5.10 Alternatives of the control loop at the effluent stream.	73
5.11 Temperature profile of C1.	74
5.12 Temperature profile sensitivity at C1.	75
5.13 Temperature profile at C2.	76
5.14 Temperature profile sensitivity at C2.	77
5.15 Control loops obtained by step 4 th and 5 th	78
5.16 Others inventory loops.	79
5.17 Cascade control at the C1.	79

Figure	Page
5.18 Control Structure of Base Case (BC).	81
5.19 Control Structure of CS1	82
5.20 Control Structure of CS2	83
5.21 Control Structure of CS3	84
5.22 Control Structure of CS4	85
5.23 Total IAE results for handling all the disturbances.	109
5.24 The summation of utility costs for each control structure when test all disturbances	111
5.25 The summation of utility costs for the base case and CS3 handling the disturbances for acetone process and heat-integrated of acetone process. ...	122

CHAPTER I

INTRODUCTION

1.1 Background

Plantwide control design has been studied widely in a couple last decades. The category of plantwide control structure approaches are two main methodologies, namely, a heuristic-based and a mathematical-based. The most well-known in the heuristic-based methodology contributors are Luyben (1997) and co-workers. A nine-step approach is developed by Luyben and co-workers based on the process experience of the group. The main consequence of this methodology is an alternative way to achieve a decentralized plantwide control structure. This philosophy is systematic in nature and addresses many of the major issues involved in the plantwide control problem, such as the effects of recycles and energy integration. The other is the mathematical-based methodology that depends on a rigorous mathematical framework of dynamic theory, constrained optimization and systems analysis. Skogestad (2000) and co-workers provided interesting results using these tools. They concentrated on the selection of self-optimizing control variables that give the smallest loss in profit. The mathematical approaches given by these authors, although rigorous, are often very difficult to formulate for large scale systems, in many cases they turn computationally very intensive. In order to achieve this purpose some useful modifications are proposed to generate a new systematic approach able to deal with the most critical problems such as size, complexity, and multiple objectives commonly found in the majority of chemical plants. Recently, Detjareansri (2009) presented the eight-step plantwide control procedure of Wongsri (2009). This procedure based on heuristics and mathematical approaches are applied on the alkylation process. One of the steps of the procedure can find the appropriate set of controlled variables to achieve form fixture

point theorem. The obtained plantwide control structure successfully copes with disturbances entering the process and be able to maintain product quality as compared by integral absolute error (IAE). Furthermore, Sukkongwaree (2009) also showed that the procedure of Wongsri (2009) be capable to provide an excellent performance of control structures though highly complexity with heat-integration recycle plants.

In this research, the proficient control structures of the acetone process which has been proposed as a benchmark problem is discussed. The first study of the acetone process is presented by Torton. Afterward, Luyben (2011) has improved the process adjusting the kinetic rate from irreversible to reversible that more realistic and the absorber pressure is raised to reduce off-gas acetone losses. Nevertheless, the increasing pressure makes higher hydrogen release in the first column feed and causes upper losses of acetone in the vent stream. Eventually, the development optimized the capital costs, energy costs, and raw material costs and also provided a plantwide control structure workable of effectively handling large disturbances in production rate. Hence, this research is focused on the developed design. The acetone process contains several standard unit operations. It comprises both gas and liquid recycle streams to constitute a typical reactor/separator system with recycle. The control structures then be designed applying the new procedure of Wongsri (2012) which is performed through the HYSYS program simulator (Version 7.0).

1.2 Research Objectives

This research aims to design and evaluate the designed plantwide control structures of the acetone process by using the procedure of Wongsri (2012).

1.3 Scope of Research

The scopes of this research are listed as follows:

1. The dynamic simulation of acetone process is performed using HYSYS dynamic simulator (Version 7.0).
2. The description of the acetone process is given by Luyben (2011)
3. The four control structures of the acetone process are designed by using the procedure of Wongsri (2012).

1.4 Contribution of Research

The rest of the research contribution is shown below:

1. Process flowsheet diagram of acetone process via dehydrogenation of 2-propanol is simulated.
2. A new heat exchanger network of the acetone process is designed.
3. The new control structures using Wongsri (2012) are simulated and discussed their performance.
4. Plantwide control structure design procedures of Luyben and Wongsri (2012) are evaluated.

1.5 Research Procedures

The research scheme is followed these steps:

1. Studying plantwide control structure design procedures.
2. Investigating thoroughly all related information of the acetone process.
3. Simulating a steady-state of the acetone process using Aspen HYSYS™.

4. Designing a heat exchanger network of the acetone process using Aspen HYSYS™ and then comparing energy cost of the process with and without heat exchanger networks.

5. Designing new plantwide control structures by using Wongsri (2012) procedure.

6. Simulating dynamic model of all designed control structures.

7. Analyzing and interpreting the dynamic performance of those control structures.

8. Drawing a conclusion of the performance of the control structures.

1.6 Conceptual Framework

The rest of this research is organized as follow;

Chapter I: provide background, objectives, scopes, contributions and outline of the research.

Chapter II: present the literature review related to plantwide control structures design procedure and heat exchanger network design strategies; the review of previous work on the acetone process design.

Chapter III: purpose the theory concerning with plantwide control and heat exchanger network design, and the design procedure based on heuristic of Luyben and of Wongsri (2012).

Chapter IV: elaborate the description of the acetone process and heat exchanger network design of the process.

Chapter V: demonstrate and compare the control structure alternatives and their dynamic simulation results.

Chapter VI: show the conclusion and recommendation of this research.

This is follow by:

References

Appendix A: Process stream data and equipment data

Appendix B: Tuning parameter of control structures

CHAPTER II

LITERATURE REVIEW

The plantwide control design procedures for chemical process have been studied by researchers over the last couple of decades. In general, the plantwide control structure design can be categorized into the heuristic-based and mathematical-based frameworks. However, the integrated framework of heuristics and simulation was proposed by a group of researchers.

One of the conceptual decide of the plantwide control methodology is a heuristic design procedure of Luyben *et al.* (1997). He applied the procedure consisting of nine-step on the three processes; the vinyl acetate monomer process, the Tennessee Eastman process, and the HDA process. The procedure produces a workable plantwide control strategy to achieve the desired objectives. However the heuristic-based methodology is needed experience and basic process understanding for their effective usage. Moreover, heuristics cannot always be totally relied upon as the solution can hardly be unconventional. Furthermore, heuristics can sometimes be contradictory and leave the designer in a dilemma. In the latter-time, the other plantwide design control procedure, an integrated framework of simulation and heuristics, is suggested by Konda, Rangaiah and Krishnaswamy (2005). This framework is successfully applied to the HDA process. A viable control system can be designed by the proposed framework which the advantages of both heuristics and simulation. It shows that plantwide control system cannot be accomplished just by heuristics without the aid of rigorous nonlinear simulation tools.

Another important plantwide design control procedure is a mathematical-based. Larsson and Skogestad (2000) presented the procedure divided in two main

parts: (1) Top-down analysis, to identify degree of freedom and primary controlled variables (look for self-optimizing variables) (2) Bottom-up analysis to determine secondary controlled variables and structure of control system (pairing). The approach based on a rigorous mathematical framework of dynamic theory, constrained optimization and systems analysis. In particular, the selection of self-optimizing control variables that give the smallest loss in profit was concerned. Skogestad (2004) proposed an expanded version of Larsson and Skogestad (2000). A systematic approach to plantwide control begins by defining the operational and economic objectives, and the degrees of freedom available to fulfill them. Other issues include inventory and production rate control, decentralized versus multivariable control, loss in performance by bottom-up design, and a definition of a the “complexity number” which can proceed to find the “optimal” controller for the secondary (regulatory) control layer.

Since the plantwide control methodologies have played an important role, the comparative studies to evaluate the effectiveness of alternate methodologies are important. Vasudevan *et al.* (2009) showed the comparison of the development of a plantwide control for the styrene monomer plant using the integrated framework (Konda *et al.*, 2005). In order to measure its effectiveness, the result was compared to the heuristics procedure of Luyben and co-workers (Luyben *et al.*, 1998) and the self-optimizing control procedure (Skogestad, 2004). An analysis of the results indicated that while all the procedures give stable control structures, the integrated framework and self-optimizing control procedures give more robust control structures than heuristics procedure. Furthermore, Zhang *et al.* (2010) applied this framework to the ammonia synthesis process. The control system was compared to the self-optimization control procedure (Skogestad, 2004). It was found that both control systems give satisfactory response; while the integrated framework of simulation and heuristics performs better in

terms of control and management of production rate during the transient period, the self-optimization control procedure gives higher steady-state profit.

It is shown that the integrated framework combining rigorous nonlinear simulation with heuristics builds synergies between the powers of both the simulation and the heuristics. Nevertheless, the appropriate of controlled variables is one of the most important tasks in plantwide control structure design. Suntisriksomol (2008) suggested the "Fixture Point Theorem" for HDA process to select appropriated set of controlled variables from a large number of candidate output as plant level variables. The fixture point control theorem states that the most disturbed points must be satisfactory controlled by giving them consideration before other controlled variables and mitigating the propagation to other units. The maximum (scaled) gain is used for selecting and pairing controlled variables with manipulated variables. The set of first rank of controlled variables are same as Luyben (1998). In addition, the two set of controlled variables (second and third rank from fixture point) is studied. The five control structures were designed and compared. The performance of designed control structures were presented in the IAE value and compared with reference structure. The designed structures are fast response and the most effective on compared with the base case.

However, a systematic approach of plantwide control using fixture point theorem was not proposed until Detjareansri (2009) proposed the eight-step plantwide control procedure of Wongsri (2009). This procedure based on heuristics and mathematical analysis applied on the alkylation process. One of the steps of the procedure can find the appropriated set of controlled variables to achieve form fixture point theorem. The dynamic performance compared with base case control structure (Luyben, 2002) by two types of disturbances: material and thermal disturbances. The

control structure successfully copes with disturbances entering the process and be able to maintain product quality as compared by integral absolute error (IAE). In the same time, Sukkongwaree (2009) also pointed out that the procedure of Wongsri (2009) not only provides the appropriated set of controlled variables but also consider the energy management via heat exchanger networks. The result of the designed control structures showed an excellent performance of control structures through highly complexity with heat-integration recycle plants.

Luyben (2011) illustrated the design trade-off of the acetone process. The process consists of a vaporizer, heated tubular reactor, flash tank, absorber, and two distillation columns. The economical optimum design is concerned capital costs, energy costs, and raw material costs. There is an optimum absorber pressure that balances the opposing effects for pressure on losses in the absorber off-gas stream and losses in the distillation column vent stream. Raising absorber pressure adversely impacts on reaction kinetics so that reactor temperature must be increased as pressure is up. However, a higher pressure in the absorber made the hot reactor effluent using cooling water instead of refrigerator in the condenser since a low temperature is not required at the higher pressure. Furthermore, the design provided a plantwide control structure workable of effectively handling large disturbances in production rate.

CHAPTER III

THEORY OF PLANTWIDE CONTROL

This chapter provides a basic of pinch technology and the previous heuristic approach of heat exchanger network design. Moreover, the fundamental of plantwide control problem and the preceding heuristic procedures of plantwide control structure are summarized in the following section. It is important to note that the plantwide control structure procedure of Wongsri 2012 is a crucial procedure of this research

3.1 Fundamental Concept of Pinch Technology

Pinch technology provides a systematic methodology for energy saving in processes. The concept was first developed based on an applied thermodynamics point of view (Flower and Linnhoff, 1978; Umeda et al., 1979).

The pinch analysis concept is originated to design the heat recovery in network for a specified design task. Starting with calculate heat and material balance of the process obtained after the core process has been design. By using thermal data from the process, we can set the target for energy saving prior to the design of the heat exchanger networks.

Table 3.1 Thermal data for pinch analysis (Linnhoff, 1998)

Stream No.	Stream Type	Start	Target	Heat Capacity
		Temperature, Ts (°C)	Temperature, Tt (°C)	Flowrate, CP (kW/°C)
1	Hot	180	80	20
2	Hot	130	40	40
3	Cold	60	100	80
4	Cold	30	120	36

Table 3.1 shows the necessary information for pinch analysis: source, start and target temperature and heat capacity flowrate for each stream. “Hot streams” are the streams that need cooling such as heat sources while cold streams are the streams that need heating such as heat sinks. The heat capacity flow rate (CP) is the mass flowrate times the specific heat capacity

$$CP = C_p \times M$$

Where C_p is the specific heat capacity of the stream (kJ/kg.°C)

M is the mass flowrate (kg/s)

The CP of a stream is measured as enthalpy change per unit temperature (kW/°C or equivalent units).

To find the location of pinch, the problem table method is an easy numerical method is used to calculate the pinch point and the minimum energy requirements. For this example, a minimum temperature difference, ΔT_{min} , is 10°C. The results obtained from this method are shown in Table 3.2

Table 3.2 Problem table for data given in Table 3.1

CP (kW/°C)				Thot (°C)	Tcold (°C)	Sum CP (kW/°C)	dT (°C)	Required Heat Qh	Interval (kW)	Cascade Heat (kW)	Sum Interval (kW)
H1	H2	C1	C2								
0	0	0	0	180	170	0		960	0	960	0
20	0	0	0	130	120	20	50	960	1000	1960	1000
20	40	0	36	110	100	24	20	1960	480	2440	1480
20	40	80	36	80	70	-56	30	2440	-1680	760	-200
0	40	80	36	70	60	-76	10	760	-760	0	-960
0	40	0	36	40	30	4	30	0	120	120	-840
										Qc	

The pinch separates the problem into 2 thermodynamic regions called hot end and cold end. The hot end is the region comprising all streams or part of stream above the pinch temperature. Only hot utility is required in this region but not cold utility. On the other hand, the cold end is the region comprising all streams or part of stream below the pinch temperature and only cold utility is instead desired regardless the hot utility. Therefore, if there is no heat transfer across the pinch, the minimum utility requirement is achieved.

3.2 Heat Exchanger Networks Synthesis and Design

To attain an optimal network, a minimum number of units that reflects on a capital cost and maximum heat recovery that reflects on operating costs must be materialized. The responsibility of a good engineering design is to deal with minimizing capital and operating costs. However, the heat exchanger network design is importantly considered operability, reliability, safety, etc. Consequently, HENs synthesis is not only focused on costs but also the operability features of a HEN. The ability of a HEN to tolerate unwanted changes in operating conditions is called *resiliency*. On the other hand, the ability of a HEN to tolerate wanted changes is called *flexibility*.

3.2.1 Heuristics

Several HENs matching rules with minimum energy and investment costs have been presented (Masso and Rudd, 1969, Ponton and Donalson, 1974 Rathore and Powers, 1975, Linnhoff and Hindmarsh, 1983, Jezowski and Hahne1986, Huang, Metha and fan, 1988, etc.). The following are heuristics from the literature classified according to the design criteria.

The heuristics to minimize the capital cost (the number of heat exchangers):

Heuristic C1: To generate a network featuring the minimum number of heat exchanger units, let each match eliminate at least one of the two streams; a tick-off rule (Hohmann, 1971).

Heuristic C2: Prefer the matches that will leave a residual stream at its cold end for a heating problem, or its hot end for a cooling problem. A match of this type will feature the maximum temperature difference.

Heuristic C3: Prefer matching large heat load streams together. The significance of this rule is that the control problem (a capital cost) of a match of this type (whether it is implemented by one or many heat exchangers) should be less than that of heating or cooling a large stream with many small streams.

The heuristics to minimize the energy cost (the minimum utility requirement):

Heuristic E1: Divide the problem at the pinch into subproblems, one a heat sink (heating subproblem or hot end problem) and the other a heat source (cooling subproblem or cold end problem), and solve them separately (Linnhoff and Hindmarsh, 1983).

Heuristic E2: Do not transfer heat across the pinch.

Heuristic E3: Do not cool above the pinch.

Heuristic E4: Do not heat below the pinch.

The laws of thermodynamics:

Heuristic T1: In a heating problem, if a supply temperature of a cold stream is less than a target temperature of a hot stream by ΔT_{\min} or more and the heat capacity flowrate of a hot stream is less than or equal to the heat capacity flowrate of a cold stream, the match between these two streams is feasible (Immediately above the pinch temperature, the heat capacity flowrate of a cold stream must be greater than or equal to that of a hot stream.).

Heuristic T2: In a cooling problem, if a supply temperature of a hot stream is greater than a target temperature of a cold stream by ΔT_{\min} or more and the heat capacity flowrate of a hot stream is greater than equal to the heat capacity flowrate of a cold stream, the match between these two streams is feasible (Immediately below

the pinch temperature, the heat capacity flowrate of a hot stream must be greater than or equal to that of a cold stream.).

Heuristic T3: For a situation different from the above rule, match feasibility must be determined by checking whether ΔT_{\min} of a match violates the minimum approach which is specific by the design.

3.2.2 Match Pattern

This is another heuristics approach based on the use of rules of thumb to provide a plausible direction in the solution of the problem. There are a number of design procedures using heuristic in structuring an optimal network featuring minimum number of matches and maximum energy recovery. Nevertheless, Match pattern is another method which used heuristics to structure a resilient network.

The heuristic approach to design or synthesis a resilient HEN was presented by Wongsri (1990). A resilient network is defined as a network that provides a down path for variable process streams so that their specified input heat load disturbances can be shifted to the heaters or coolers in their network without violation in the specified target temperatures and MER. HENs synthesis is usually considered as a combinatorial matching problem. Match patterns are the descriptions of the match configuration of two, and possibly more, process streams and their properties that are thermally connected with the heat exchangers.

Match patterns are classified following criteria are considered important in this research:

1. Position of a Match

One heuristic prefers a match at the cold end and another prefers a match at the hot end. Pinch heuristics prefers a match at the cold end in a heating subproblem and a match at the hot end in a cooling subproblem. However, there are other possibilities by using the tick-off heuristics. There are four ways that two streams can match. This leads to the basic four match patterns (Wongsri, 1990)

2. Heat capacity flowrate (between hot and cold stream)

See *Heuristic T.1* and *T.2*

3. Heat Load (between hot and cold streams)

The heuristic that concerns heat load state that one must match large heat load hot and cold streams first. This leads to two additional heuristic:

Heuristic N1: For a heating subproblem, a match where the heat load of a cold stream is greater than that of a hot stream should be given higher priority than the other. The reason is that the net heat load heating subproblem is in deficit. The sum of heat loads of cold streams is greater than of hot streams. The purposed match will likely be part of a solution (Wongsri, 1990).

Heuristic N2: Conversely, a match where the heat load of a hot stream is greater than that of a cold in a cooling subproblem are preferred (Wongsri, 1990).

4. Residual Heat Load.

No heuristics for this quantity have thus far appeared in the literature. Two new heuristics are introduced:

For a match in a heating subproblem that satisfies the heat load preference heuristics N.1;

Heuristic N3: a match where the residual heat load is less than or equal to the minimum heating requirement are preferred (Wongsri, 1990).

For a match in a cooling subproblem that satisfies the heat load preference or heuristics N.2;

Heuristic N4: a match where the residual heat load is less than or equal to the minimum cooling requirement are preferred (Wongsri, 1990).

The reason behind the above two heuristics N3 and N4 is that the residual may be matched to a utility stream. One has the possibility of eliminating two streams at once.

In the next section, class of match patterns is illustrated thoroughly. There are four match patterns for a pair of hot and cold streams according to the match position and the length (heat load) of stream. The four match patterns are considered as the basic match pattern classes simply called A, B, C and D shown in Figure 3.1-3.4. Any eligible match must belong to one of the four match pattern classes.

Class A Match Pattern

The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the cold end of the cold stream. The residual heat load is on the hot portion of the cold stream (Figure 3.1).

Class B Match Pattern

The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the hot end of the hot stream. The residual heat load is on the cold portion of the hot stream (Figure 3.2).

Class C Match Pattern

The heat load of a hot stream is greater than the heat load of a cold stream in a pattern, i.e. the cold stream is totally serviced. The match is positioned at the cold end of the hot stream. The residual heat load is on the hot portion of the hot stream (Figure 3.3).

Class D Match Pattern

The heat load of a cold stream is greater than the heat load of a hot stream in a pattern, i.e. the hot stream is totally serviced. The match is positioned at the hot end of the cold stream. The residual heat load is on the cold portion of the cold stream (Figure 3.4).

When the residual heat load in a match pattern is matched to a utility stream, it is a closed or completed pattern. Otherwise, it is an open or incomplete pattern. It can be seen that if the heat load of the residual stream is less than the minimum heating or cooling requirements then the chances that the match pattern will be matched to a utility stream is high. Therefore, we give a match pattern which residual less than the minimum heating or cooling requirement a high priority in match pattern.

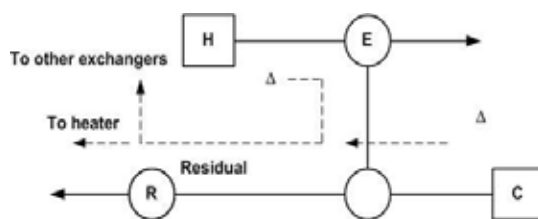


Figure 3.1 Class A Match Pattern

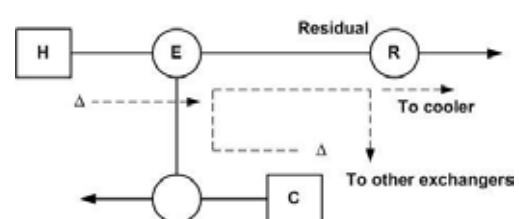


Figure 3.2 Class B Match Pattern

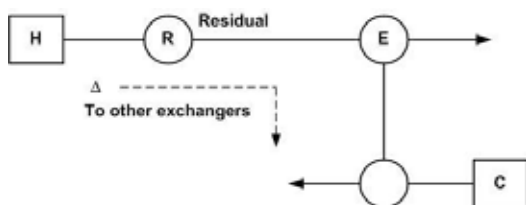


Figure 3.3 Class C Match Pattern

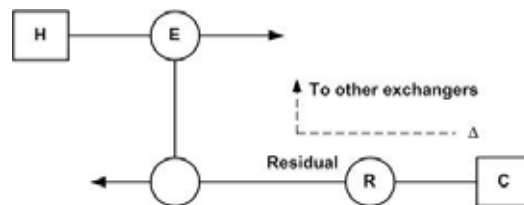


Figure 3.4 Class D Match Pattern

A match of Class A or Class C will leave a residual at the hot end, while a match of class B or D will leave a residual at the cold end. Heuristics N.3 and N.4 will be use heuristics to further subclassify matches of class A and B into matches of high priority.

To make use Heuristic N.3 and N.4 to further subclassify matches, class A and B are given the following subclass match high priorities.

Subclass AH

A match of this subclass is a member of Class A, a heating problem where the residual is less than or equal to the minimum heating requirement. (A letter H in the subclass name denotes that the residual is matched to a heating utility.)

Subclass BK

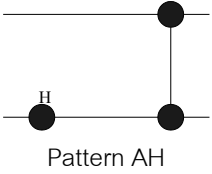
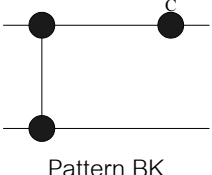
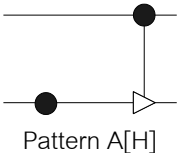
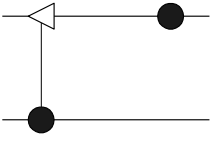
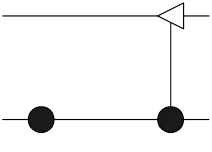
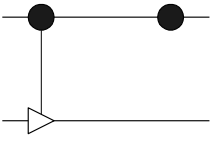
A match of this subclass is a member of Class B, a cooling problem where the residual is less than or equal to the minimum cooling requirement. (A letter K in the subclass name denotes that the residual is matched to a cooling utility).

As it might be expected, a match of subclasses AH in a heating subproblem and BK in a cooling subproblem given in the highest priorities as illustrated in Table 3.3.

To discriminate match patterns according to heat capacity flowrate, by following pinch heuristics, in a heating problem, a match where the heat capacity flowrate of a cold stream is greater than or equal to that of a hot stream are satisfied. For example, A[H]H is a match in which the heat capacity flowrate of the cold stream is greater than that of the hot stream and the residual of the cold stream is matched to the heating utility. Similarly in a cooling problem, a match in which the heat capacity flowrate of a hot stream is greater than or equal to that of a cold stream are preferred. For example, B[C]K is a match in which the heat capacity flowrate of the hot stream is greater than that of the cold stream and the residual of the hot stream is matched to the cooling utility.

In summary, the rankings of the match patterns in a heat problem are AH, A[H], B[C], A[C], B[H],C[H], D[C] and D[H]. For a cooling problem, BK, B[C], A[H], B[H], A[C], D[C], C[H], D[H] and C[C].

Table 3.3 Match Pattern Operators of Class A and B

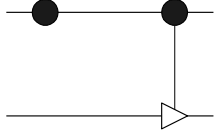
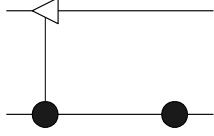
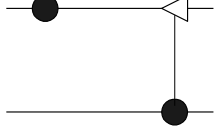
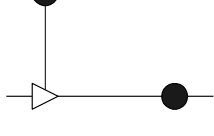
Match Operators	Conditions	Actions
	$T_H^s \geq T_C^t$ $L_H \leq L_C$ $T_H^s \geq T_C^s + L_H W_C^{-1}$ $L_C - L_H \leq Q_{\min}^{\text{heating}}$	Match H and C Status of H \Leftarrow Matched*** $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
	$T_H^s \geq T_C^t$ $L_C \leq L_H$ $T_C^s \leq T_H^s - L_C W_H^{-1}$ $L_H - L_C \leq Q_{\min}^{\text{cooling}}$	Match H and C Status of C \Leftarrow Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
	$T_H^t \geq T_C^s$ $L_H \leq L_C$ $W_C \geq W_H$	Match H and C Status of H \Leftarrow Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
	$T_H^s \geq T_C^t$ $L_C \leq L_H$ $W_C \leq W_H$	Match H and C Status of C \Leftarrow Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
	$T_H^t \geq T_C^s$ $L_H \leq L_C$ $W_C < W_H$ $T_H^s \geq T_C^s + L_H W_C^{-1}$	Match H and C Status of H \Leftarrow Matched $T_C^s \Leftarrow T_C^s + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
	$T_H^s \geq T_C^t$ $L_C \leq L_H$ $W_H < W_C$ $T_C^s \leq T_H^s - L_C W_H^{-1}$	Match H and C Status of C \Leftarrow Matched $T_H^s \Leftarrow T_H^s - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$

* T^t = Target temp, T^s = Supply temp, W =Heat capacity flowrate, L , Q =Heat load.

** Cold stream temperatures are shifted up by ΔT_{\min} .

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set of process streams to be selected next.

Table 3.4 Match Pattern Operators of Class C and D.

Match Operators	Conditions	Actions
 <p>Pattern C[H]</p>	$T_H^t \geq T_C^s$ $L_H > L_C$ $W_H \leq W_C$	<p>Match H and C</p> <p>Status of C \Leftarrow Matched</p> $T_H^t \Leftarrow T_H^t - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 <p>Pattern D[C]</p>	$T_H^s \geq T_C^t$ $L_H < L_C$ $W_H \geq W_C$	<p>Match H and C</p> <p>Status of H \Leftarrow Matched</p> $T_C^t \Leftarrow T_C^t + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$
 <p>Pattern C[C]</p>	$T_H^t \geq T_C^s$ $L_H > L_C$ $W_C < W_H$ $T_C^t \leq T_H^t + L_C W_H^{-1}$	<p>Match H and C</p> <p>Status of C \Leftarrow Matched</p> $T_H^t \Leftarrow T_H^t - L_C W_H^{-1}$ $L_H \Leftarrow L_H - L_C$
 <p>Pattern D[H]</p>	$T_H^s \geq T_C^t$ $L_H \leq L_C$ $W_H < W_C$ $T_H^t \geq T_C^t - L_H W_C^{-1}$	<p>Match H and C</p> <p>Status of H \Leftarrow Matched</p> $T_C^t \Leftarrow T_C^t + L_H W_C^{-1}$ $L_C \Leftarrow L_C - L_H$

* T^t = Target temp, T^s = Supply temp, W =Heat capacity flowrate, L , Q =Heat load.

** Cold stream temperatures are shifted up by ΔT_{\min} .

*** There are two statuses of process streams, 'active' and 'matched'. This will exclude this stream from a set of process streams to be selected next.

3.3 Plantwide Control Issues

Most continuous processing plants contain many units, such as reactor, heat exchangers, and distillation columns. The goal of process design is to minimize capital costs while operating with optimum utilization of materials and energy. Unfortunately, achieving lower plant capital costs and higher processing efficiencies inevitably makes the individual units interact more with each other and thus makes them harder to control. The process control engineer deals with these unit-to-unit interactions by designing a control system that counteracts disturbances before they propagate from their source to other units. Therefore, there are general problems a control system is called on to satisfy.

3.3.1 Motivations of integrated process

Three basic features of integrated chemical processes must be taken into the account for plantwide control problems: (1) The effect of material recycle, (2) the effect of energy integration and (3) the effect of chemical component inventories. However, there are fundamental reasons why each of these exists in virtually all real processes.

3.3.1.1 Material recycles

Material is recycled for six basic and important reasons.

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

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

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

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

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

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

3.3.1.2 Energy Integration

The fundamental reason for the use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost. For energy-intensive processes, the savings can be quite significant.

3.3.1.3 Chemical component inventories

There are three types of chemical species in a chemical process: reactants, products, and inert. A material balance for each of these components must be satisfied. This is typically not a problem for products and inerts. However, the real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every molecule of reactants fed into the plant must either be consumed via reaction or leave as impurity or purge. The loss of reactants exiting the process is minimized since this represents a yield penalty. Therefore, we must ensure that every mole of reactant fed to the process is consumed by the reactions.

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

3.4 Plantwide Control Problem

3.4.1 Internal feedback of material and energy

Processes that include recycle systems have an important design requirement—namely, that there must be an exit path for every chemical species. For example, inert components can be kept at reasonable levels by “bleeding off” a small portion of the recycle stream. However, Luyben (1994) discussed a subtle problem with recycle systems, the snowball effect, which is characterized by a large sensitivity of one or more of the variables in a recycle loop to small changes in a disturbance variable. This problem arises from both a small reactor holdup and a particular control structure.

In particular, if changes in fresh feed composition “load the reactor excessively”—that is, beyond its ability to provide the required conversion—then the separator/recycle system will be called on to make up the deficiency. For the case where extra reactor capacity is available through an increase in the reactor level, the particular choice of level/flow control structure within the recycle loop can radically affect plant gains (sensitivities). In the following, we assume that the reactor design is fixed and its level is set at less than full capacity. The question to be considered is how alternative designs of level and flow loops mitigate the effect of fresh feed flow rate or composition disturbances.

3.4.1.1 Steady-state behavior: the snowball effect

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

This high sensitivity of the recycle flowrates to small disturbances called the snowball effect. It is important to note that this is not a dynamic effect; it is a steady-state phenomenon, it can be analyzed by considering a steady-state model. However, it does have dynamic implications for disturbance propagation and for inventory control. There is nothing to do with closed-loop stability. Furthermore, this does not imply that it is independent of the control structure. On the contrary, the extent of the snowball effect is very strongly dependent upon the control structure used. The large swings in recycle flowrates are undesirable in a plant because they can overload the capacity of the separation section or move the separation section into a flow region below its minimum turndown. Therefore, it is important to select a plantwide control structure that avoids this effect.

3.4.1.2 Transient behavior: the slowdown in overall system dynamics

A second characteristic of using material recycle and/or heat integration is that the plant may respond to disturbances much more slowly than would be anticipated based on the time constants of individual units.

3.4.1.3 Propagation and recirculation of disturbances

A third major effect often encountered with recycle and heat integration is the propagation of disturbances from unit to unit, and their recirculation around internal process flow paths. This understanding why this plantwide control issue differs so substantially from single-unit issues.

In a single unit regulation, one desirable effect of using feedback control to attenuate disturbances in a process unit is to transfer these variations to a utility stream. For example, if a reactor temperature is disturbed, the cooling water flow rate will be changed by the temperature controller so as to reduce the effect of the disturbance. Even so, some variation in reactor temperature inevitably will remain, and this will propagate to downstream units as a disturbance.

A minor side effect of these actions is that the supply header temperature itself will change slightly as cooling water demand is raised/lowered by actions of a reactor temperature controller. Although utility supply systems are built with their own internal controllers, and these are designed to attempt to regulate the utility outputs in the face of process disturbances, it is not possible to attenuate utility disturbances entirely. These propagate directly throughout the plant.

In older plants, surge tanks were used to damp flow variations between units. Material holdup in a surge tank can also serve as a thermal capacitance and thus reduce effluent temperature variations; only reduced flow and temperature variations propagate to downstream units. In today's more highly integrated plants, containing material recycle and/or heat integration but little surge capacity, unattenuated disturbances propagate directly to downstream units, even to adjacent (coupled) units and to upstream units.

3.4.2 Interaction of plant design and control system design

In the past, when the continuous processing plants were designed to be much less interaction than now, it was possible to complete the plant design before considering control system design. After the proposed plant's flowsheet and equipment specifications were completed, process control engineers were responsible for specifying instruments and controllers. By providing an excess of measurements (instruments) and control valves, plus a feedback controller for every important process variable, the control system designer was reasonably sure that the new plant could be started up and controlled. Continuous processing plants designed or retrofitted today no longer can utilize a sequential design process in which plant design is followed by control system design (Keller and Bryan, 2000), nor can designers specify redundant equipment, except for safety purposes.

Without careful attention to design, highly integrated plants may have too few control degrees of freedom, which makes them difficult to start up and operate safely. For example, in designing the heat exchanger and related equipment for heat integration the heating and cooling loads first must be approximately balanced by the process designer. Then the designer must establish whether the approach temperatures are satisfactory to meet the heat transfer requirements with a reasonably sized heat exchanger; in this step, adjustment of column operating pressures may be required (Seider et al., 2003). Because the energy supply capability in one unit usually will not balance the demand in another unit exactly, a "trim exchanger" (small heat exchanger sized to make up the difference in heating/cooling capability) generally has to be provided in the steady-state design.

A heat integration scheme also causes two control degrees of freedom to be “lost”: the cooling water flow rate control valve that would have been located in the Column 1 condenser, plus the steam control valve that would have been used in the Column 2 reboiler. If process control engineers are not involved in the plant design process from the beginning, the critical process dynamic and control evaluations may be omitted that would provide such information and an opportunity to resolve any problems (Keller and Bryan, 2000). In short, a suitably sized trim unit must be available to make up for any steady-state heating/cooling deficiency plus lost control degrees of freedom necessary for normal operations. It also can assist in start-up and shutdown operations.

The control system designer must determine whether a proposed plant design will be controllable and operable (Fisher et al., 1988b; Downs and Ogunnaike, 1995). For example, highly integrated distillation columns can cause problems in a number of ways:

1. One or both column products cannot be controlled at the desired set point(s).
2. Disturbances in the Column 1 overhead cannot be prevented from propagating to Column 2.
3. The “lost degrees of freedom” from plant integration need to be restored by the addition of one or two trim heat exchangers operated and controlled using plant utility supplies.
4. The plant cannot be started up easily because of the need to have Column 1 “hot” before Column 2 can be brought into service.

Consequently, there are three main functions of the control system, namely, disturbance rejection. It is the main objective in installing control system. The external disturbance is uncertain so the operator cannot monitor the changing in process. As a result, the control system must be installed to follow the changing of process and manipulate the process variable to compensate for the disturbance from external factors. Another function is to maintain stability. The stability is necessary for every process. As a result the control system is set to improve the process stability for the guarantee of quality of product, safety to equipment of process and plant. The other is to keep the process performing highest efficiency. Besides rejecting disturbance and maintaining stability, the control system can achieve the great profit because it losses less energy and raw materials during the operating. Moreover, the product will meet the required specification and have high production rate.

3.5 Fundamental Procedures for Plantwide Control

3.5.1 Buckley basics

Page Buckley (1964) was the first to suggest the idea of separating the plantwide control problem into two parts: material balance control and product quality control. He suggested looking first at the flow of material through the system. A logical arrangement of level and pressure control loop is established, using the flowrates of the liquid and gas process streams. No controller tuning or inventory sizing is done at this step. The idea is to establish the inventory control system by setting up this “hydraulic” control structure as the first step. Then, he proposed to establishing the product-quality control loops by choosing appropriate manipulated variables. The time constants of the closed-loop product-quality loops are estimated. They try to make these as small as possible so that good, tight control is achieved, but stability constraints impose limitations on the achievable performance.

3.5.2 Douglas doctrines

Jim Douglas (1988) has devised a hierarchical approach to the conceptual design of process flowsheets. Although he primarily considers the steady-state aspects of process design, he has developed several useful concepts that have control structure implications. He points out that in the typical chemical plant the costs of raw materials and the value of the products are usually much greater than the costs of capital and energy. This leads to the two Douglas doctrines:

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

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

3.5.3 Downs drill

Jim Dows (1992) pointed out the importance of looking at the chemical component balances around the entire plant and checking to see that the control structure handles these component balances effectively. The concepts of overall component balances go back to our first course in chemical engineering, where they learned how to apply mass and energy balances to system, microscopic or macroscopic. They did these balances for individual unit operations, for section of a plant, and for entire processes. He must ensure that all components (reactants, products, and inerts) have a way to leave or be consumed within the process.

3.5.4 Luyben laws

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

1. A stream somewhere in all recycle loops should be flow controlled.

This is to prevent the snowball effect

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

3. If the final product from a process comes out the top of a distillation column, the column feed should be liquid. If the final product comes out the bottom of a column, the feed to the column should be vapor (Cantrell et al., 1995). Changes in feed flowrate or feed composition have less of a dynamic effect on distillate composition than they do on bottoms composition if the feed is saturated liquid. The reverse is true if the feed is saturated vapor: bottom is less affected than distillate. If our primary goal is to achieve tight product quality control, the basic column design should consider the dynamic implications of feed thermal conditions.

3.5.5 Richardson rule

Richardson (1995) suggested the heuristic that the largest stream should be selected to control the liquid level in a vessel. This makes good sense because it provides more muscle to achieve the desired control objective. An analogy is that it is much easier to maneuver a large barge with a tugboat than with a life raft. The point is that the bigger the handle you have you have to affect a process, the better you can control it.

3.5.6 Shinskey schemes

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

3.5.7 Tyreus tuning

Tyreus and Luyben (1997) suggested one of the vital steps in developing a plantwide control system, once both the process and the control structure have been specified, is to determine the algorithm to be used for each controller (P,PI, or PID) and to tune each controller. They strongly recommend the use of P-only controllers for liquid levels (even in some liquid reactor applications) and the use PI controller for other control loops. The relay-feedback test is a simple and fast way to obtain the ultimate gain (K_u) and ultimate period (P_u). Then either the Ziegler-Nichols settings (for very tight control with a closed-loop damping coefficient of about (0.1) or the Tyreus-Luyben (1992) settings (for more conservative loops where a closed-loop damping coefficient of 0.4 is more appropriate) can be used:

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

$$K_{TL} = K_u/3.2 \quad \tau_{TL} = 2.2P_u$$

3.6 Step of Plantwide Control Design Procedure

Plantwide control design procedure is importantly satisfying the principles of the overall conservation of energy and mass. Furthermore, economic criterion is essentially taken into account.

Luyben et al., (1997) proposed a nine-step heuristic design procedure for a workable plantwide control strategy. The nine-step of the design procedure essentially concentrate on: energy management; production rate; product quality; operational; environmental and safety constraints; liquid-level and gas-pressure inventories; makeup of reactants; component balances; and economic or process optimization.

Step 1: Establish control objectives

Assess the steady-state design and dynamic control objectives for the process. This is probably the most important aspect of the problem because different control objectives lead to different control structures. The chosen control structure for a plant depends upon the design and control criteria established. 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 degree of freedom

Count the number of control valves available. This is the number of degrees of freedom for control, that is, the number of variables that can be controlled. The valves must be legitimate (flow through a liquid-filled line can be regulated by only one control valve). The placement of these control valves can sometimes be made to improve dynamic performance, but often there is no choice in their location

Step 3: Establish energy management system

Term “energy management” indicates two functions. Firstly, it is necessary that the design is provided 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. The other function, if heat integration does occur between process streams, then this second function of energy management is to provide a control system that prevents the propagation of thermal disturbances and ensures the exothermic reactor heat is dissipated and not recycled. Process-to-process heat exchangers and heat-integrated unit operations must be analyzed to determine that there are sufficient degrees of freedom for control.

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. To obtain higher production rate, the overall reaction rates must be increased. This can be accomplished by increasing temperature, pressure, reactant concentrations, or reactor holdup.

A variable that has the least effect on the separation section and a rapid and direct effect on reaction rate in the reactor without hitting an operational constraint must be selected.

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

Select the “best” valves to control each of the product-quality, safety, and environmental variables. The tight controls of these important quantities are required for economic and operational reasons. Hence, the manipulated variables should be selected such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead times and large steady-state gains. The former gives small closed-loop time constants and the latter prevents problems with the range-ability of the manipulated variable (control valve saturation).

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

Determine the valve to control each inventory variable. These variables include all liquid levels (except for surge volume in certain liquid recycle streams) and gas pressures. An inventory variable should typically be controlled with the manipulated variable that has the largest effect on it with that unit.

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 flow in the recycle loop are controlled by levels. For gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields.

Step 7: Check component balances

Ensure that the overall component balances for each chemical species can be satisfied either through reaction or exit streams by accounting for the composition of a component or inventory at some point in the process.

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

Step 8: Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations. For example a tubular reactor usually requires control of inlet temperature. High-temperature endothermic reactions typically have a control system to adjust the fuel flowrate to a furnace supplying energy to the reactor. Liquid solvent feed flow to an absorber is controlled as some ratio to the gas feed.

Step 9: Optimize economics or improve dynamic controllability

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

Afterward, the procedure of Wongsri (2009) presented the eight-step of design procedure which based on heuristics analysis. In this procedure, the precedence of control variables is established. The major disturbances are directed or managed explicitly to achieve the minimal interaction between loops by using the extended (thermal) disturbance propagation method (Wongsri, 1990) to cover the material disturbances. The purposed plantwide control structure design procedure for selection the best set of control structure is intuitive, simple and straightforward.

Step1. Establishment of control objective

Step2. Selection of controlled variables

Step3. Selection of manipulated variables and measurements via DOF analysis

Step4. Energy management via heat exchanger networks

Step5. Selection of control configuration using various tools available

Step6. Completing control structure design by checking the component balance

Step7. Selection of controller type: single loop or MPC

Step8. Validation via rigorous dynamic simulation

Fixture Point theorem

The selected controlled variables are ranked using the Fixture point theorem. The step of fixture point theorem analysis is followed below.

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

3.7 Plantwide Energy Management

Plantwide control issue around energy conservation has played an important role in process design. It is general practical to install feed-effluent heat exchangers (FEHs) around reactors and distillation columns. In any process flowsheet, a number of streams must be heated, and other streams must be cooled. For example, in HDA process, the toluene fresh feed, the makeup hydrogen, the recycle toluene, and the recycle gas stream must be heated up to reaction temperature. Furthermore, the reactor effluent stream must also be cooled to the cooling water temperature to accomplish a phase split. Hence, the energy integration is required to reduce the utility cost and also to improve thermodynamic efficiency of the process.

3.7.1 Heat recovery

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

3.7.2 Control of process-to-process exchanger

Process-to-process (P/P) exchangers are used for heat recover within a process. The two exit temperatures provided the two inlet flowrates independently manipulated. However, these flowrates are normally unavailable to manipulate. Hence, two degrees of freedom for temperature control are neglected. One of these degrees of freedom can be restored fairly easily. It is possible to oversize the P/P exchanger and provides a controlled bypass around it as in Fig. 3.5a. It is possible to combine the P/P exchanger with a utility exchanger as in Fig. 3.5b.

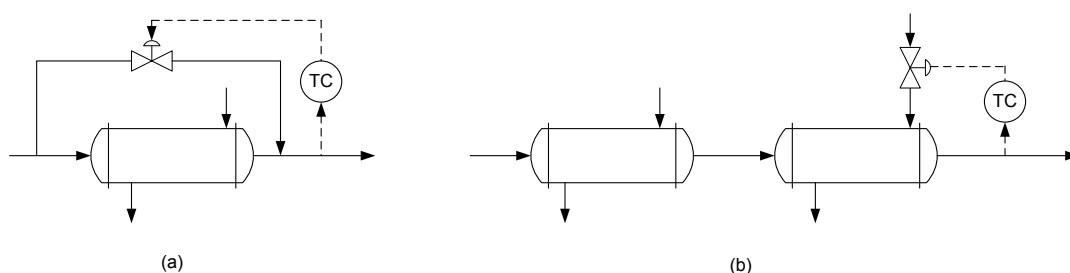


Figure 3.5 Control of P/P heat exchangers: (a) Use of bypass; (b) use of auxiliary utility exchanger.

3.7.2.1 Use of bypass control

When the bypass method is used for unit operation control, there are several choices about the bypass location and the control point. Figure 3.6 shows the most common alternatives. The question “Which option is the best?” may be asked. It depends on “the best” option is defined. As with many other examples, it boils down to a trade-off between design and control. Design considerations might suggest the measure and bypass on the cold side since it is typically less expensive to install a measurement device and a control valve for cold service than high-temperature service. Cost considerations would also suggest a small bypass flow to minimize the exchanger and control valve sizes. From a control standpoint the most important stream should be measured, regardless of temperature, and bypassed on the same side. This minimizes the effects of exchanger dynamics in the loop. A large fraction of the controlled stream needs to be bypassed since it improves the control range. This requires a large heat exchanger.

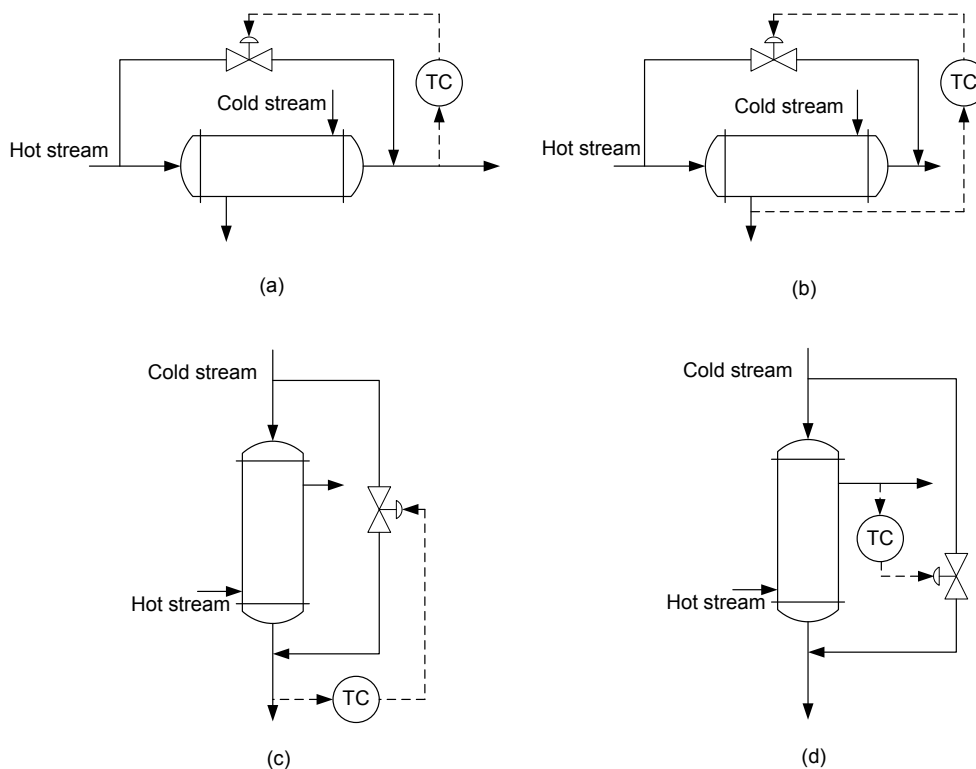


Figure 3.6 Bypass controls of process-to-process heat exchangers. (a) Controlling and bypassing hot stream; (b) controlling cold stream and bypassing hot stream; (c) controlling and bypassing cold stream; (d) controlling hot stream and bypassing hot stream.

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

3.7.2.2 Use of auxiliary utility exchangers

When the P/P exchanger is combined with a utility exchanger, there are a few design decisions to make. Firstly, the relative sizes between the recovery and the utility exchangers are established. From a design standpoint, the recovery exchanger large and the utility exchanger small are considered to give the most heat recovery. It is also the least expensive alternative from an investment standpoint. However, a narrow control range and the inability to reject disturbances make this choice the least desirable from a control standpoint.

Next step, the decision which how to combine the utility exchanger with the P/P exchanger is inquired. This could be done either in a series or parallel arrangement. Physical implementation issues may dictate this choice but it could affect controllability. Finally, the decision is made that how to control the utility exchanger for best overall control performance.

Consider a distillation column that uses a large amount of high-pressure steam in its thermo siphon reboiler. To reduce operating costs, this column will be heat-integrated with the reactor. Practically, this is to generate steam in a waste heat reboiler connected to the reactor as suggested. Then, some or all of these streams are used to help reboiling the column by condensing the steam in the tubes of a stab-in reboiler. However, the total heat from the reactor may not be enough to reboil the column, so the remaining heat must come from the thermo siphon reboiler that now serves as an auxiliary reboiler. The column tray temperature controller would manipulate the steam to the thermo siphon reboiler.

CHAPTER IV
ACETONE PROCESS AND
NEW CONTROL STRUCTURES DESIGN PROCEDURE

4.1 Introduction

Acetone is widely used as solvents and a precursor to other chemical products. The largest usage of acetone is to make methyl methacrylate (MMA) and methacrylic acid. About 80% of the MMA is polymerized to produce homo- and co-polymers. In addition, acetone is consumed by production of bisphenol-A (BPA), methyl isobutyl ketone (MIBK) and methyl isobutyl carbinol. Other applications include coatings, film, adhesives, pharmaceuticals and antioxidants. The production of acetone has two important routes. Approximately 90% of acetone is produced via the cleavage of cumene hydroperoxide into phenol as by-product. The other route is the catalytic dehydrogenation of isopropyl alcohol (IPA). This process assures that acetone is free from aromatic compounds, particularly benzene. For this reason, the pharmaceutical manufacturing may advocate the acetone production via dehydrogenation of IPA due to the strictly limitation imposed on solvents by Food and Drug Administration (FDA).

4.2 Process Studied

4.2.1 Process description

Figure 4.1 shows the detail of the acetone production via dehydrogenation of IPA. In the reaction section, this section comprises of a vaporizer, plug flow reactor. The liquid fresh feed 51.96 kmol/h consisting of 67 mol % IPA and 33 mol % water is combined with a small recycled stream. The mixture is fed to the vaporizer using high-pressure steam (HPS) to increase temperature around 451 K. Afterward, such stream is dehydrogenated in the plug flow reactor at around 753.5 K with 90 % conversion. The optimization operation design of Luyben (2011) is at 17.5 atm and using 200 tubes. The effluent of the reactor is the mixtures of acetone, hydrogen, water, and IPA. The heating medium of the reactor is accomplished using a molten salt recycling stream, which is not modeled in our process. The molten salt stream is continuously heated using a furnace.

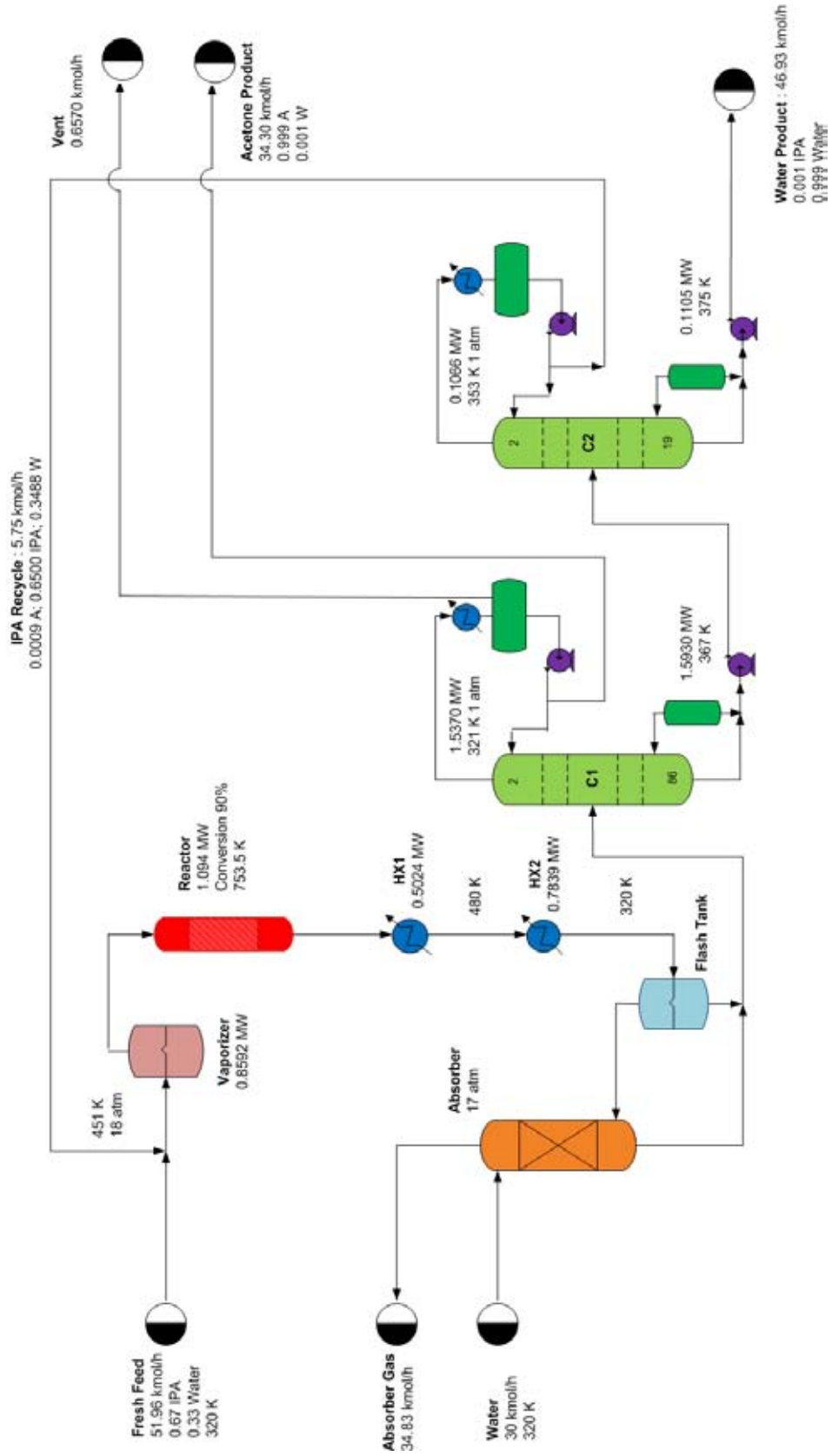


Figure 4.1 Acetone flowsheet

In the separation section, this section is composed of two heat exchangers, flash tank, absorber and two distillation columns. Before operating with distillation columns, the very high temperature product stream is cooled by the two heat exchangers. The first one decreases the temperature of the stream to 480 K using low-pressure steam (LPS) and the second one drops the temperature of the stream to 320 K using cooling water (CW). The reason that the cooling section is divided into two stages is the low-pressure steam is cheaper than cooling water so that only using cooling water to bring the stream down from 753.5 K is highly expensive. The cooled stream is continuously passed through the flash tank to release the most of the hydrogen from the denser liquids. The hydrogen dominant stream is fed into the bottom of the 10-stage absorber to scrub with water at 17 atm to recover additional acetone. Water is fed on the top tray at 30 kmol/h and 320 K. The diameter of the absorber is 0.710 m.

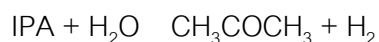
The both of bottom streams of the flash tank and the absorber are mixed which is a combination of acetone, water and IPA, with a smaller percentage of hydrogen. Such combined stream is fed on stage 73 of the first column (C-1) which has 87 stages. The operating pressure is 1 atm so that a reflux-drum temperature is 320 K. This column produces the high-purity acetone as a distillate 99.9 mol% acetone and a bottom 0.01 mol% acetone impurity; removes the small amount of hydrogen dissolved in the feed out using partial condenser as a vent gas. The reflux ratio is 4.37, and the column diameter is 3.424 m.

Then, the bottom of the first column is fed on stage 15 of the second column which has 20 stages. Similar to the first column, the operation pressure is 1 atm so that a reflux-drum temperature is 353 K. The reflux ratio is 0.617, and the column diameter is 0.790 m. The function of this column is to separate IPA from the mixture which gives a water bottom 0.1 mol% IPA and a distillate 65 % mol IPA in which a

composition close to the IPA/water azeotrope. Finally, such distillate is recycled back to the vaporizer as mention earlier.

4.2.2 Reaction Kinetics

The catalytic dehydrogenation of 2-IPA occurs at high temperature and in gas-phase which is a reversible reaction. This reaction is endothermic with a standard heat of reaction of 62,900 kJ/kmol.



The kinetics for the forward and reverse reactions is based on those given by Luyben (2011). The reaction rates are given in units of $\text{kmol s}^{-1} \text{m}^{-3}$:

$$R_F = C_{\text{IPA}} k_F e^{(-72380/RT)}$$

$$R_R = C_{\text{acetone}} C_{\text{H}_2} k_R e^{(-9480/RT)}$$

The reaction occurs in the plug flow reactor with a solid catalyst (assumed to have 0.5 void fraction and 2000 kg/m^3 solid density) to achieve 90 % conversion. Table 4.1 shows the reaction kinetic parameters for reversible dehydrogenation of 2-IPA.

Table 4.1 Reaction kinetic parameters (Luyben, 2011)

Parameters	Forward	Reverse
k	2.2×10^7	1.0×10^3
E (kJ/kmol)	72380	9480
Concentration terms (kmol/m^3)	C_{IPA}	$C_{\text{acetone}} C_{\text{H}_2}$

4.2.3 Steady-State Simulation of Acetone Process

In the steady-state simulation, the information of the process flowsheet is mainly given by Luyben (2011). The UNIQUAC physical property is chosen to predict the properties of the components in the Aspen HYSYS simulations. All data of material stream and the equipment specifications are presented in Appendix A.

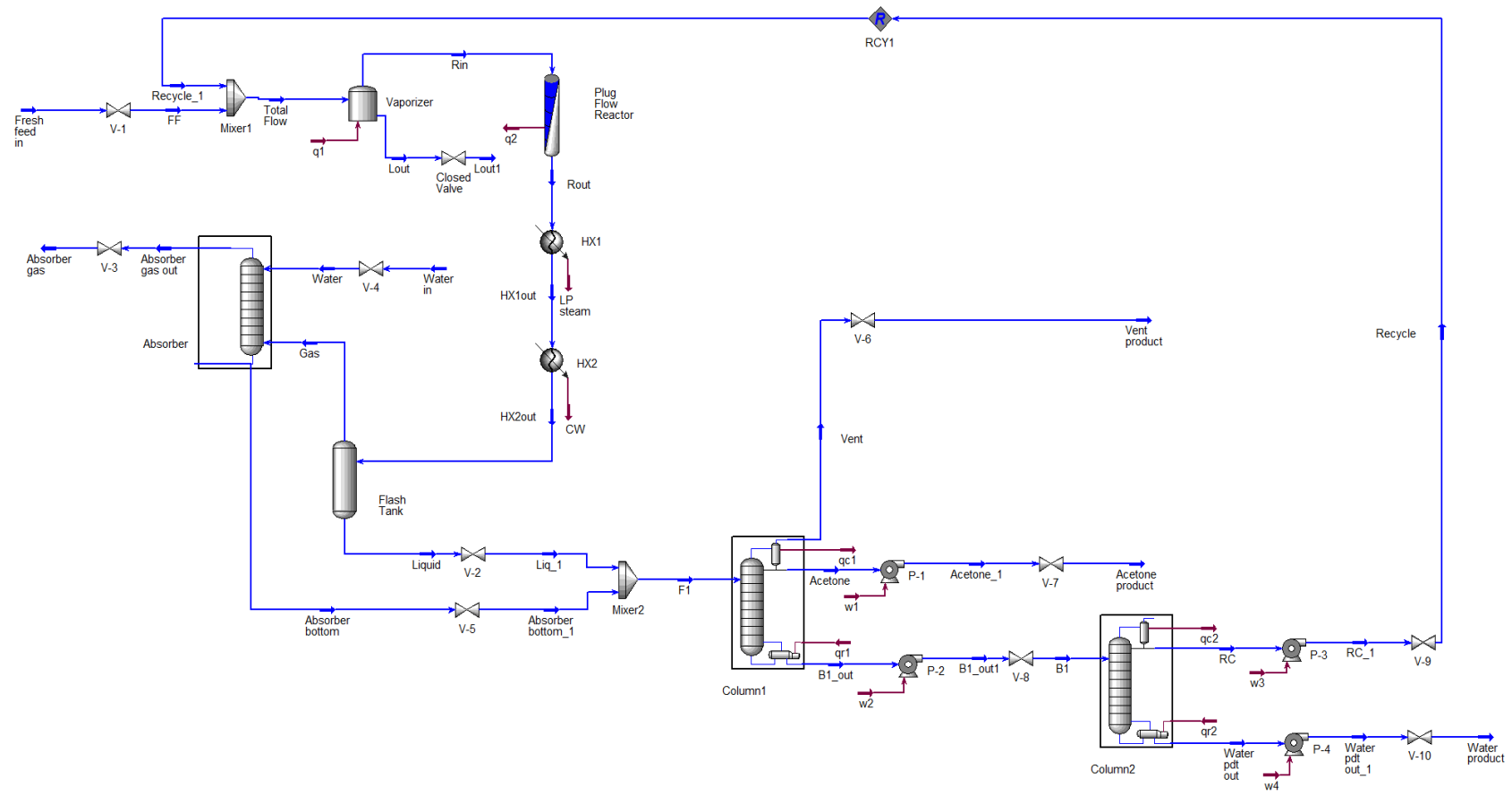


Figure 4.2 Steady-state simulation of acetone process using Aspen HYSYS simulators

4.3 Heat-integrated Plant for Acetone Process

4.3.1 Design of HIPs for Acetone Process

In this process, there are hot stream and cold stream available for design heat-exchanger network. Table 4.2 shows all available hot streams and cold streams for design HENs. This problem is no pinch since the ΔT_{\min} is large called "Threshold problems". The hot stream (H1) exchanges heat to the cold stream (C1) as shown in Figure 4.3. Then the residue of heat is completed by a cold utility.

Table 4.2 Process data for heat-integration plant of acetone process

Stream Name	Start Temperature, T_s (K)	Target Temperature, T_t (K)	W (MW/K)	Duty (MW)
H1: Outlet stream of reactor	753.5	420	1.90	0.5971
C1: Total feed stream (fresh feed + recycle)	323.5	450	2.78	0.3512

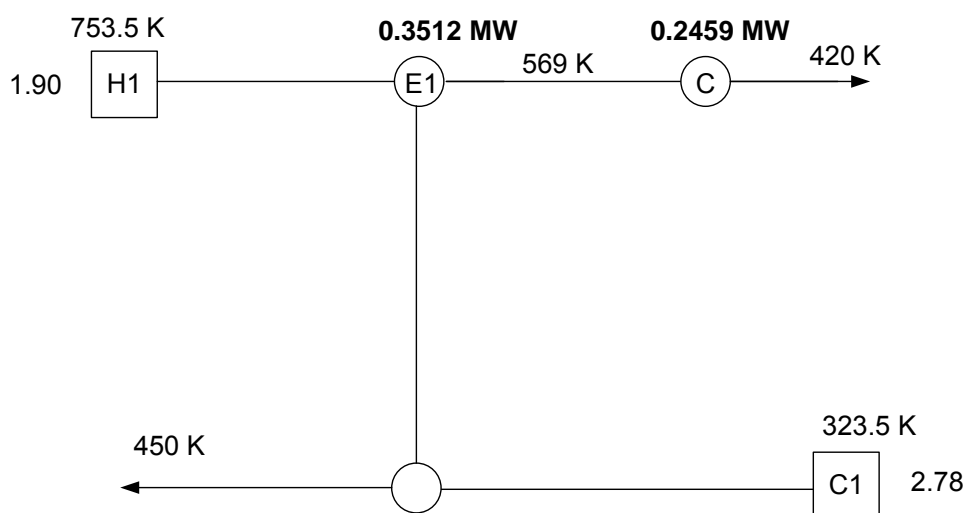


Figure 4.3 Heat-exchanger networks representation in grid diagram

Table 4.3 Utility costs (Luyben, 2011)

Utility	Description	Cost (\$/GJ)
Steam from boilers	Process steam : latent heat only	
	HP steam	9.83
	MP steam	8.22
	LP steam	7.78
Cooling water*		0.345
Fired furnace		9.83

*Turton R. *et al*, 2009

Table 4.4 Energy consumption and energy cost of acetone process

Unit	Base case		HENs	
	Amount	Cost	Amount	Cost
	(MW)	(10 ⁶ \$/year)	(MW)	(10 ⁶ \$/year)
Vaporizer	0.8592	0.2115	0.5080	0.1251
Reactor	1.0940	0.3403	1.0940	0.3403
HX1	0.5024	0.1237	0.1512	0.0372
HX2	0.7839	0.0088	0.7839	0.0088
ReboilerC1	1.5930	0.3922	1.3476	0.3318
CondenserC1	1.5370	0.0172	1.5370	0.0172
ReboilerC2	0.1105	0.0272	0.1105	0.0272
CondenserC2	0.1066	0.0012	0.1066	0.0012
Total	6.5866	1.1209	5.6388	0.8876
% Saving	-	-	14.4	20.8

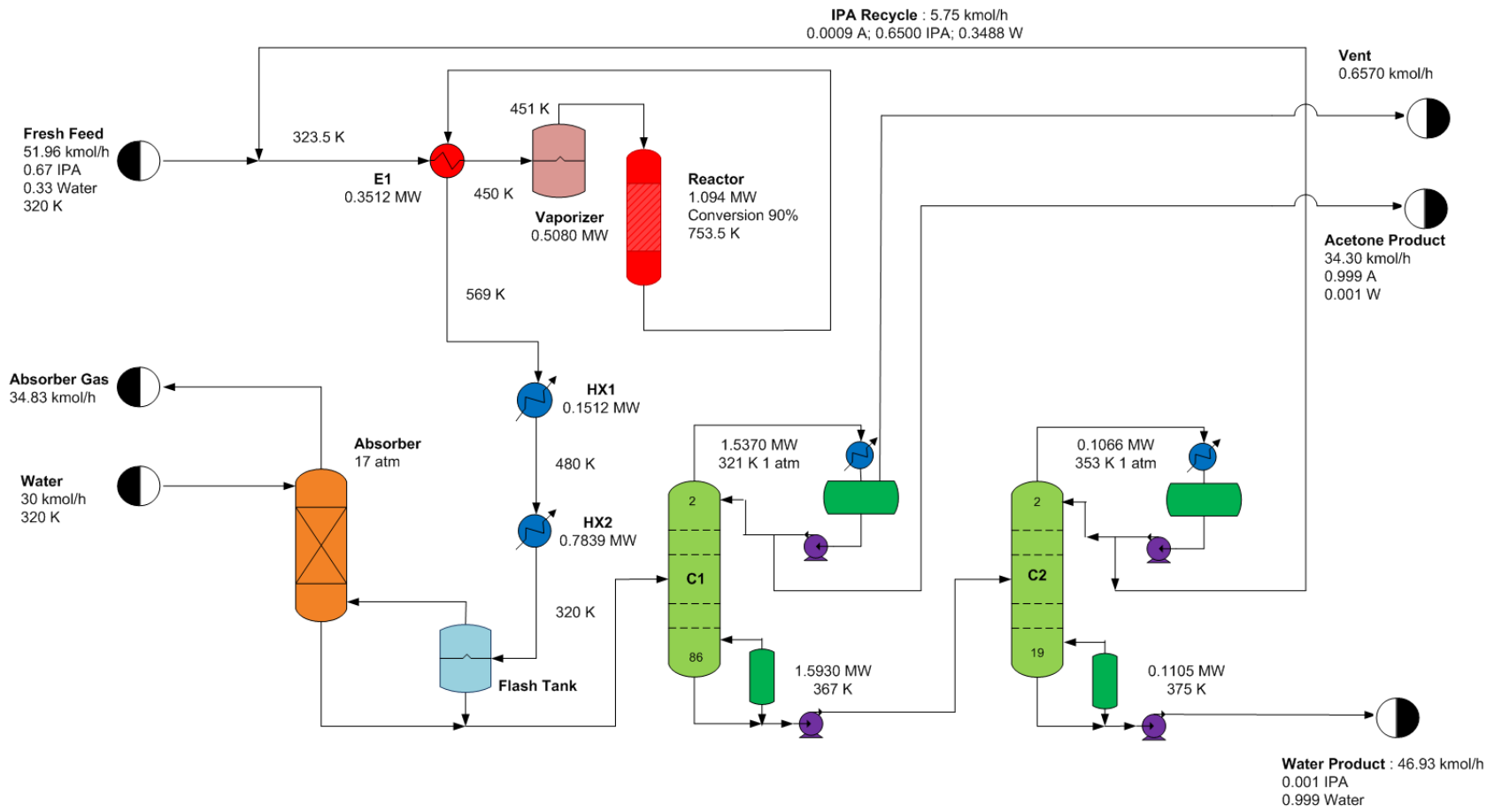


Figure 4.4 Acetone process with heat exchanger network flowsheet

4.3.2 Steady-State Simulation of the Heat-Integrated Plant for Acetone Process

Figure 4.5 shows the steady-state HENs design for acetone process by adding a process to process heat exchanger to save energy consumption. The design can save energy 20.8% which lowering cost of energy 14.4% for a year as shown in Table 4.4. This new alternative of acetone production; acetone flowsheet with HENs, is also used to evaluate performance control structures which imply more complex process.

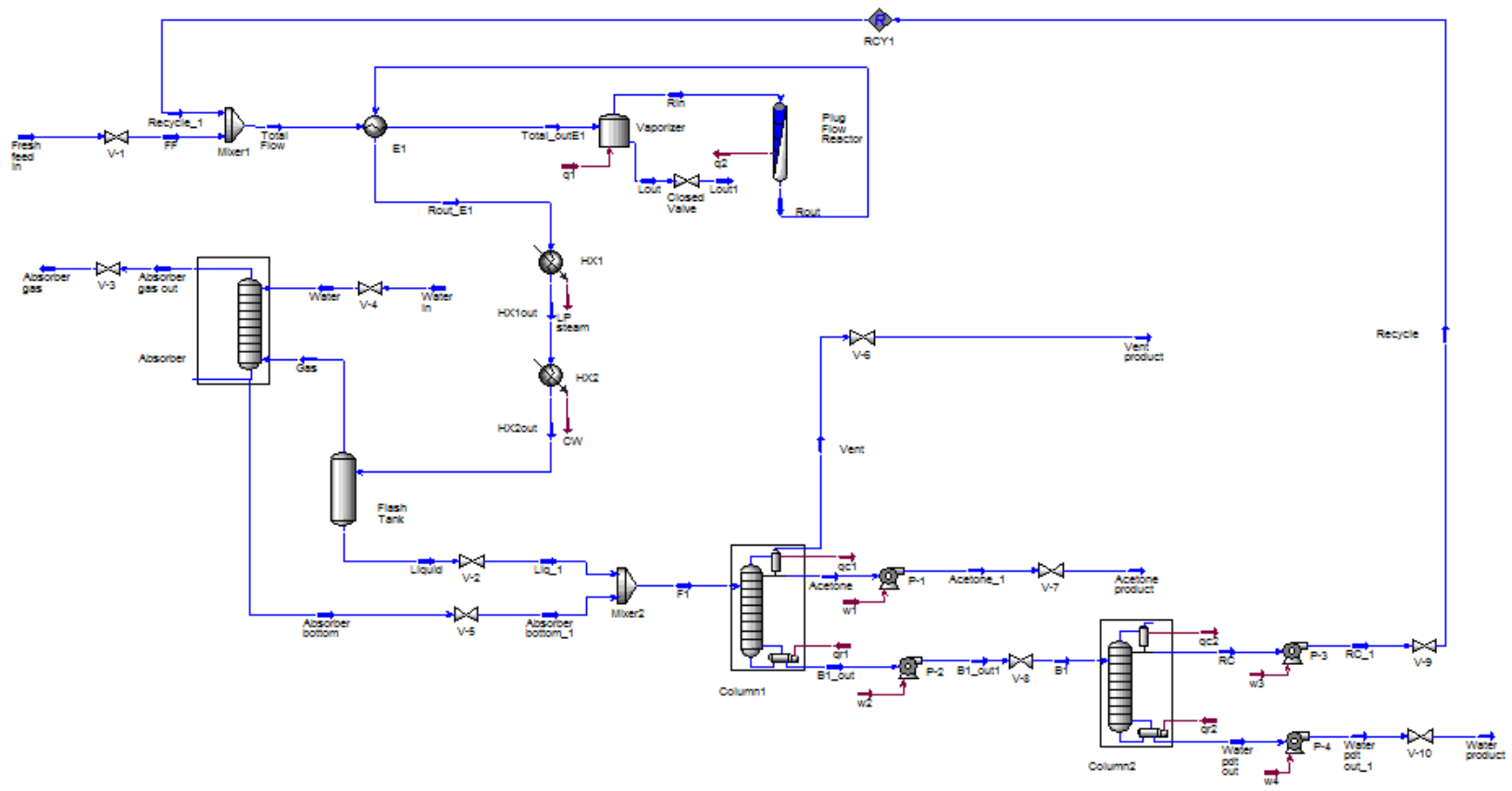


Figure 4.5 Steady-state simulation of acetone process with heat exchanger

4.4 New control structures design procedure, Wongsri 2012

The methodology of designing control structures is described below.

Step1: Gather relevant plant information and control objectives.

List all control variables and available manipulated variables (number of DOF)

List all control variables:

- i. An independent stream must have a control valve (1 DOF)
- ii. A heater, cooler, pump, or compressor has one degree of freedom (to adjust heat load or duty or work load)
- iii. A process to process heat exchanger has one degree of freedom by adding a by-pass line.
- iv. A reactor has zero or one degree of freedom depends on its type.
- v. A flash separator has two degree of freedom.
- vi. A simple distillation column has five degree of freedom.

How to select manipulated variables

- i. A control variable and manipulated variable must have strong causal relationship (high gain)
- ii. The manipulated variables should not be far from the control variables (zero or minimal dead time)
- iii. The time constant of the quality loops should be short and the time constant of the inventory loops should be longer.
- iv. The manipulated variables should not be saturated for the whole range of the disturbances.

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

Step2: Energy management via heat exchanger networks.

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

Step3: Establish fixture plant

The principal idea of establishing a fixture plant is to first have entire plant fluid-filled and material-balanced. This idea is similar to creating “hydraulic” control structure proposed by Buckley* (1964).

3.1 Keep the raw materials entered and reentered fixed

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

3.3 Locate the quantifiers for the rest of the components and design the control loops to regulate their inventories in the plant. The material flow in the plant should be fixed. In the case that this cannot be done the change of the material flow must be slow.

Step4: Handling the disturbances

In this step, we configure the quality control loops by employing the notion of all disturbances management.

4.1 Heat Disturbances

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

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

4.2 Material disturbances

The configuration of the control loops depend on the desired material pathways by analyzing the material disturbance tests on changes of composition, total flow, component flow: At reactor, we adjust the reactor inlet temperature in order to keep the reactor outlet composition or the product component flow fixed. For distillation columns, to control top or bottom temperature depend on the material disturbance rejection policy.

Step5: Find the most disturbed point and design the control loops to alleviate the effects of disturbances

Step6: Design the control loops for the rest of the control variables or adding enhanced controls, i.e. cascade, feed forward controls.

Step7: Optimize economics and improve control performance

Step8: Validate the designed control structures by rigorous dynamic simulation

CHAPTER V

CONTROL STRUCTURES DESIGN

AND DYNAMIC SIMULATION

5.1 Plantwide Control Strategies

In this research, the 8 steps of Wongsri procedure (2012) are applied to the acetone process. This procedure is sort of the heuristic method which concerned about the direction of the disturbance propagation through entire the process. Both of material and heat disturbances are managed in the proper path way that eliminating out of the process. For all designed control structures are discussed thoroughly below.

Step 1: Gather relevant plant information and control objectives.

The important thing of designing control structure is to achieve the control objectives with stably and smoothly operation. Additionally, constraints of each unit have to be considered. The control objectives and plant information for the acetone process are:

Control objectives:

1. Production capacity: more than 17,000 tonnes a year
2. Product quality: acetone composition more than 99.9 mol%

Plant information:

1. The temperature of the reactor outlet maintains at 753.5 K to keep conversion at 90% and to ensure the loss of catalyst activity due to the temperature.
2. Both of heat exchanger effluent streams are fixed the temperature at 480 and 320 K respectively to minimize the loss of acetone in the gas stream leaving the flash tank.

3. The operation pressure of the absorber is at 17 atm in order to maximize the acetone recovery (Luyben, 2011).

All potential control variables and available manipulated variables (number of DOF) are listed in Table 5.1 and 5.2 respectively.

Table 5.1 Potential controlled variables of each unit operation

Unit operation	Controlled variables
Independent stream	Flow rate
Vaporizer	Outlet temperature and Liquid level
Reactor	Outlet temperature and Outlet composition
Heat exchanger	Outlet temperature
Flash tank	Liquid level and Pressure
Absorber	Liquid level and Pressure
Distillation column	Composition of distillate and bottom, Level of reflux drum and base column, and Pressure

Table 5.2 Manipulated variables and number of control degree of freedom

Unit operation	Manipulated variables	Number	DOF
Independent stream	Fresh feed flow, Water flow	2	2
Vaporizer	Vaporizer duty	1	1
Reactor	Reactor duty	1	1
Heat exchanger	HX duty	2	2
Flash tank	Bottom flow, Gas flow	1	2
Absorber	Absorber gas flow, Absorber bottom flow	1	2
Distillation column	Reflux flow rate, Condenser duty, Reboiler duty, Distillate flow, Bottom flow	2	11*
Pump	Work	4	4
Total number control degree of freedom			25

*There is a vent flow stream as a manipulated variable added in acetone column (C1).

Step 2: Energy management via heat exchanger networks.

The energy management via heat exchanger network is elaborated in Chapter IV in design of heat exchanger network topic.

Step 3: Establish fixture plant

3.1 Keep the raw materials entered and reentered fixed

Raw materials are very important for on-demand production. Fixing the raw materials is considered. Therefore, the fresh feed stream can be a manipulated variable to control the total feed flow rate (fresh feed + recycle). Another control loop is to fix fresh feed water entering in the process by manipulating water flow rate. Figure 5.1 shows all control loops provided by this step.

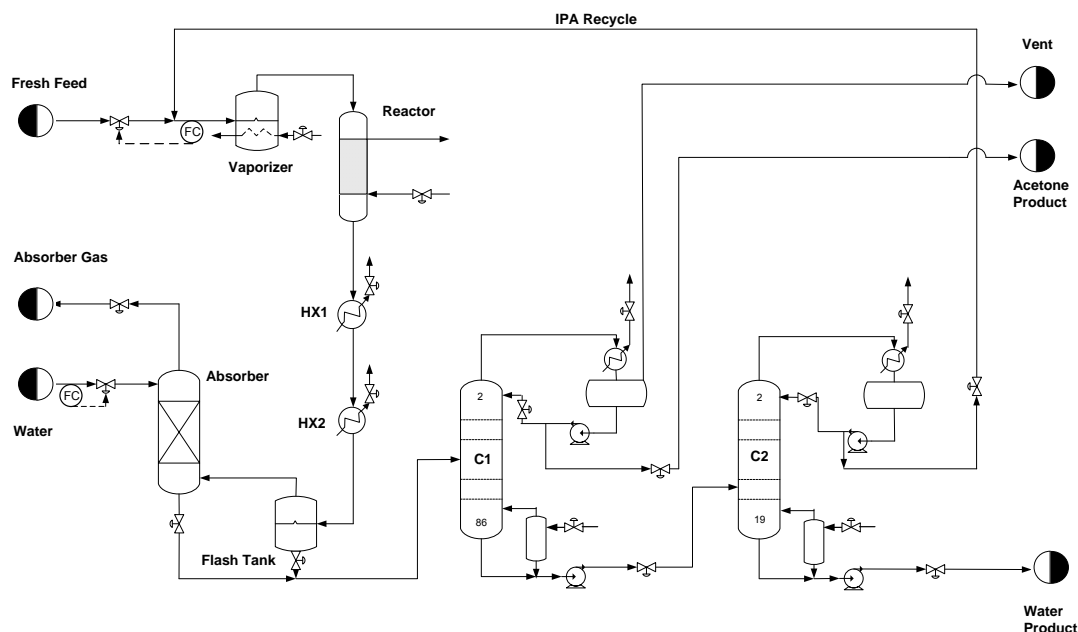


Figure 5.1 Control loops to fix the raw materials entered and reentered in the process

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

There are 4 exit points of material stream in the process; absorber gas, distillate of product C1, vent and bottom of product C2. Such exit points can balance the accumulation of hydrogen, acetone and water. As Richardson rule, the control loops should be established to the larger flow which carried out more impacts to the process. Therefore, this step obtains 2 control loops shown in Figure 5.2 which can balance the exit point are listed below.

1. To balance amount of hydrogen, control top stage pressure of the absorber by manipulating the absorber gas flow.

2. To balance amount of water, control reboiler level of C2 by the bottom flow of product C2.

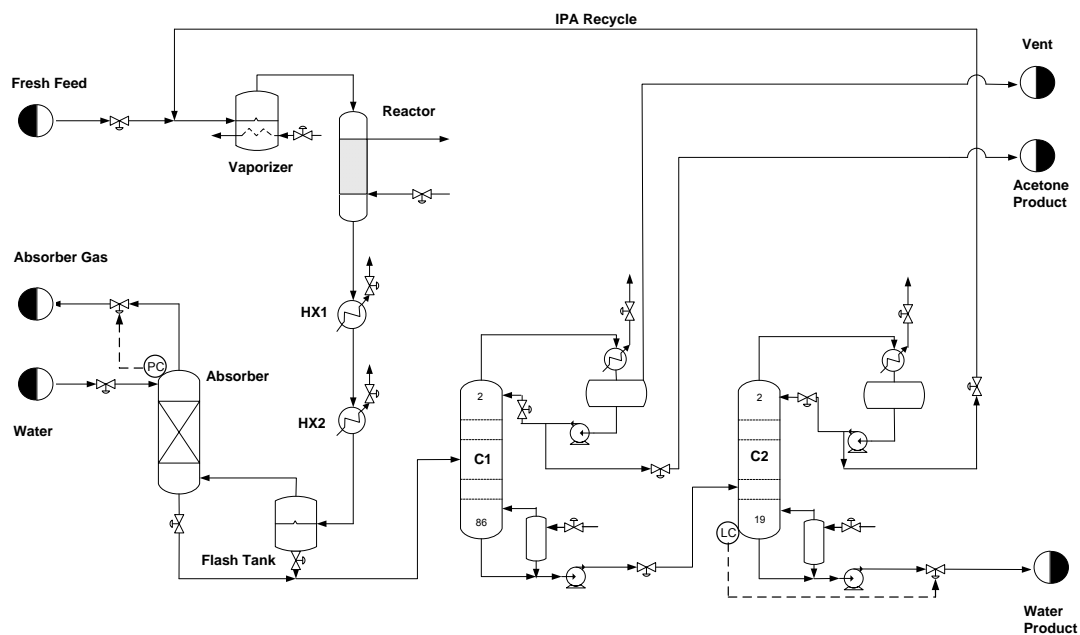


Figure 5.2 Control loops to balance the accumulation of products, by-products, and inert

3.3 Locate the quantifiers for the rest of the components and design the control loops to regulate their inventories in the plant. The material flow in the plant should be fixed. In the case that this cannot be done the change of the material flow must be slow.

There are 4 components; IPA, water, acetone and hydrogen, in the process. The quantifiers of each component which has a potential to balance their inventories; level and pressure, are reflux drum C2, column base C2, reflux drum C1 and absorber, respectively. This step provides the control loops below.

1. The reflux drum C2 is a quantifier of IPA is manipulated by the distillate flow of product C2.

2. The column base C2 is a quantifier of water is manipulated by the bottom flow of product C2.

3. The reflux drum C1 is a quantifier of acetone is manipulated by the reflux flow rate of C1.

4. The absorber is a quantifier of hydrogen is manipulated by the absorber gas flow.

However, there are 2 control loops is similar to the control loop providing by step 3.2 means that the leftover control loops regulated the inventory in the process are level control loop of reflux drum C1 and C2 as shown in Figure 5.3.

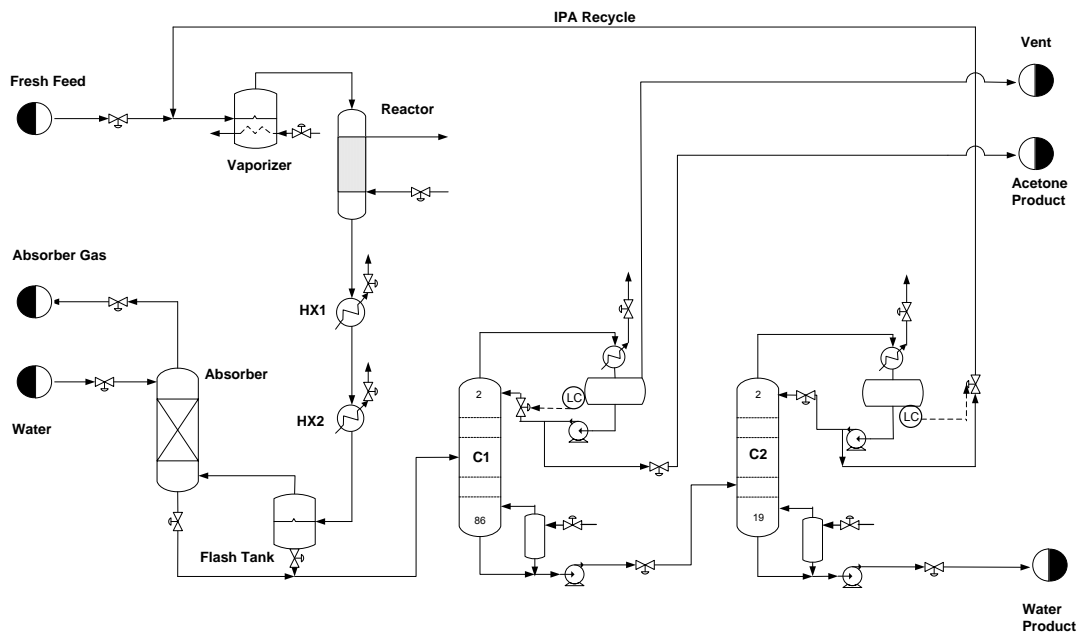


Figure 5.3 Control loop to balance the amount of acetone and IPA

Step 4: Handling the disturbances

In this step, we configure the quality control loops by employing the notion of all disturbances management.

4.1 Heat Disturbances

4.1.1 Direct the heat disturbances that are not directly related to quality to the environmental via the next and nearest exit points to keep the thermal conditions of process stream constants.

Heat disturbances normally can be handled by heat duty in/out the process. In this process, the unit operation which is capable of cope with the heat

disturbances are vaporizer duty, reactor duty, heat exchanger duty, compressor duty and reboiler duty. There are 2 loops that they are not related to quality of product; outlet temperature of HX1 and outlet temperature of HX2, as shown in Figure 5.4.

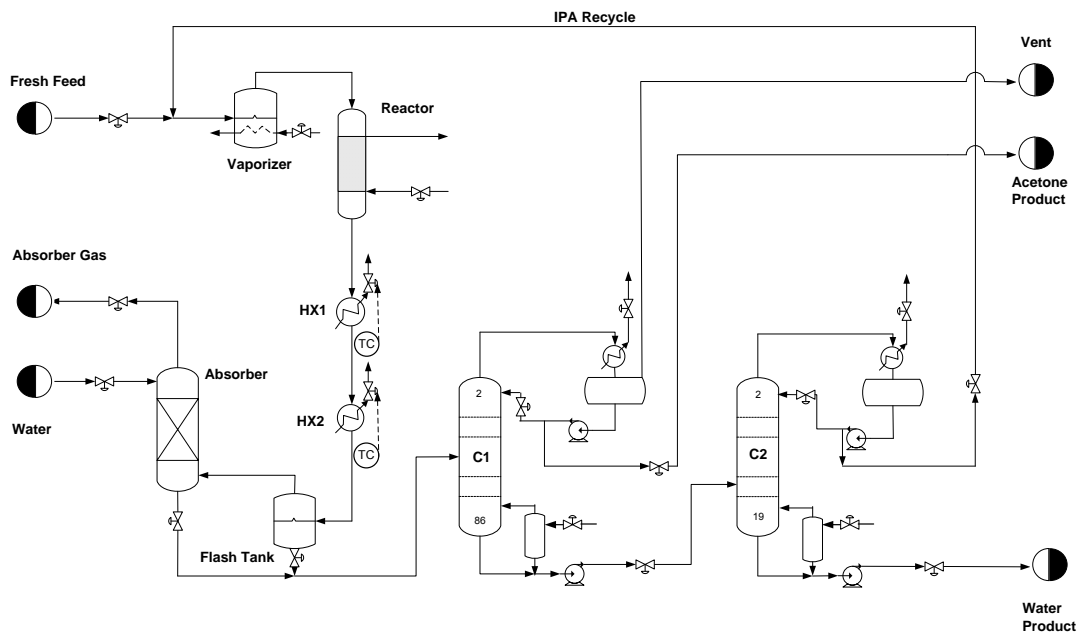


Figure 5.4 Control loops not related to quality of product

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

This step is to the quality of product which involving 3 loop; outlet temperature of reactor, tray temperature of C1 and tray temperature of C2 as shown in Figure 5.5. At the reactor, the catalyst activity is limiting at 773 K (Howard, 2001) so that controlling the outlet temperature of reactor is taken into account to prevent losing of the catalyst activity. At the columns, both distillation columns; C1 and C2, tray temperature are controlled by manipulating the reboiler duty as an energy to separate light key and heavy key in the column.

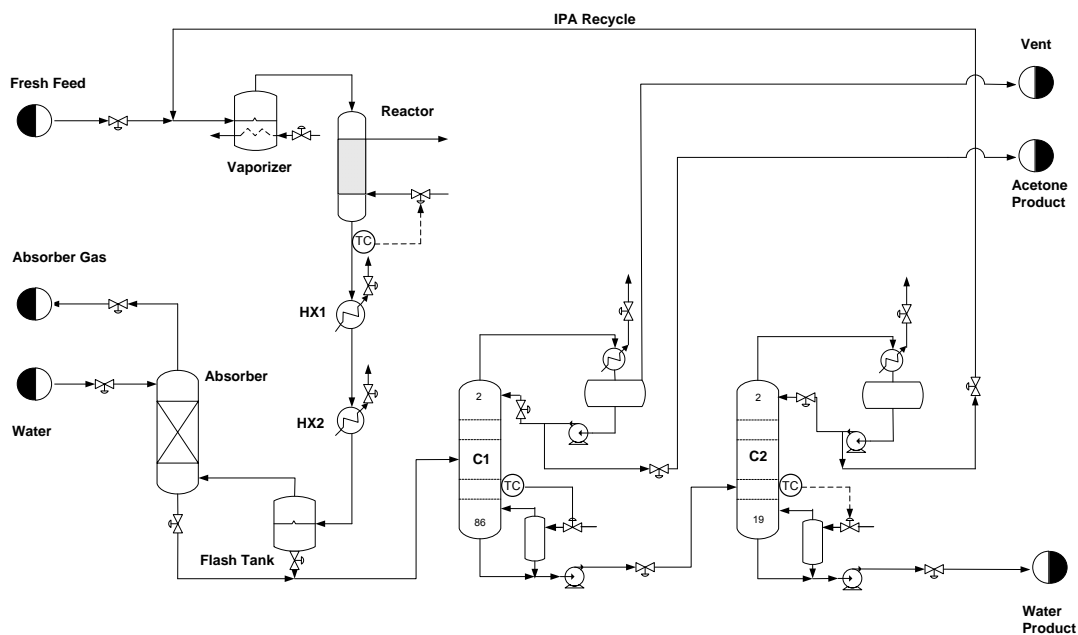


Figure 5.5 Control loops related to quality of product

4.2 Material disturbances

First of all, the directions of each component are considered so as to map out the component through the process. Figure 5.6-9 show the pathway of each component in the process. IPA pathway is shown in Figure 5.6. IPA is fed to the process then dehydrogenated at the reactor to acetone and hydrogen. In the separation section, IPA is scrubbed back at the absorber and separated from water at the C2 in order to recycle back to the process.

Figure 5.7 shows the pathway of water in the process. Water is fed with IPA as an inert in fresh feed and as a solvent to scrubbed acetone and IPA at the absorber and then distilled out in the C2.

Figure 5.8-9 show acetone and hydrogen which generated at the reactor. After condensed the product at the heat exchanger, acetone is carried out to the flash tank to separate from hydrogen and then removed out at the C1 as a distillate (Figure 5.8). Hydrogen is mainly released at the absorber and the residue is removed at the reflux drum of C1 (Figure 5.9).

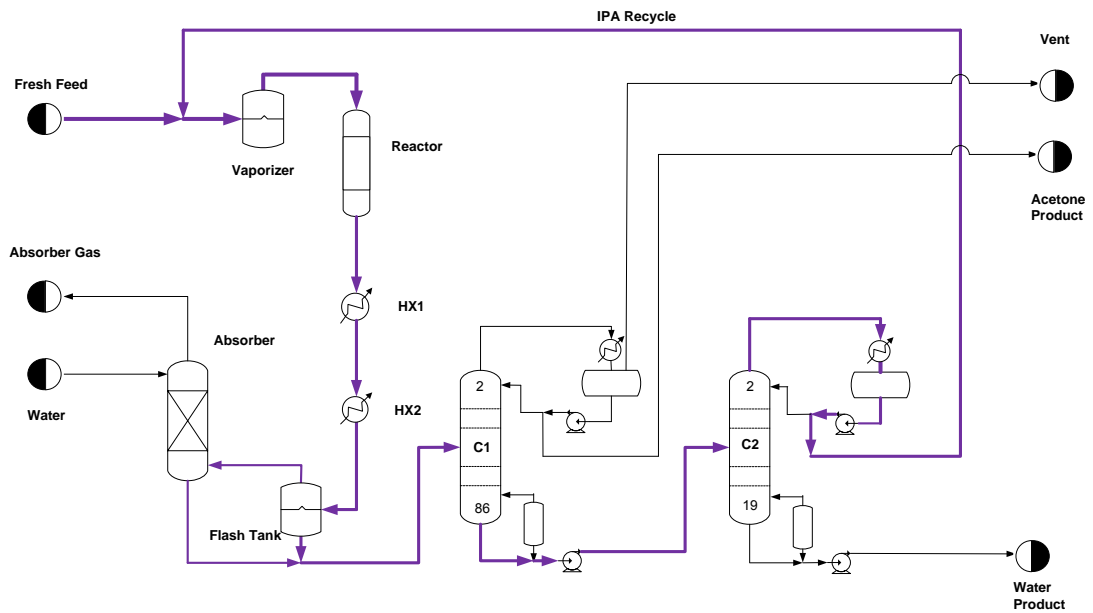


Figure 5.6 IPA pathway through the process

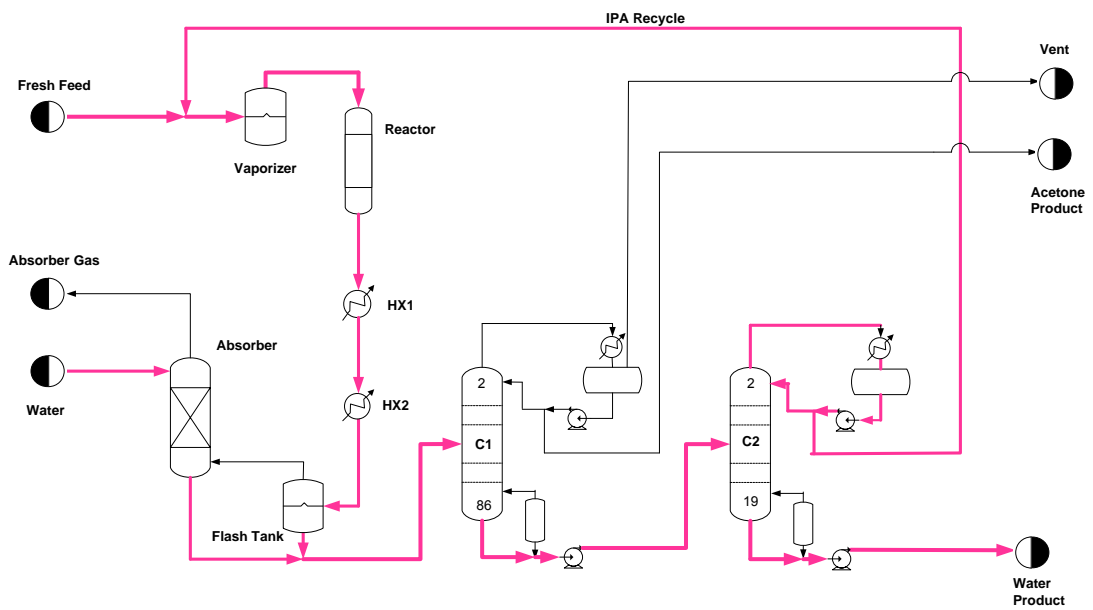


Figure 5.7 Water pathway through the process

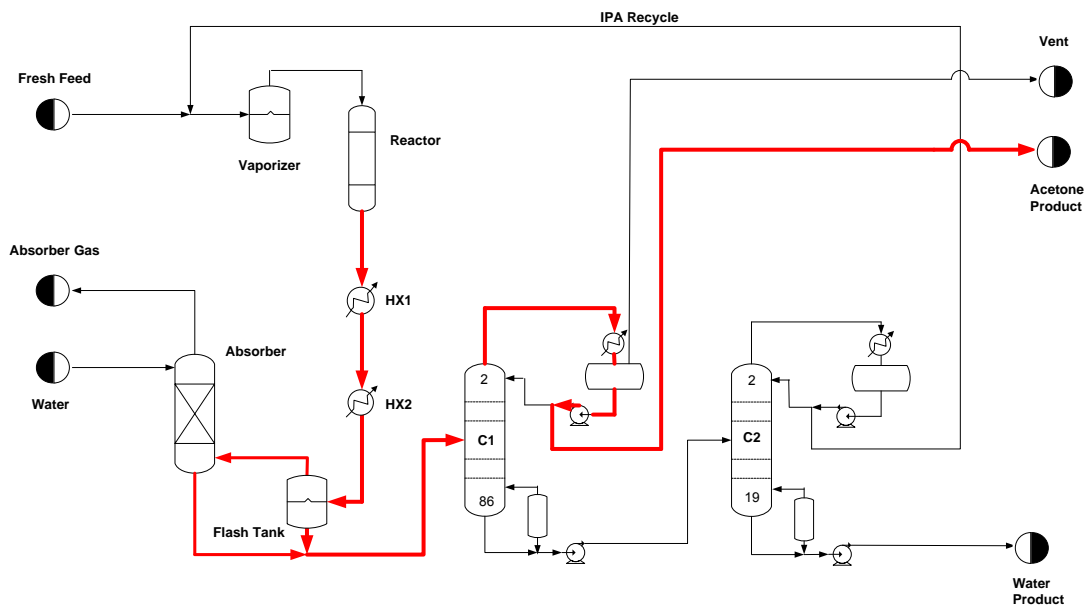


Figure 5.8 Acetone pathway through the process

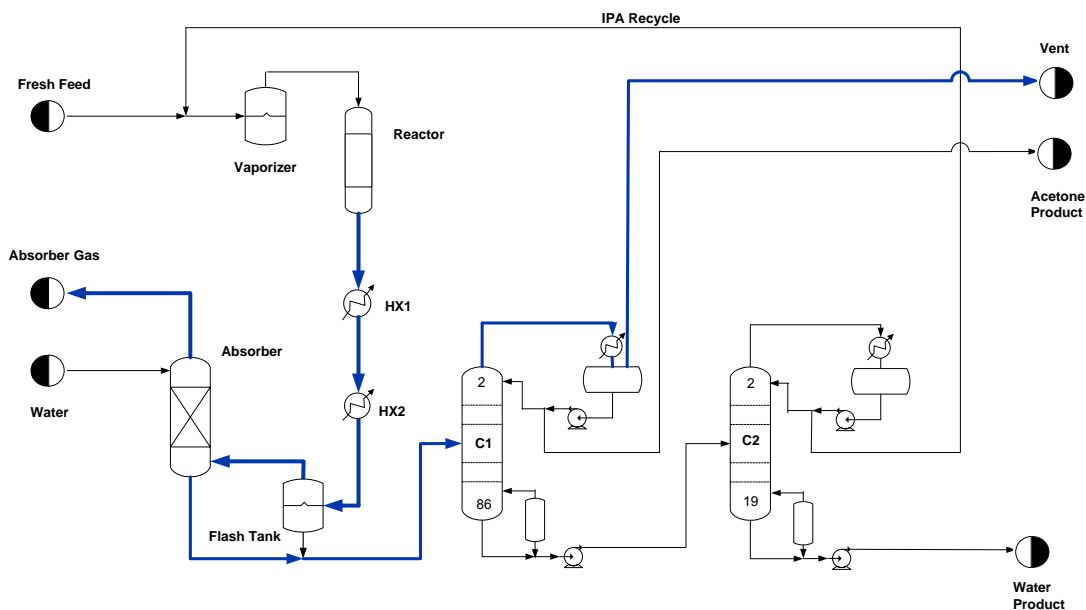


Figure 5.9 Hydrogen pathway through the process

For each component pathway indicates their direction through the process. In the separation section, absorber and distillation columns are the units which closed to the exit point of each component. The large amount of hydrogen is release at the top of the absorber as mentioned in step 3. The amount of acetone is regulated to exit the top stage of the C1 by the reboiler duty. The amount of water and IPA are

regulated by the reboiler duty which exit at the bottom and top stage of the C2 respectively.

Step5: Find the most disturbed point and design the control loops to alleviate the effects of disturbances

At the reactor

The study of disturbances by changing the inlet stream of reactor while fixing the reactor duty shows the result that the temperature and composition of acetone are significantly changed (Table 5.3-5). Table 5.3 shows the effect of flowrate on the effluent stream. The outlet temperature and composition of product decrease as the amount of reactant increases since the endothermic reaction needs more energy to convert more reactant flow into the reactor. In addition, the flowrate change causes the conversion decreased when the flowrate increased. Table 5.4 shows the effect of composition of the reactant on the effluent stream. The outlet temperature drops when the amount of reactant lifts because of the energy is fixed at the normal value. Although the outlet composition of product rises, the conversion decreases same as the effect of flow rate. Because of the inlet temperature is close to the dew point temperature, the disturbance test is considered only increasing case. When the inlet temperature raises as shown in Table 5.5, the outlet temperature and composition of product lifts up because the amount of heat flow of the inlet stream up. In this case, the conversion is also increased. Therefore, another alternative to design the control loop is to control the outlet composition of acetone in the effluent stream as shown in Figure 5.10.

Table 5.3 Case study of flowrate in reactor inlet stream

Changed	Flowrate (kmol/h)	Outlet stream	
		Temperature(K)	Composition of Acetone
-10%	52.05	799.7	0.3865
Normal	57.83	753.5	0.3755
+10%	63.61	719.9	0.3617

Table 5.4 Case study of composition in reactor inlet stream

Changed	Composition of IPA	Outlet stream	
		Temperature (K)	Composition of Acetone
-10%	0.6012	789.3	0.3609
Normal	0.6680	753.5	0.3755
+10%	0.7348	726.3	0.3853

Table 5.5 Case study of temperature in reactor inlet stream

Changed	Temperature (K)	Outlet stream	
		Temperature (K)	Composition of Acetone
Normal	450.6	753.5	0.3755
+5 K	455.0	755.7	0.3762
+10 K	460.0	758.5	0.3771

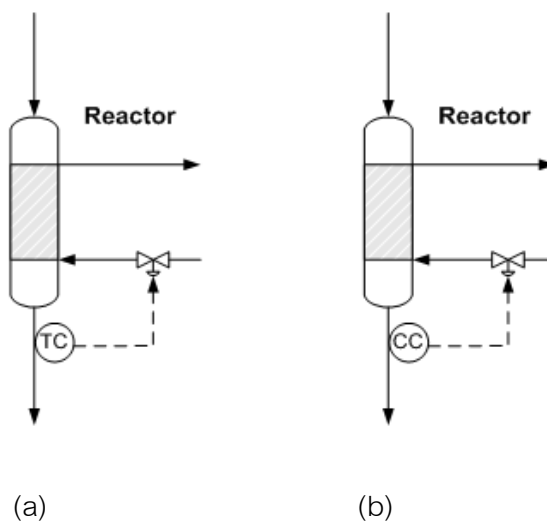


Figure 5.10 Alternatives of the control loop at the effluent stream (a) controlling the outlet temperature (b) controlling the outlet composition of acetone

At the acetone column (C1)

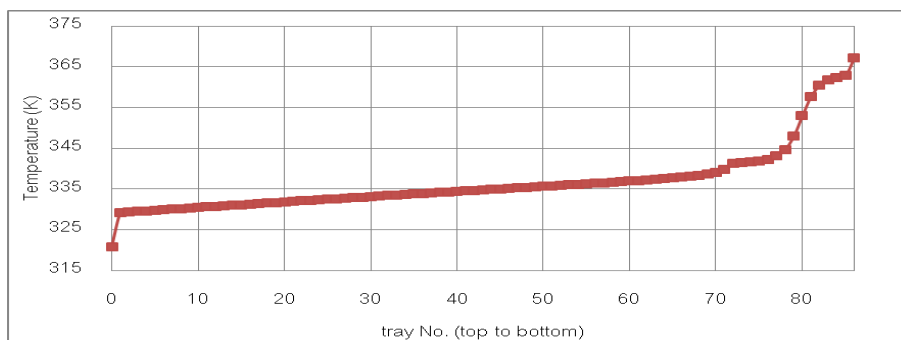


Figure 5.11 Temperature profile of C1

Figure 5.12 shows the temperature profile sensitivity which is investigated by composition, total material flowrate and temperature of column feed while fixing reflux ratio and reboiler duty. The study gives the controlled criteria tray changed significantly around the steepest point of normal temperature profile; tray 81 as shown in Figure 5.11. Testing conditions for the temperature profile are shown in Table 5.6-8.

This step gives the controlled tray which is near the bottom stage not the top stage of the column so that another control variable is considered. Reflux flowrate is a manipulated variable for controlling the temperature and composition at the column. However, the reflux flowrate is not available because it is used to control level of reflux drum of the column as mentioned in step 3. Therefore, reflux ratio is another alternative to control the composition at the top stage of the column.

Table 5.6 Case study of total flow in feed C1

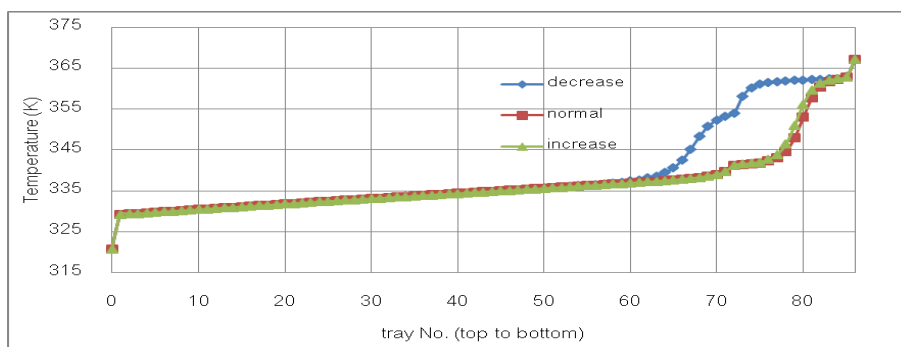
Changed	Total flow (kmol/h)
-0.02%	87.75
Normal	87.77
+0.02%	87.79

Table 5.7 Case study of composition in feed C1

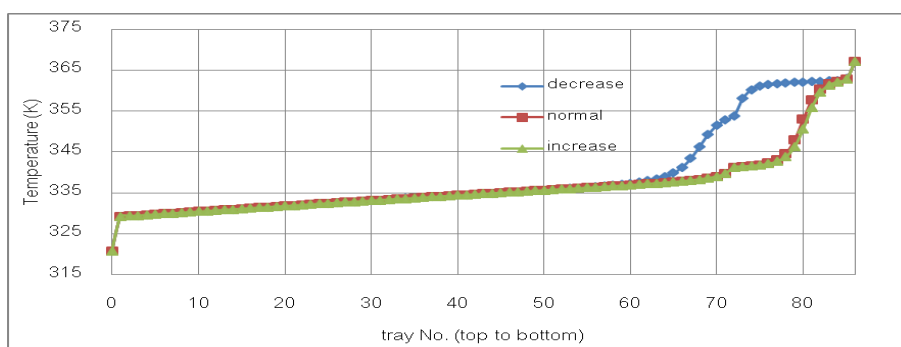
Changed	Mole fraction of acetone (LK)
-0.02%	0.3960
Normal	0.3961
+0.02%	0.3962

Table 5.8 Case study of feed temperature C1

Changed	Temperature (K)
-0.2 K	322.7
Normal	322.9
+0.2 K	323.1

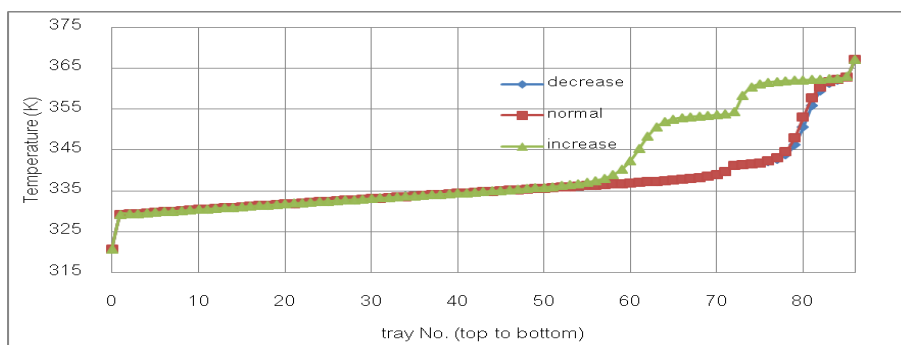


(a)



(b)

Figure 5.12 Temperature profile sensitivity at C1 (a) by changing in total flow rate (b) by changing in composition of light key and (c) by changing in temperature feed



(c)

Figure 5.12(Continued) Temperature profile sensitivity at C1 (a) by changing in total flow rate (b) by changing in composition of light key and (c) by changing in temperature feed

At water column (C2)

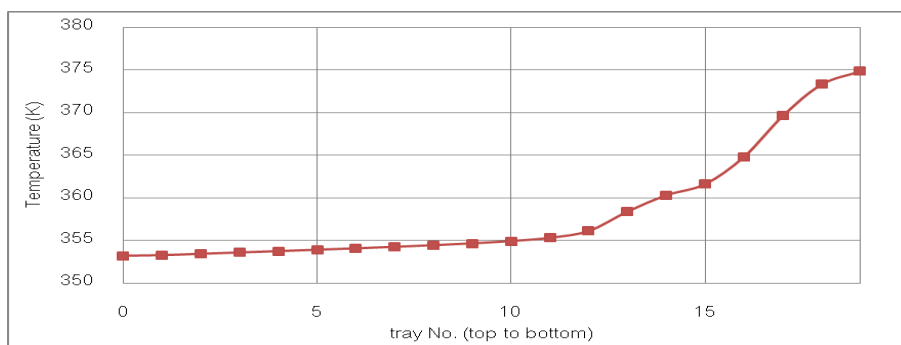


Figure 5.13 Temperature profile at C2

The study of disturbances (Figure 5.14) give the controlled criteria tray changed significantly around the steepest point of normal temperature profile; tray 17 as shown in Figure 5.13. Testing conditions for the temperature profile are shown in Table 5.9-11.

Table 5.9 Case study of total flow in feed C2

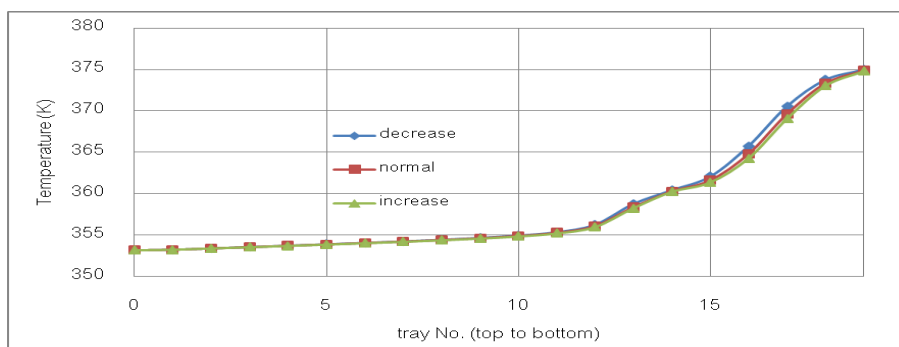
%Changed	total flow (kmol/h)
-0.5%	52.54
Normal	52.80
+0.5%	53.07

Table 5.10 Case study of total flow in feed C2

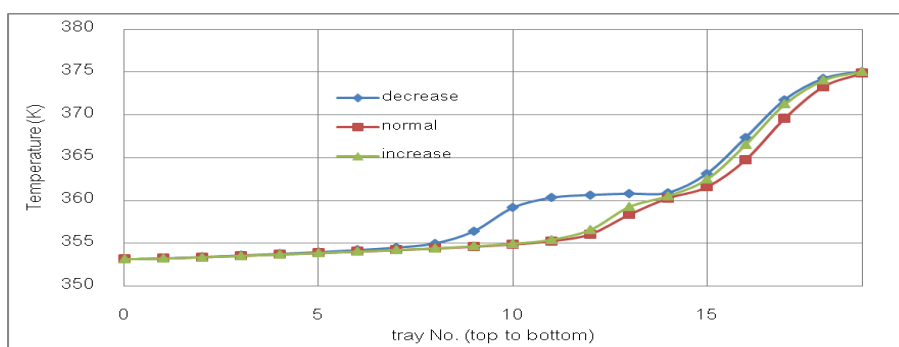
%Changed	Mole fraction of IPA (LK)
-1.0%	0.06585
Normal	0.07317
+1.0%	0.08049

Table 5.11 Case study of total flow in feed C2

Changed	Temperature (K)
-0.10	360.0
Normal	360.1
+0.10	360.2

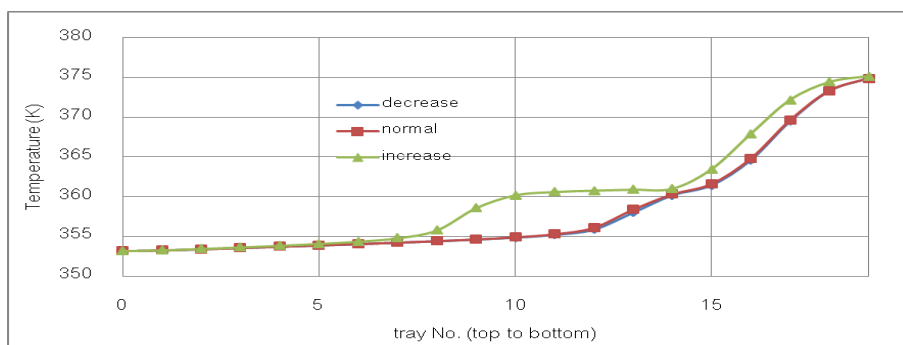


(a)



(b)

Figure 5.14 Temperature profile sensitivity at C2 (a) by changing in total flow rate (b) by changing in composition of light key and (c) by changing in temperature feed



(c)

Figure 5.14(Continued) Temperature profile sensitivity at C2 (a) by changing in total flow rate (b) by changing in composition of light key and (c) by changing in temperature feed

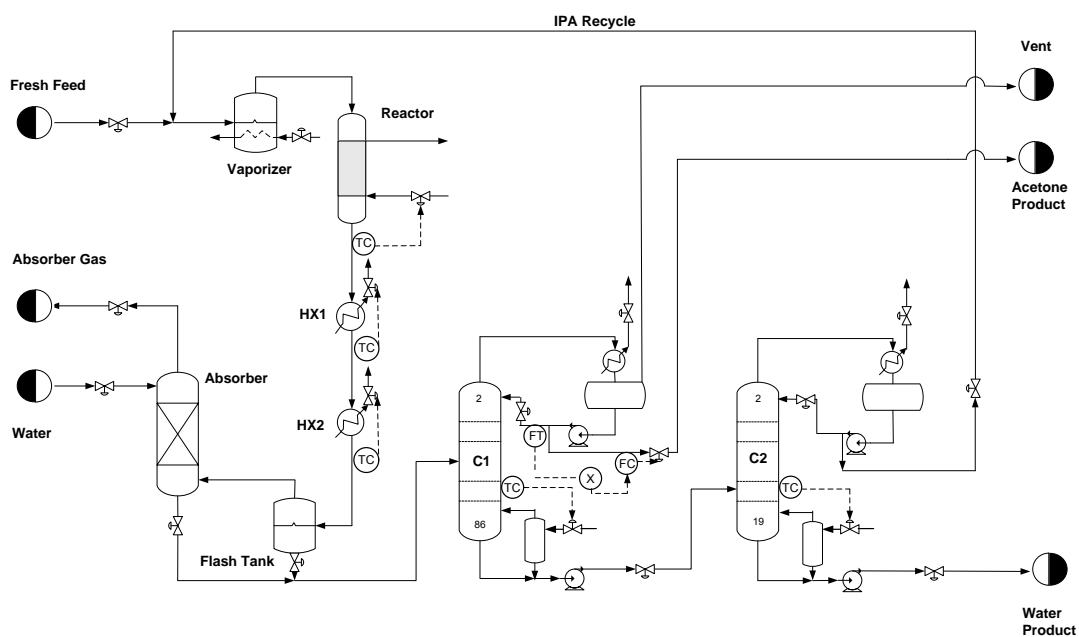


Figure 5.15 Control loops obtained by step 4th and 5th

Step6: Design the control loops for the rest of the control variables or adding enhanced controls, i.e. cascade, feed forward controls.

The rest control loops are the other inventory loops; level of vaporizer, flash tank, absorber and column base C1, reflux drum pressure of C1 and C2 as shown in Figure 5.16.

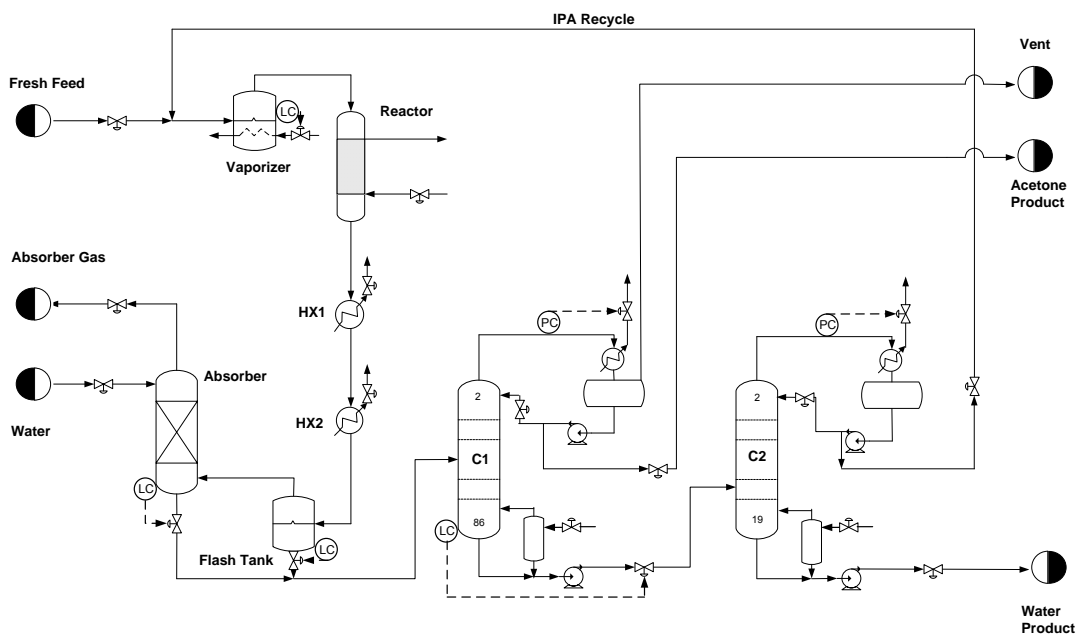


Figure 5.16 Others inventory loops

Additionally, another alternative design of control loop at the top stage of C1 (acetone column) is to design a cascade control loop. This loop is controlled the composition of water (impurity) by manipulating the distillate which is adjusted by ratio of distillate flowrate to reflux flowrate as shown in Figure 5.17.

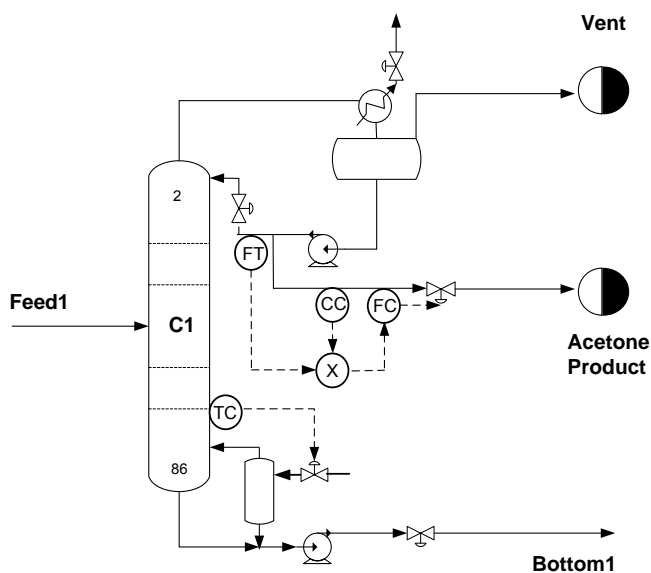


Figure 5.17 Cascade control at the C1

Step7: Optimize economics and/or improve control performance

The flowsheet by Luyben (2011) is already done economic optimization. The control performance is improved by the cascade control at the product column as mentioned in step 6th to ensure that the product quality is maintained at the specification. Furthermore, the PID controllers are taken into account to use in the process.

Step8: Validate the designed control structures by rigorous dynamic simulation

This step uses the software HYSYS to evaluate performance for acetone process. Material and thermal disturbances are used to test the control structure performance.

5.2 Plantwide Control Structures for Acetone Process

By the procedure, there are four plantwide control structures designed; CS1-4. Figure 5.18-22 show the control structure of base case (BC) and the designed control structures. The list of all control loops of each control structure are listed in Table 5.12 below. The main difference between CS1 and CS3, CS2 and CS4 is at the C1 in which the distillate composition of water controlled by adjusting the ratio of distillate to reflux ratio manipulating the distillate flowrate (CS3,4) instead of distillate to reflux ratio controlled (CS1,2). For the difference between CS1 and CS2, CS3 and CS4 are at the reactor in which the composition of acetone controlled instead of the outlet temperature.

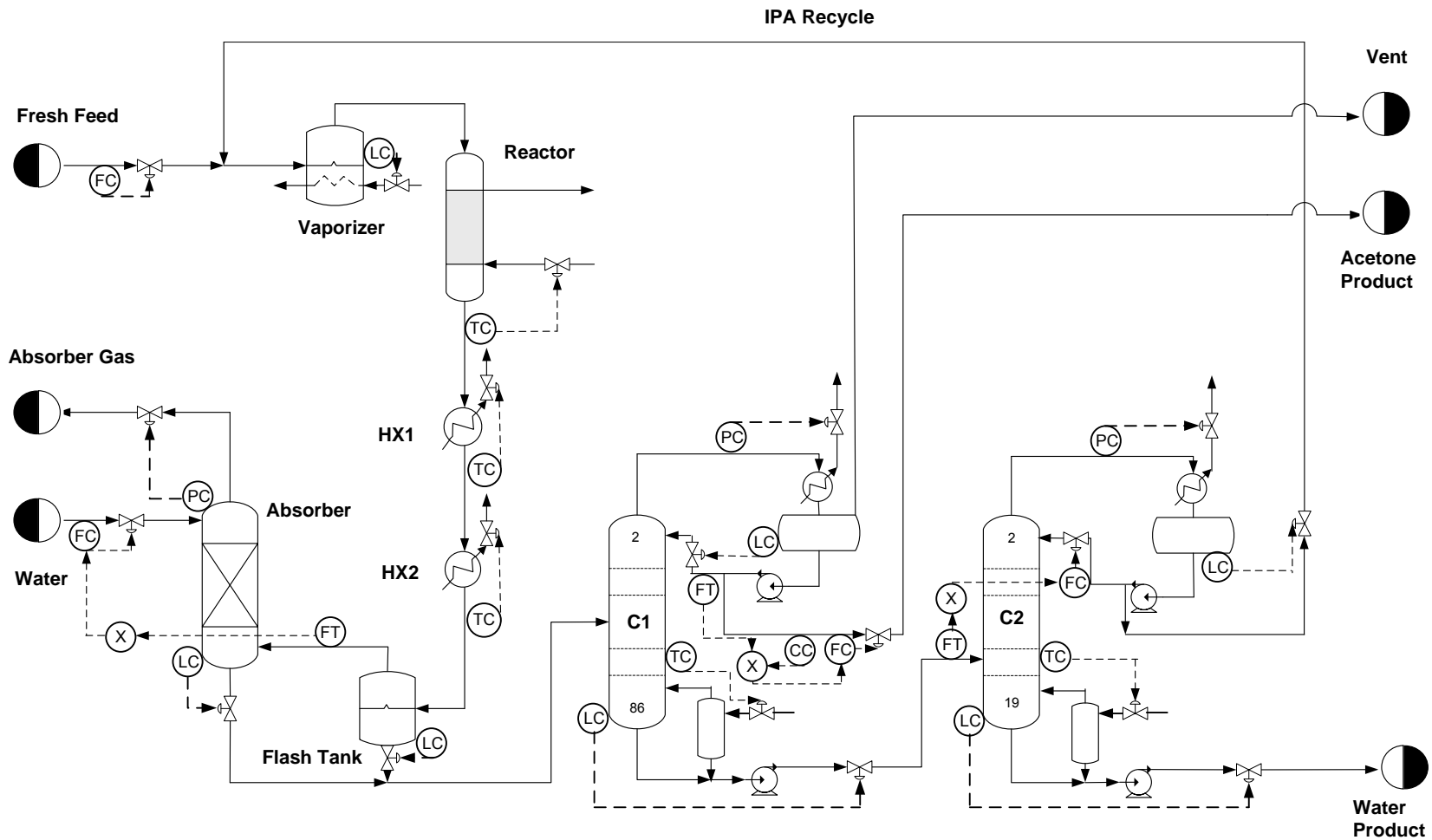


Figure 5.18 Control Structure of Base Case (BC)

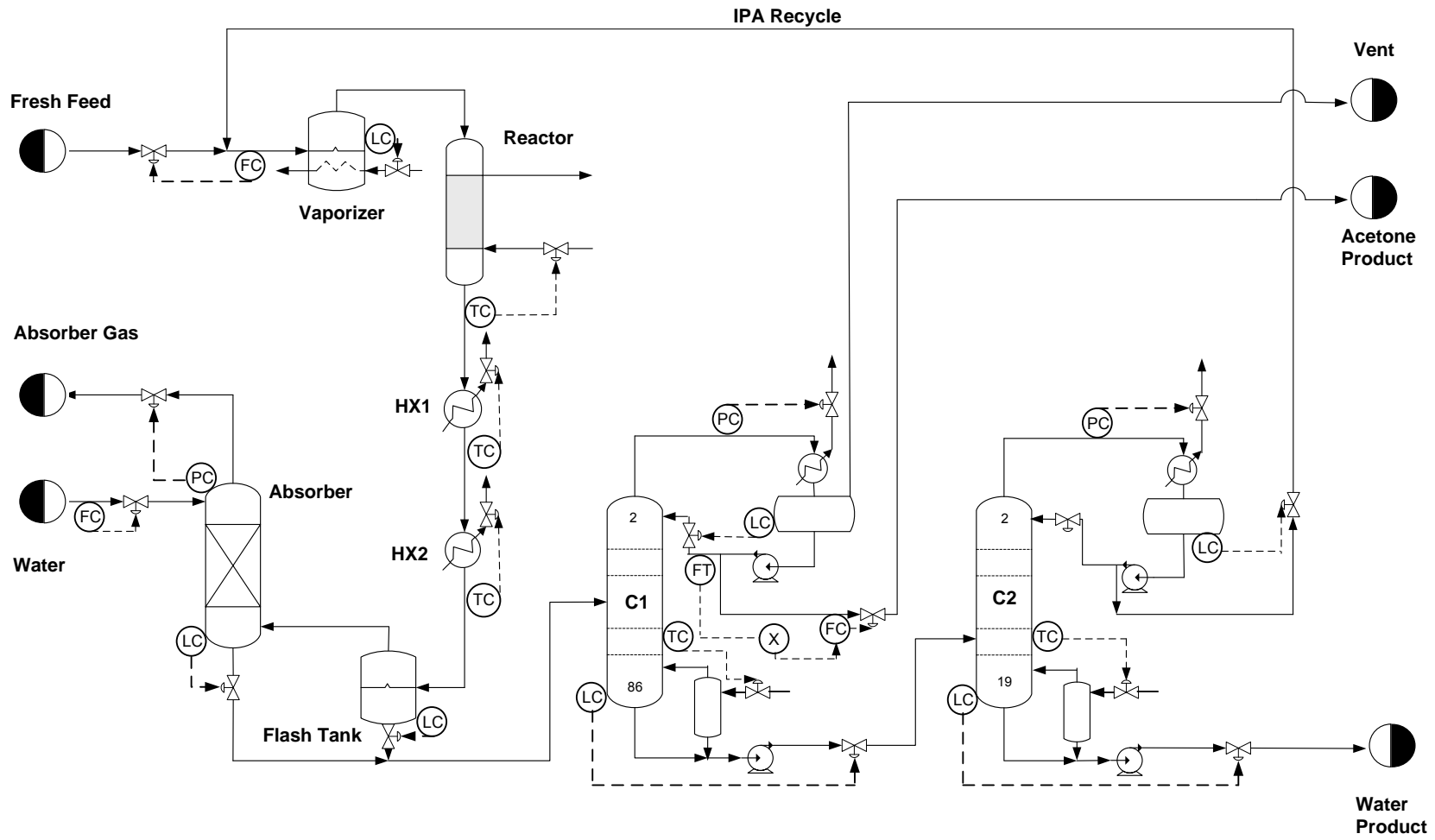


Figure 5.19 Control structure 1 (CS1)

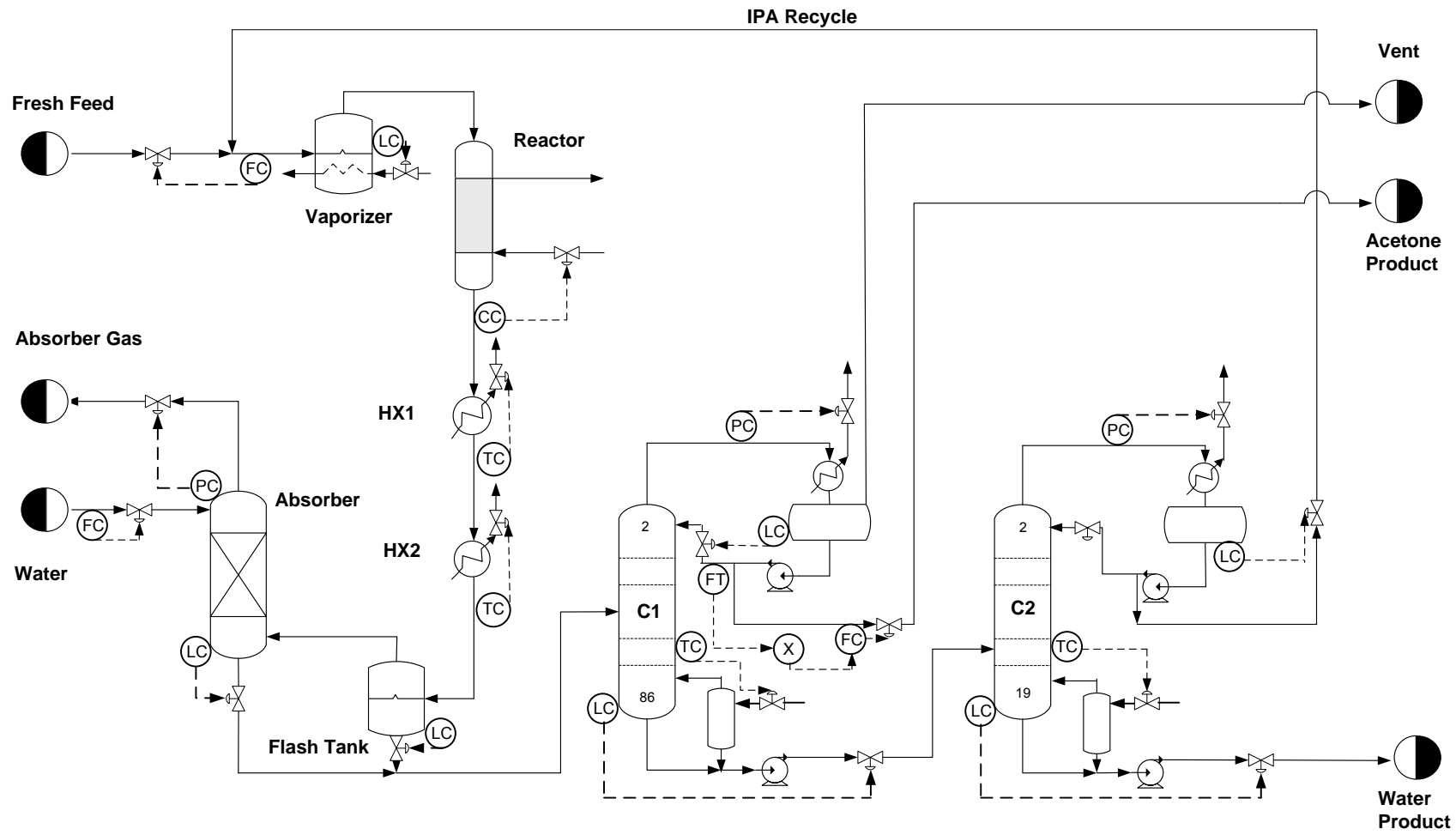


Figure 5.20 Control structure 2 (CS2)

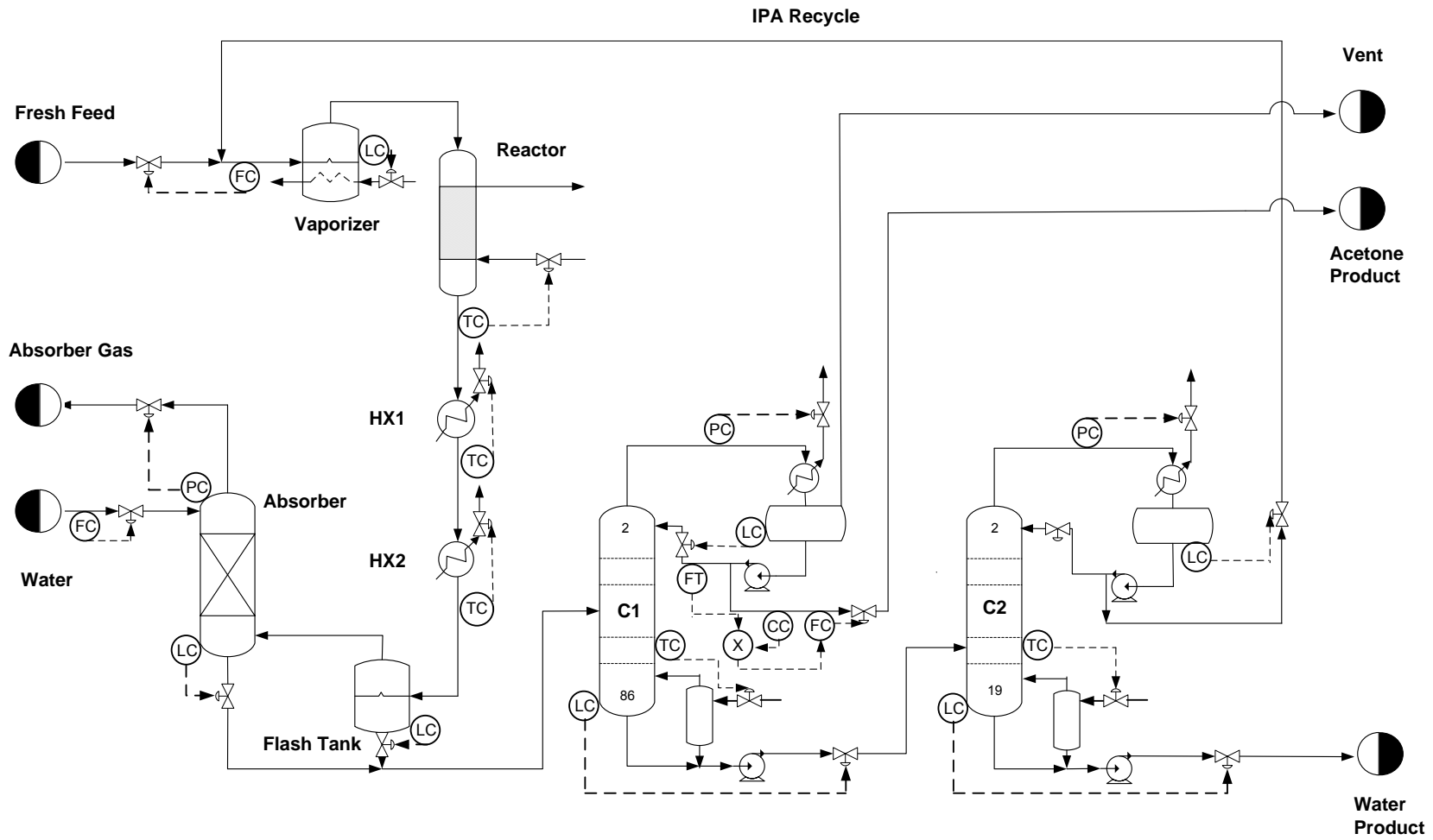


Figure 5.21 Control Structure 3 (CS3)

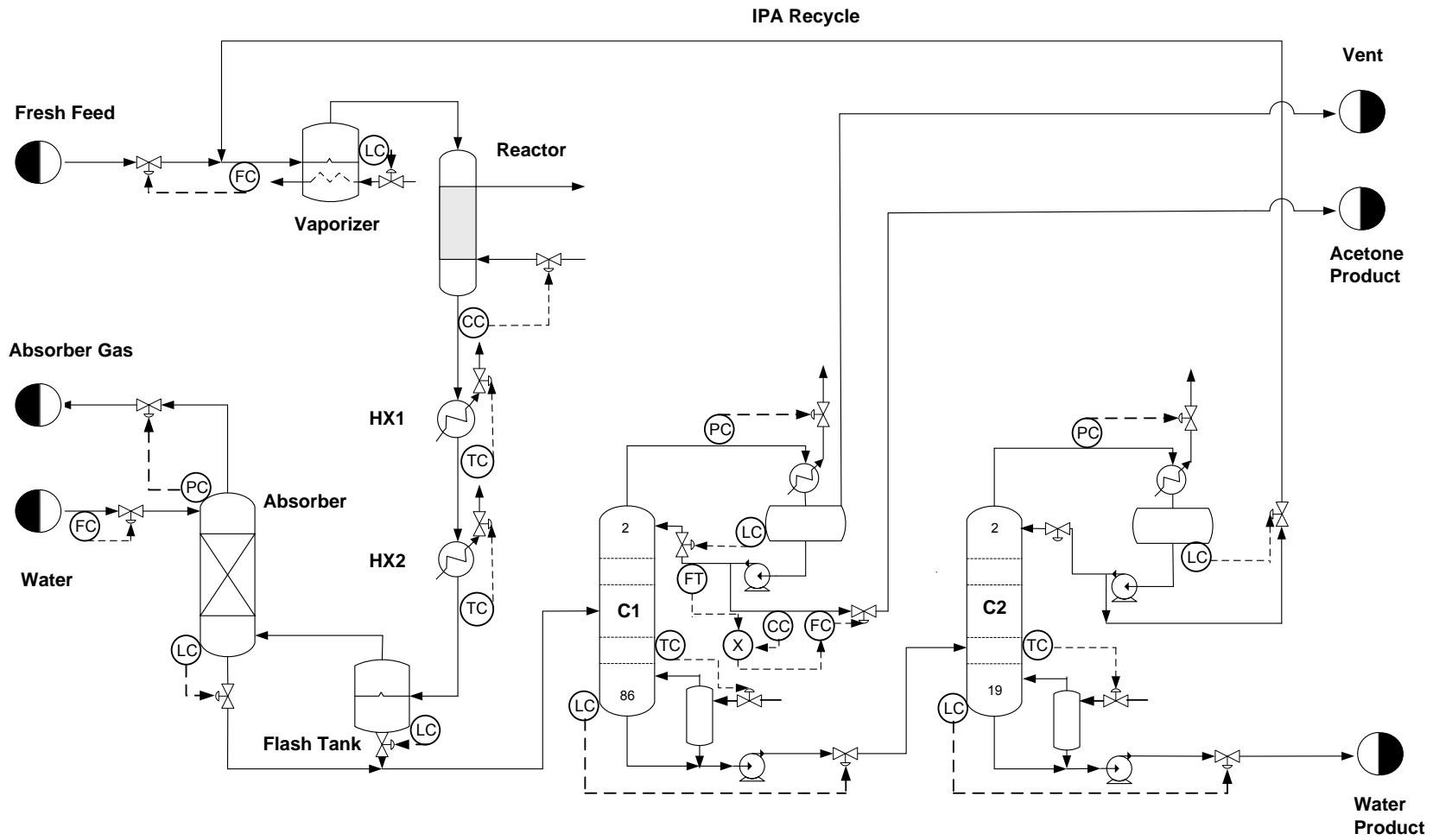


Figure 5.22 Control Structure 4 (CS4)

Table 5.12 Summary control loops of all control structure for acetone process

Equipment	Controlled Variables	Manipulated Variables				
		BC	CS1	CS2	CS3	CS4
Fresh feed	Fresh feed flow rate	Fresh feed flow rate	-	-	-	-
	Total flow rate	-	Fresh feed flow rate	Fresh feed flow rate	Fresh feed flow rate	Fresh feed flow rate
Water feed	Water flow rate	-	Water flow rate	Water flow rate	Water flow rate	Water flow rate
Vaporizer	Level	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate
Reactor	Outlet temperature	Duty flow rate	Duty flow rate	-	Duty flow rate	-
	Outlet composition	-	-	Duty flow rate	-	Duty flow rate
Exchanger(HX1)	Outlet temperature	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate
Exchanger(HX2)	Outlet temperature	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate	Duty flow rate
Flash tank	Level	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate
Absorber	Level	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate
	Vessel pressure of condenser	Absorber gas out flow rate	Absorber gas out flow rate	Absorber gas out flow rate	Absorber gas out flow rate	Absorber gas out flow rate
	Water feed to gas ratio	Water flow rate	-	-	-	-
Acetone	Reboiler level	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate
Column(C1)	Reflux drum level	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate

Table 5.12 (Continued) Summary control loops of all control structure for acetone process

Equipment	Controlled Variables	Manipulated Variables				
		BC	CS1	CS2	CS3	CS4
Acetone	Top stage pressure	Condenser duty	Condenser duty	Condenser duty	Condenser duty	Condenser duty
Column(C1)	Stage Temp tray80	Reboiler duty	Reboiler duty	Reboiler duty	Reboiler duty	Reboiler duty
	Water composition in distillate	Distillate to reflux SP	-	-	Distillate to reflux SP	Distillate to reflux SP
	Distillate to reflux ratio	Distillate flow rate	-	-	Distillate flow rate	Distillate flow rate
	Distillate to reflux ratio	-	Distillate flow rate	Distillate flow rate	-	-
Water	Level	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate	Bottom flow rate
Column(C2)	Level	Distillate flow rate	Distillate flow rate	Distillate flow rate	Distillate flow rate	Distillate flow rate
	Top stage pressure	Condenser duty	Condenser duty	Condenser duty	Condenser duty	Condenser duty
	Stage Temp tray17	Reboiler duty	Reboiler duty	Reboiler duty	Reboiler duty	Reboiler duty
	Reflux to feed ratio	Reflux flow rate	-	-	-	-
	Reflux flow rate	-	Reflux flow rate	Reflux flow rate	Reflux flow rate	Reflux flow rate

5.3 Dynamic Simulation Results

For all the control structures, material (flowrate and composition), thermal disturbances are applied to test the response of the system which referred to dynamic performance of those control structures. Furthermore, heat-integrated plant for acetone process is evaluated the dynamic performance as well.

All level loops use proportional (P) controllers only. The other loops use proportional integral (PI) and proportional integral derivative (PID) controllers namely flow, temperature and pressure loops. Temperature and composition controllers are tuned by using relay-feedback tests following Tyreus-Luyben tuning rules. Controller tuning parameters are shown in Appendix B.

To be more realistic, the temperature and composition loops are installed lags and/or dead times. All temperature loops have 1 minute dead times and composition loop has 3 minute dead times.

5.3.1 Disturbance in fresh feed flowrate

Testing condition starts at 0.5 h by change the set point value of the fresh feed flowrate controller from normal value 51.96 kmol/h to 57.16 kmol/h and 46.76 kmol/h for control structure of base case. For CS1-4, the set point value of total flowrate controller is changed instead form normal value 57.76 kmol/h to 62.96 kmol/h and 52.56 kmol/h. The dynamic responses of fresh feed flowrate disturbance are shown in Table 5.13.

When the set point of fresh feed flow rate change as shown in Table 5.13(a),(b).Table 5.13(c) show that the base case, CS1 and CS3 is well handled at about 6 h. For the CS2 and CS4, the outlet temperature is settled at the new steady-state value since the outlet composition of acetone is controlled. The larger change in the outlet composition of acetone, the CS1 and CS3, as shown in Table 5.13(d) originate in the composition of IPA and the flowrate in recycle stream change shown in Table

5.13(k)-(l). For the product column (C1), the impurity of water is maintained at the set point for all control structures as shown in Table 5.13(e) since the tray temperature is well controlled at the set point by the reboiler duty as shown in Table 5.13 (g)-(h). The product flowrate changes directly when the fresh feed flowrate changed shown in Table 5.13(f). At the water column (C2), the composition of IPA is also kept at the set point as shown in Table 5.13 (i) and the water product change in the same way of the fresh feed flowrate change (Table 5.13 (j)). Table 5.13(n) show that the supply energy at the C2 is less in the CS1-CS4 than the base case because the water fresh feed in the absorber is fixed not varied with the gas flow in the absorber. The tray temperature is well handled by the reboiler duty shown in Table 5.13 (m).

5.3.2 Disturbance in fresh feed composition

Testing condition starts at 0.5 h by change fresh feed composition of IPA at 0.67 to 0.65. The dynamic responses of the composition disturbance are shown in Table 5.14. Table 5.14(a) show that the fresh feed response is pulse around 0.5 hours because the molar flowrate is changed by the density. The calculated volume flow rate is varied by composition of the raw material flow in. The fresh feed flowrate of CS2 and CS4 has larger change than CS1 and CS3 since the variation of the recycle flowrate shown in Table 5.14 (k)-(l). The change occurs from the increasing of reaction rate when controlling the outlet composition of acetone (Table 5.14(d)). Table 5.14(c) show that the outlet temperature of the reactor changes significantly for the CS2 and CS4. The less reactant need to be more converted to the product, the more energy need to be more supplied (endothermic reaction). At the C1, the impurity of water is kept at the set point for all control structures as shown in Table 5.14(e). The product flowrate drops off as the amount of reactant decreased shown in Table 5.14(f). The tray temperature of the C1 is well controlled by the reboiler duty as shown in Table 5.14 (g). In Table 5.14(h), for CS2 and CS4 energy supply is used more than the base case, CS1 and CS3, because the product increased. At the C2, the composition of IPA has more deviation in the CS2 and CS4 and the water product increases because of the composition of water in fresh feed

changed (Table 5.13 (j)). Table 5.13(n) show that the CS2 and CS4 use the energy supply less than the base case, CS1 and CS3 because more IPA is converted in the reactor. The tray temperature is well handled by the reboiler duty in the CS1 and CS3 as shown in Table 5.13 (m).

5.3.3 Disturbance in fresh feed temperature

Testing condition starts at 0.5 h by change fresh feed temperature at normal value 320 K to 330 K and 310 K. The dynamic responses of thermal disturbance are shown in Table 5.15. When the fresh feed temperature change, the reactor and heat exchangers can cope with the disturbance as shown in Table 5.15(a)-(d). At the both column, the C1 and C2 is less effect to the disturbance so that the purity of the product is maintained at the set point as shown in Table 5.15(e)-(f).

Table 5.13 Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

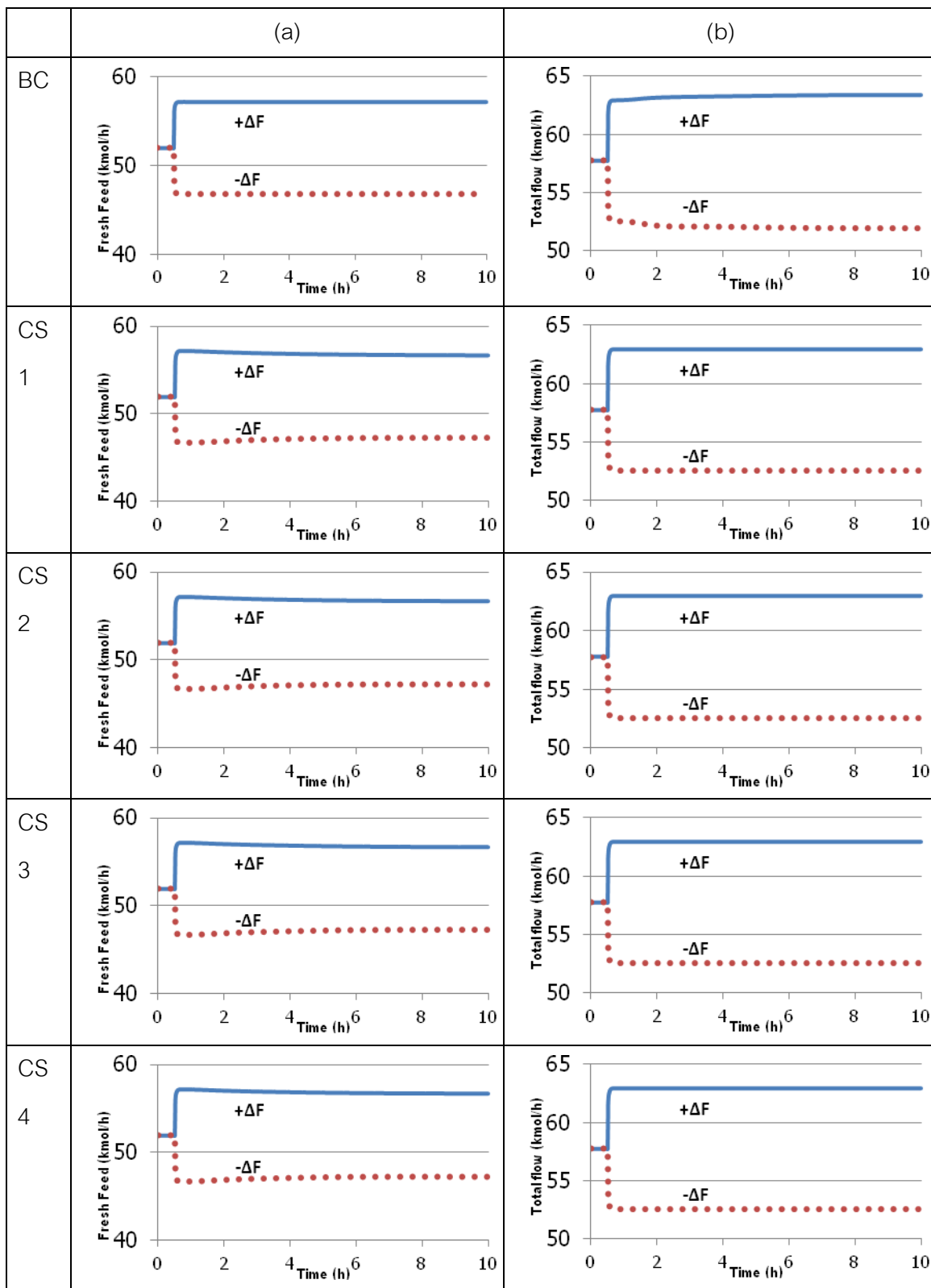


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

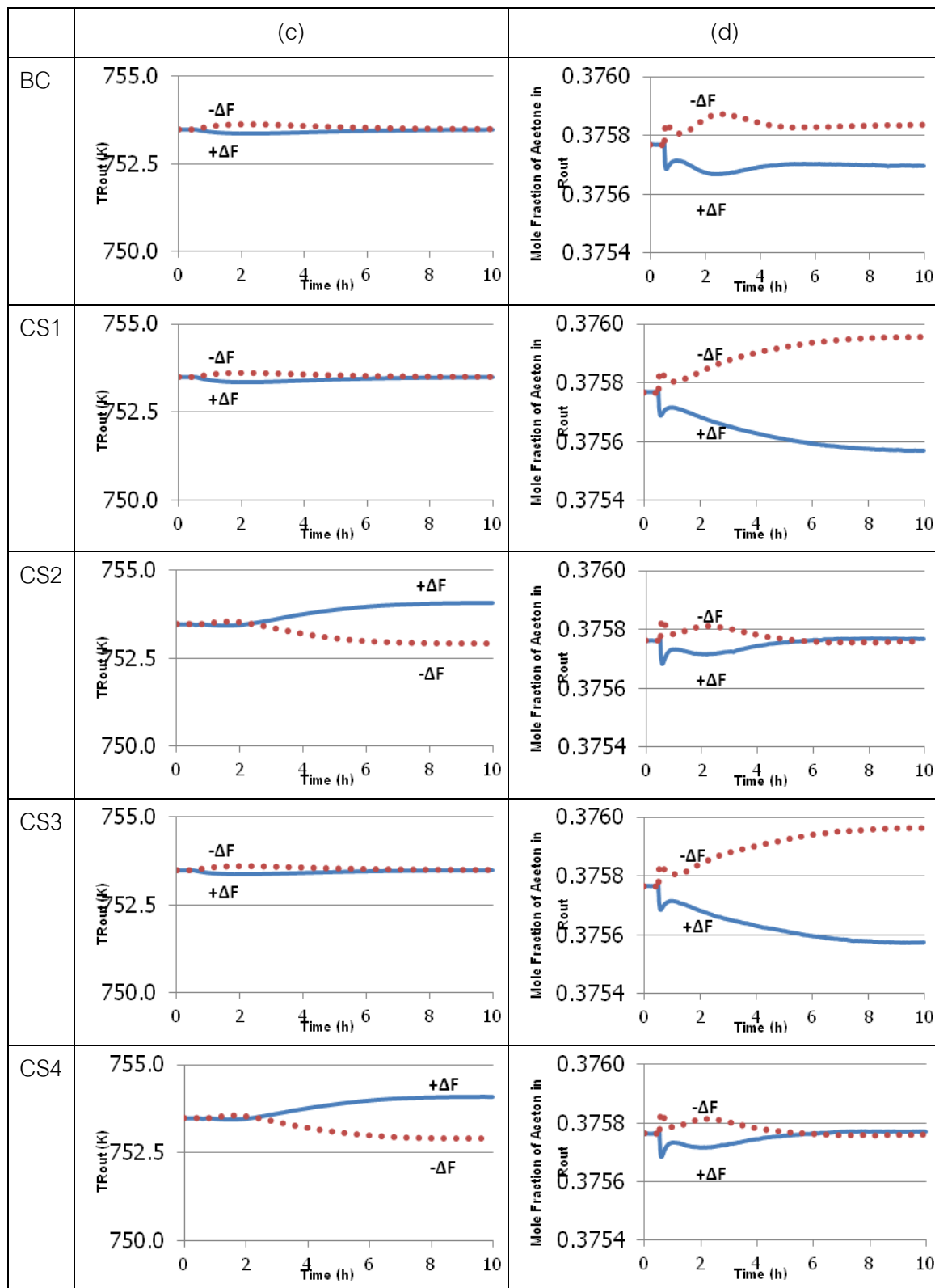


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

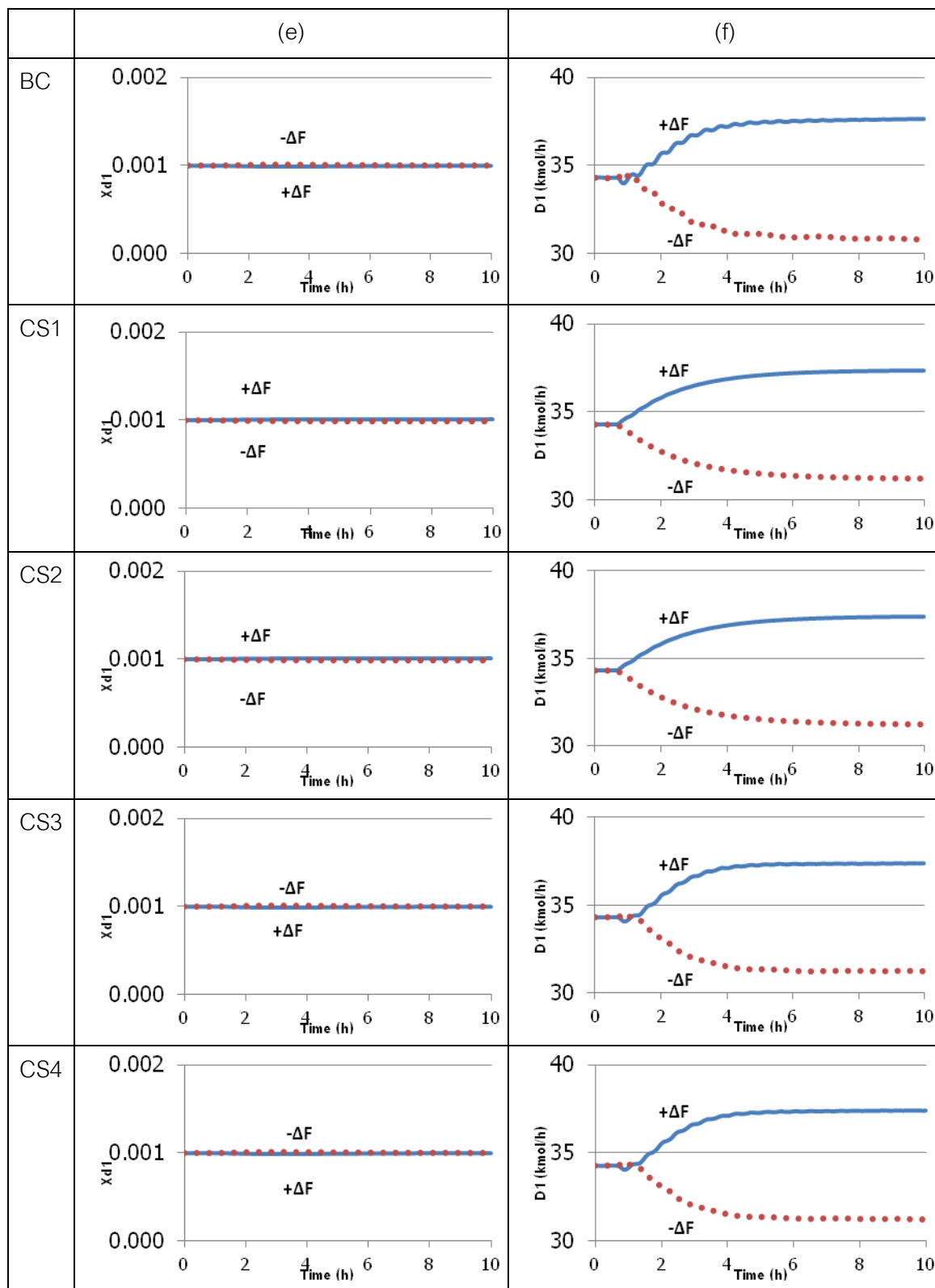


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

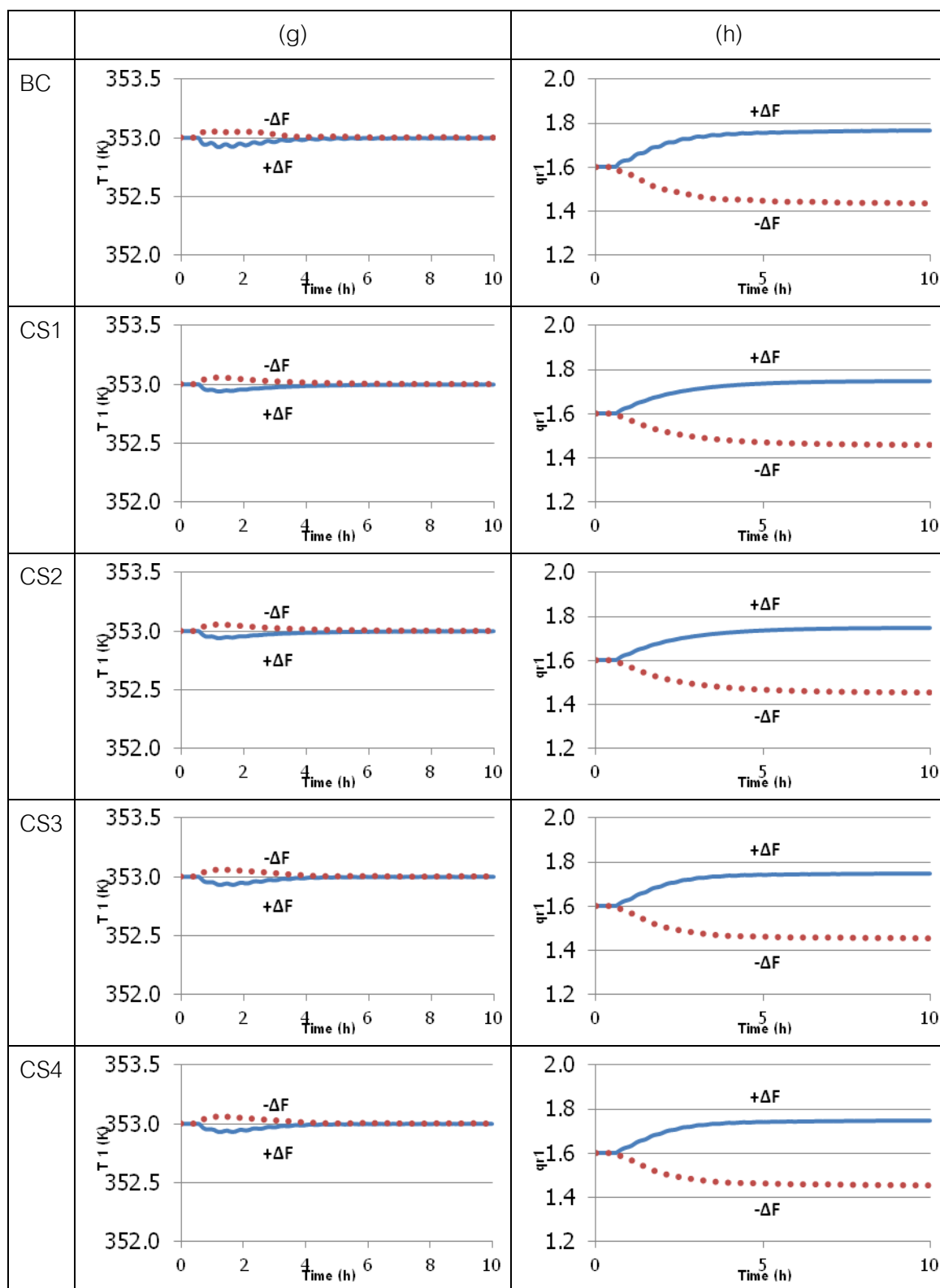


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

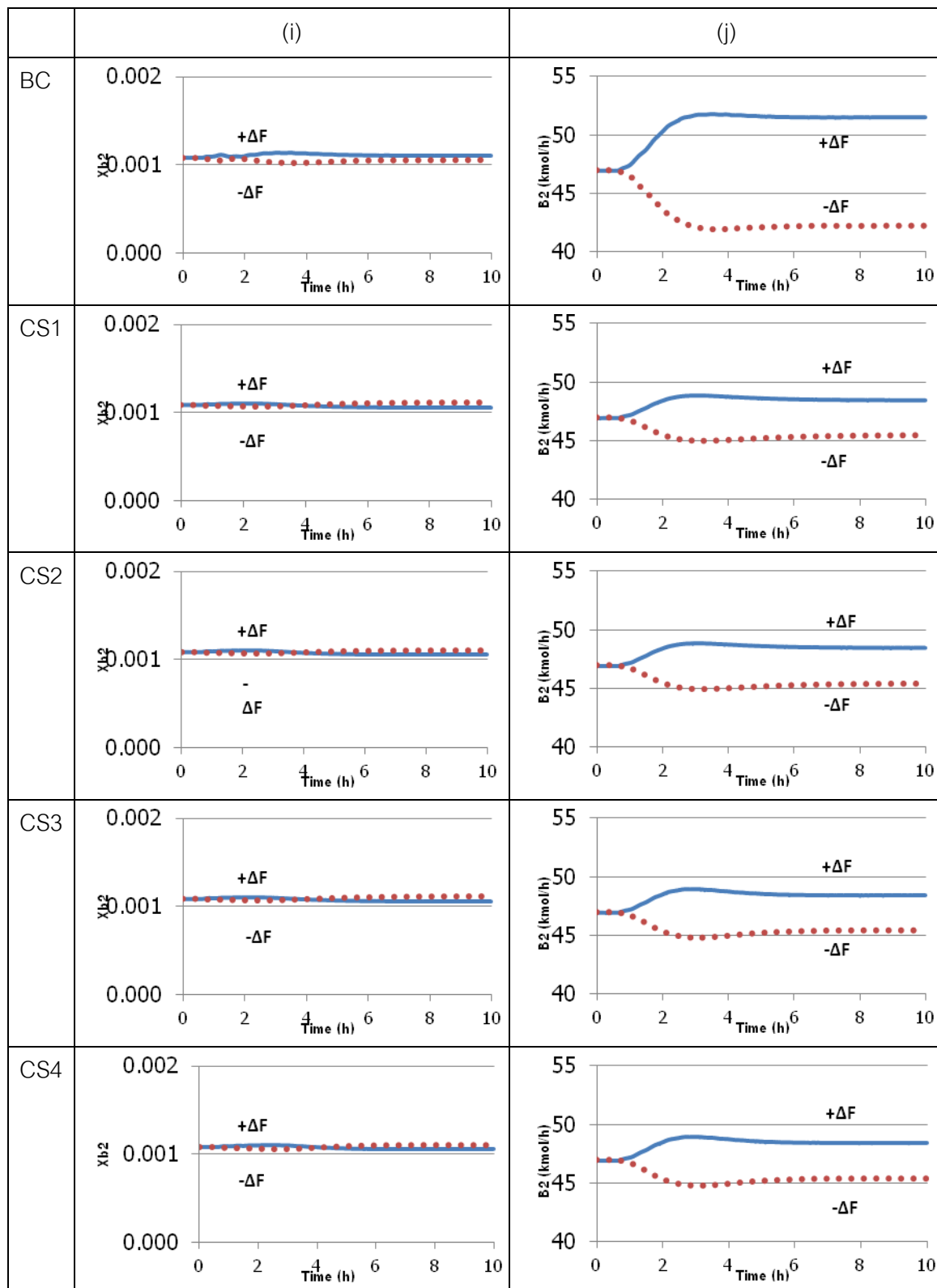


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

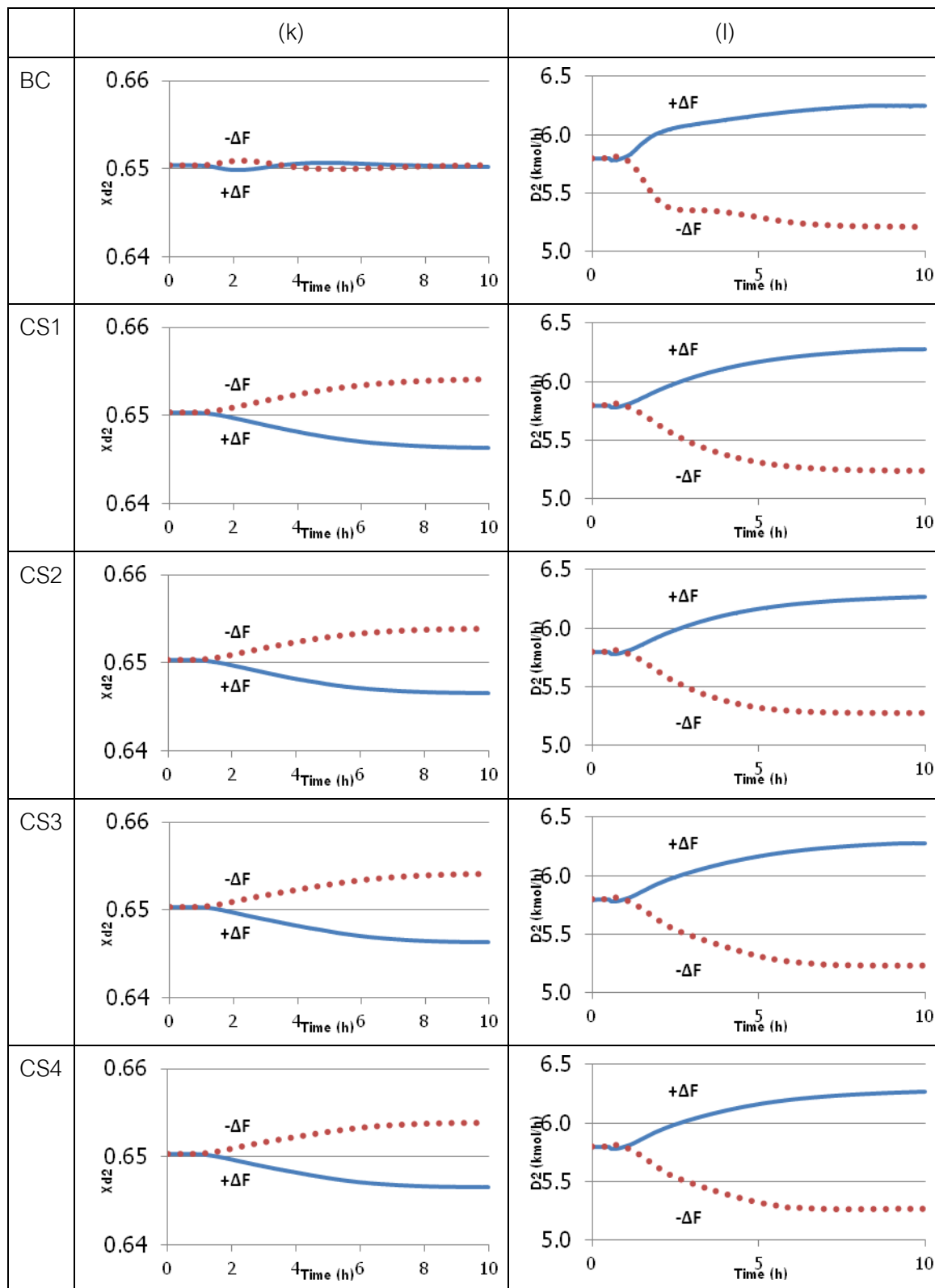


Table 5.13(Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for acetone process

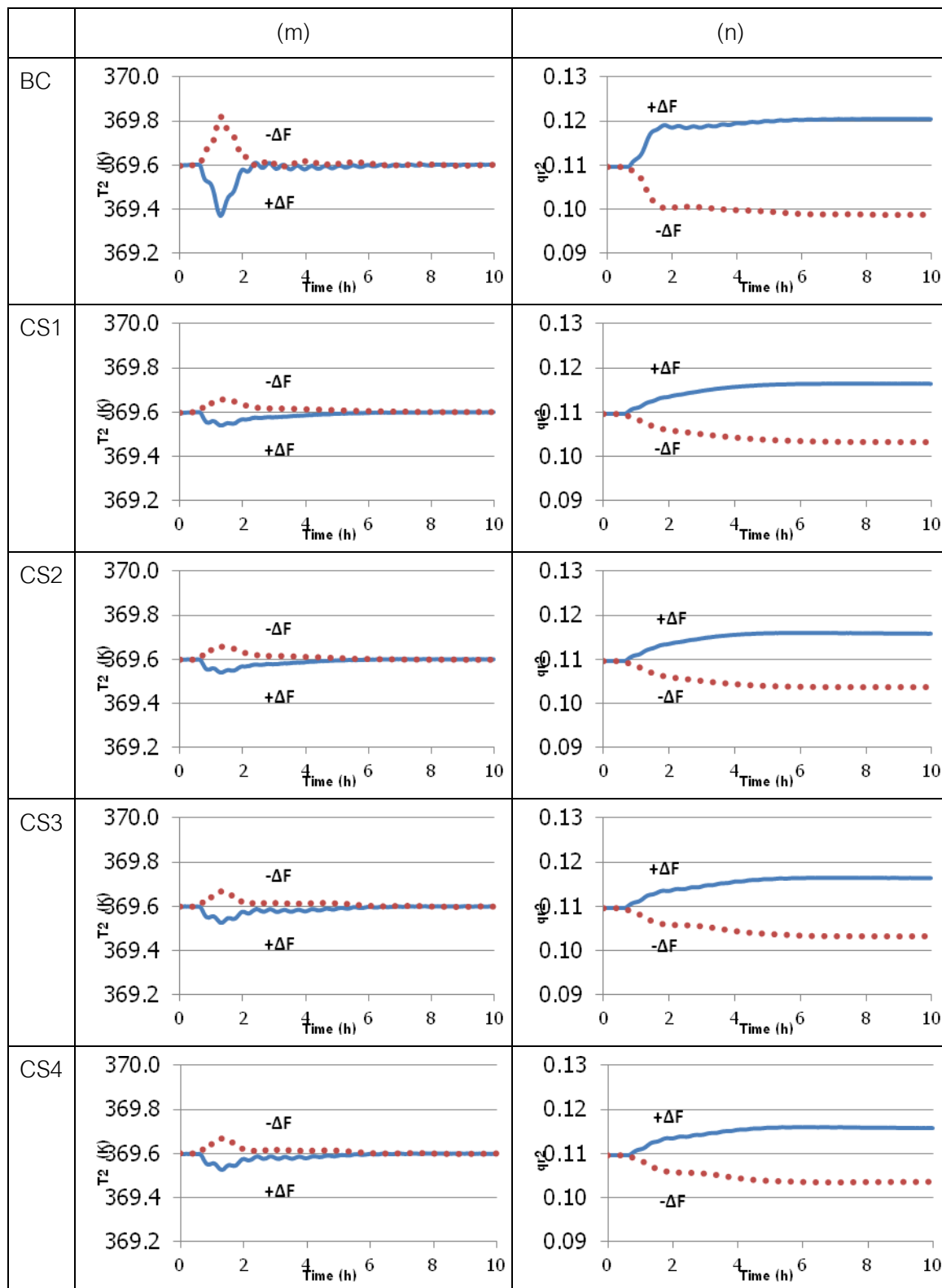


Table 5.14 Dynamic responses of the system to disturbance in fresh feed composition for acetone process

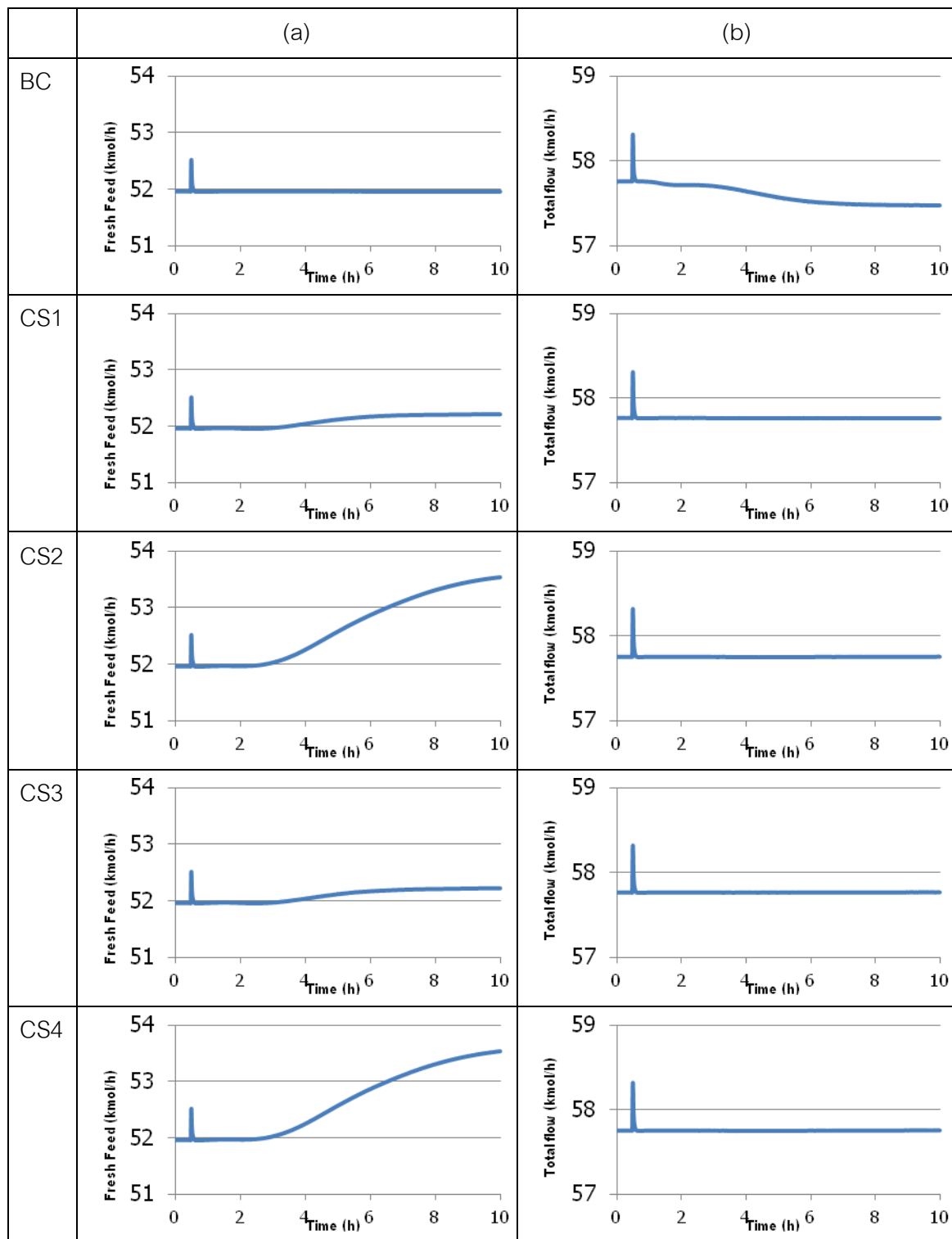


Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

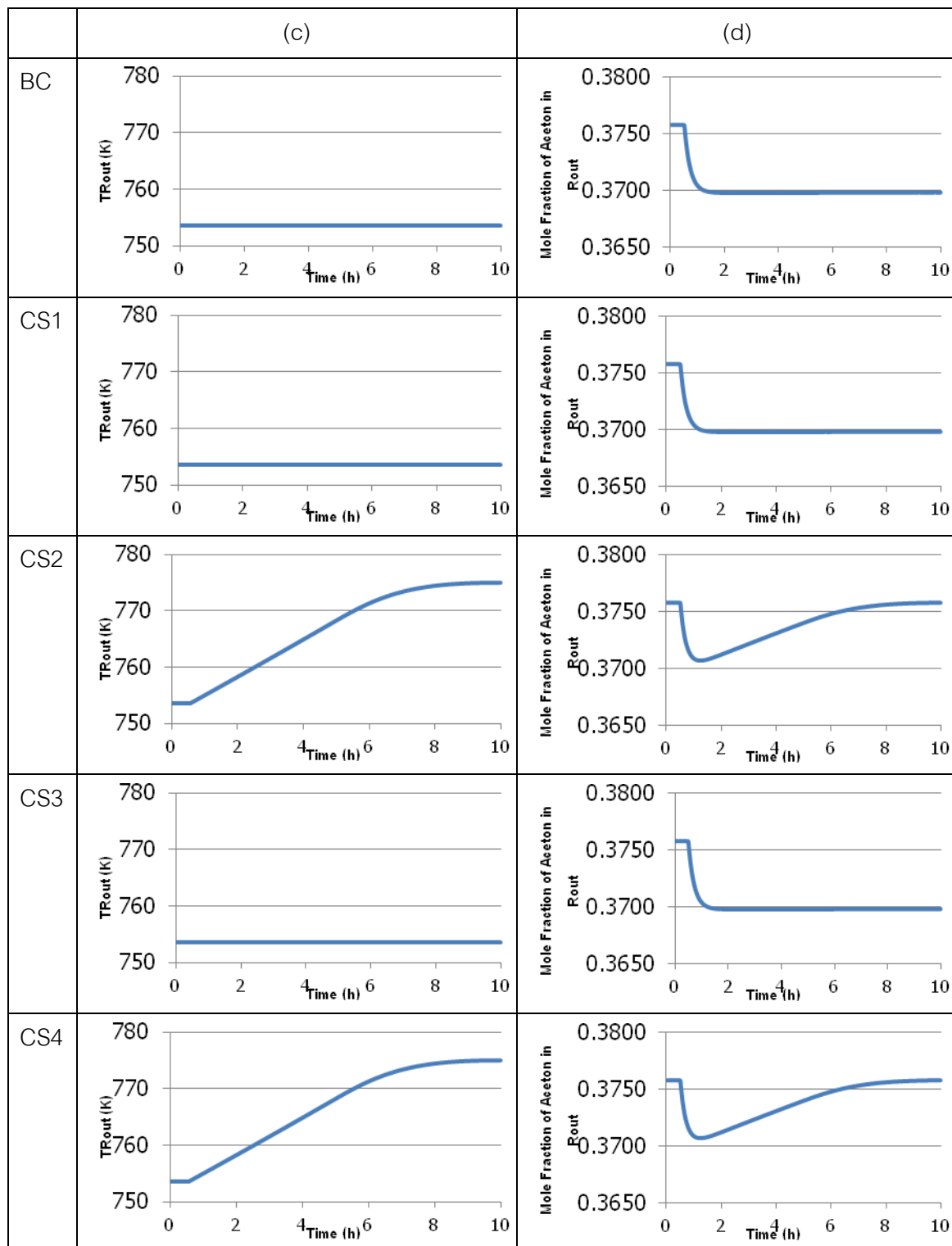


Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

	(e)	(f)
BC		
CS1		
CS2		
CS3		
CS4		

Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

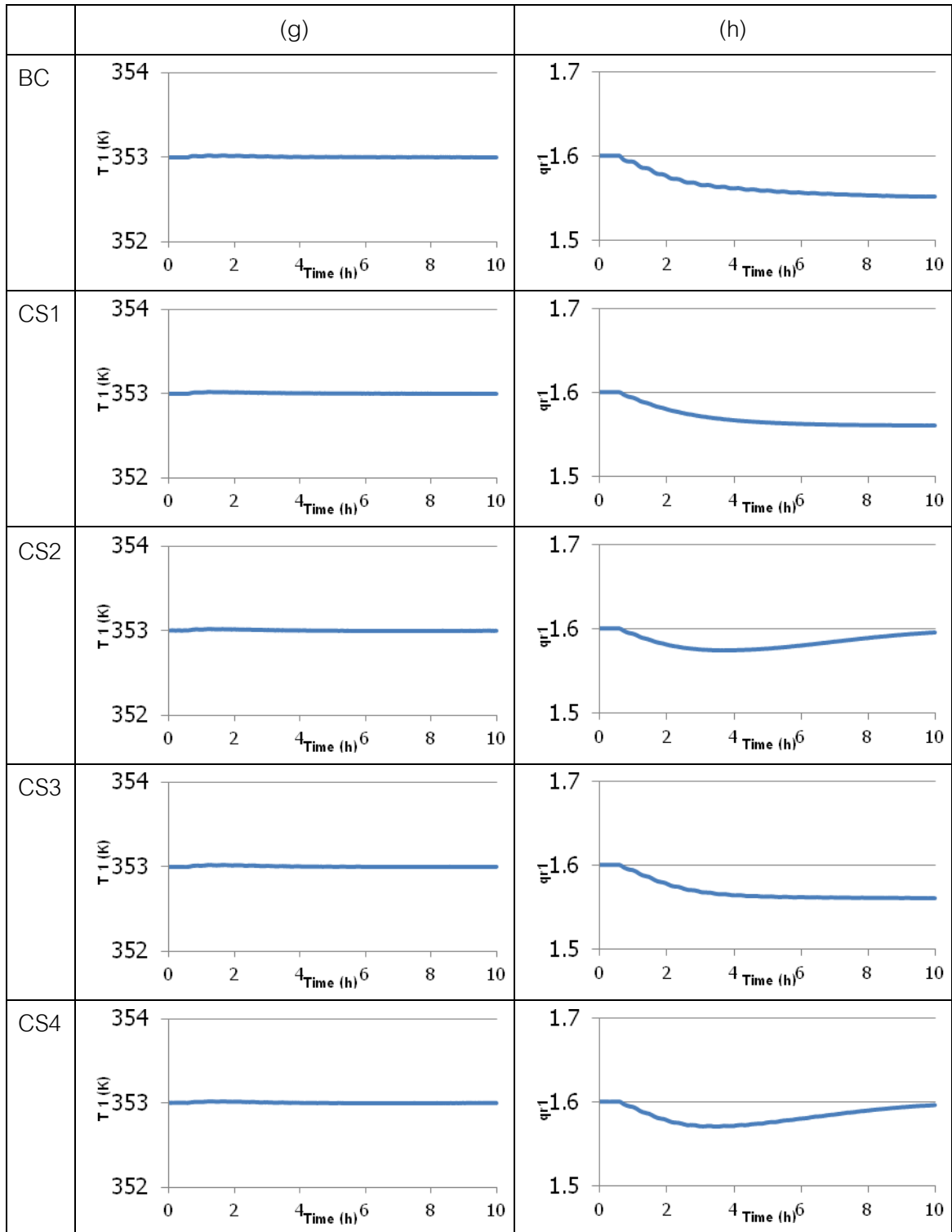


Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

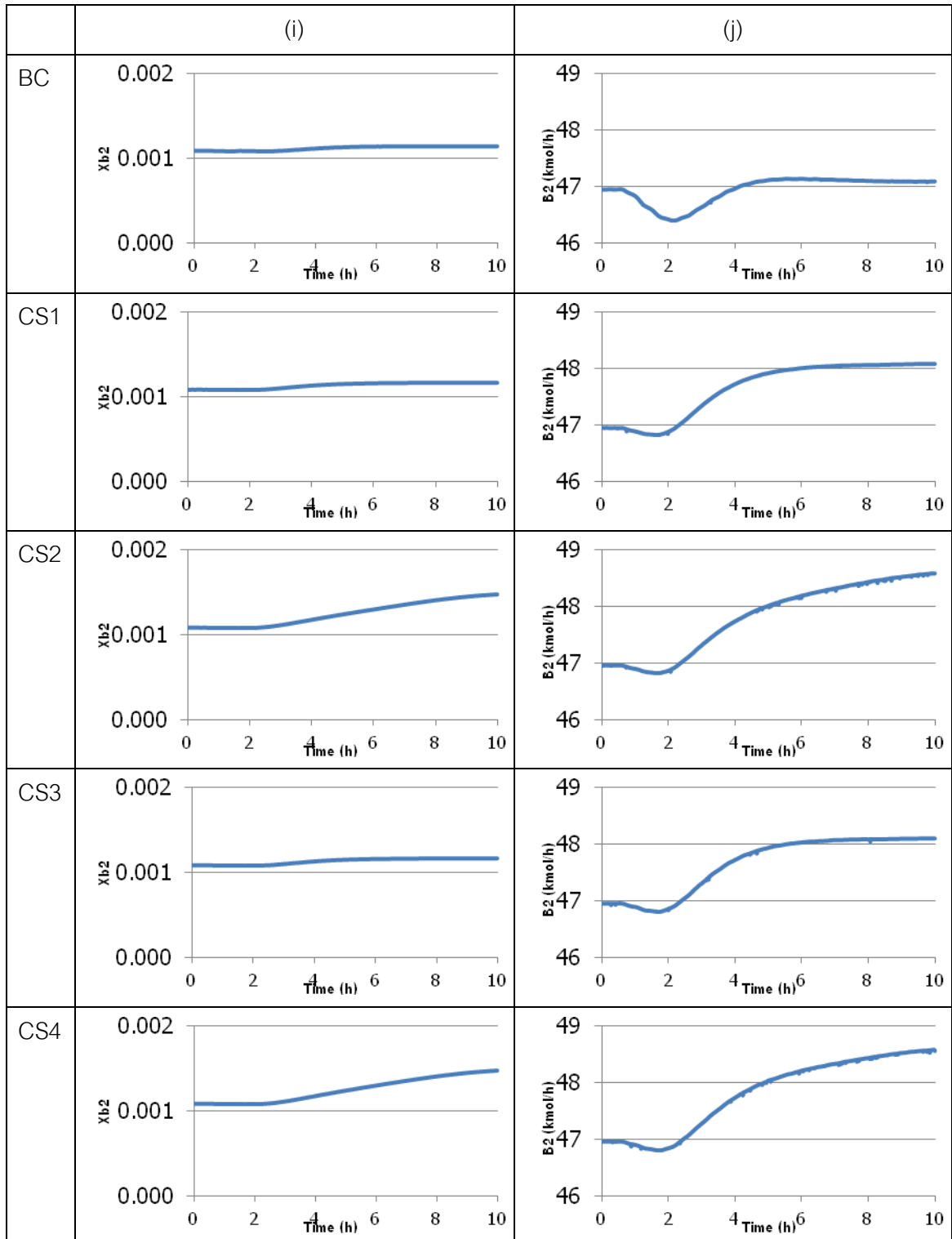


Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

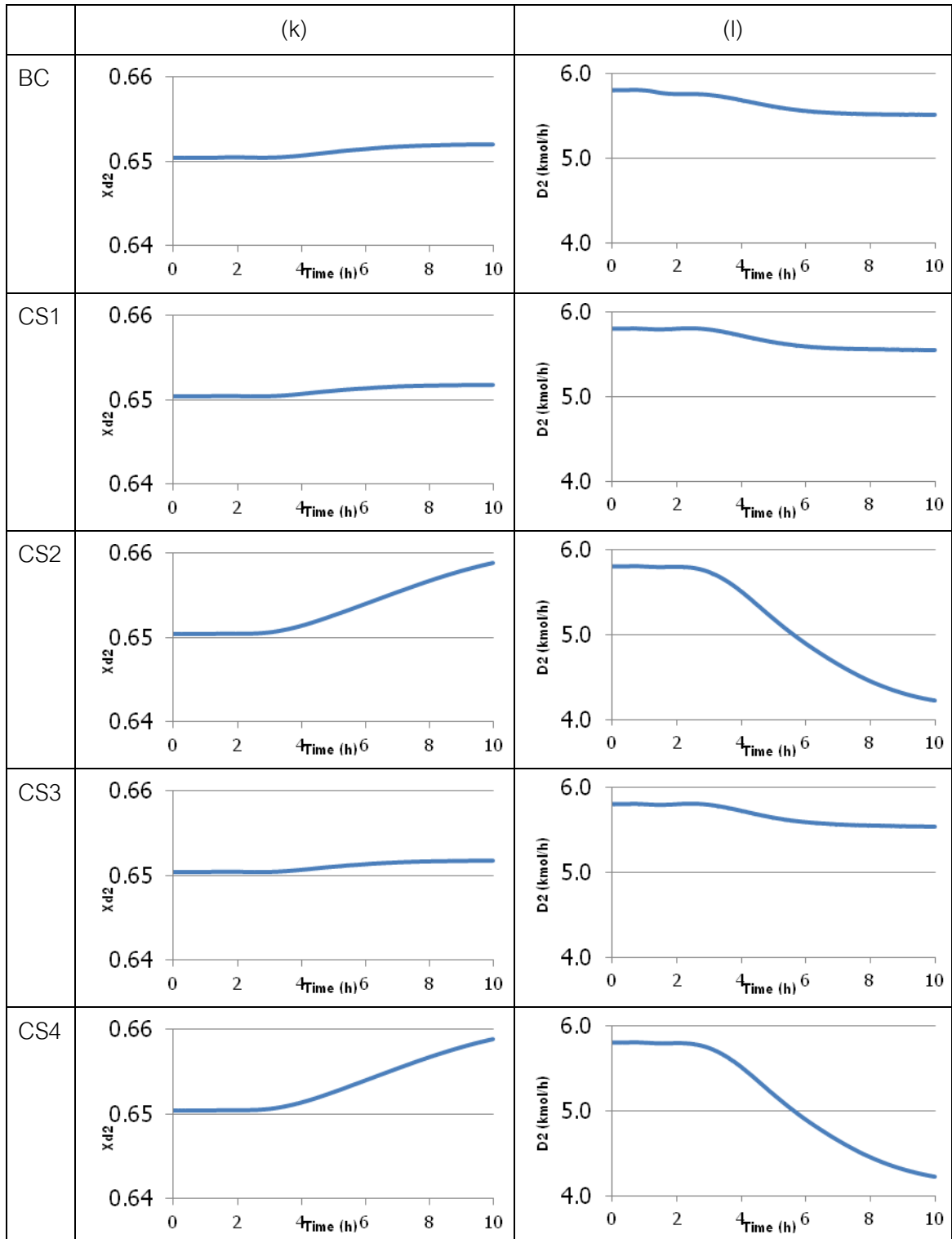


Table 5.14 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for acetone process

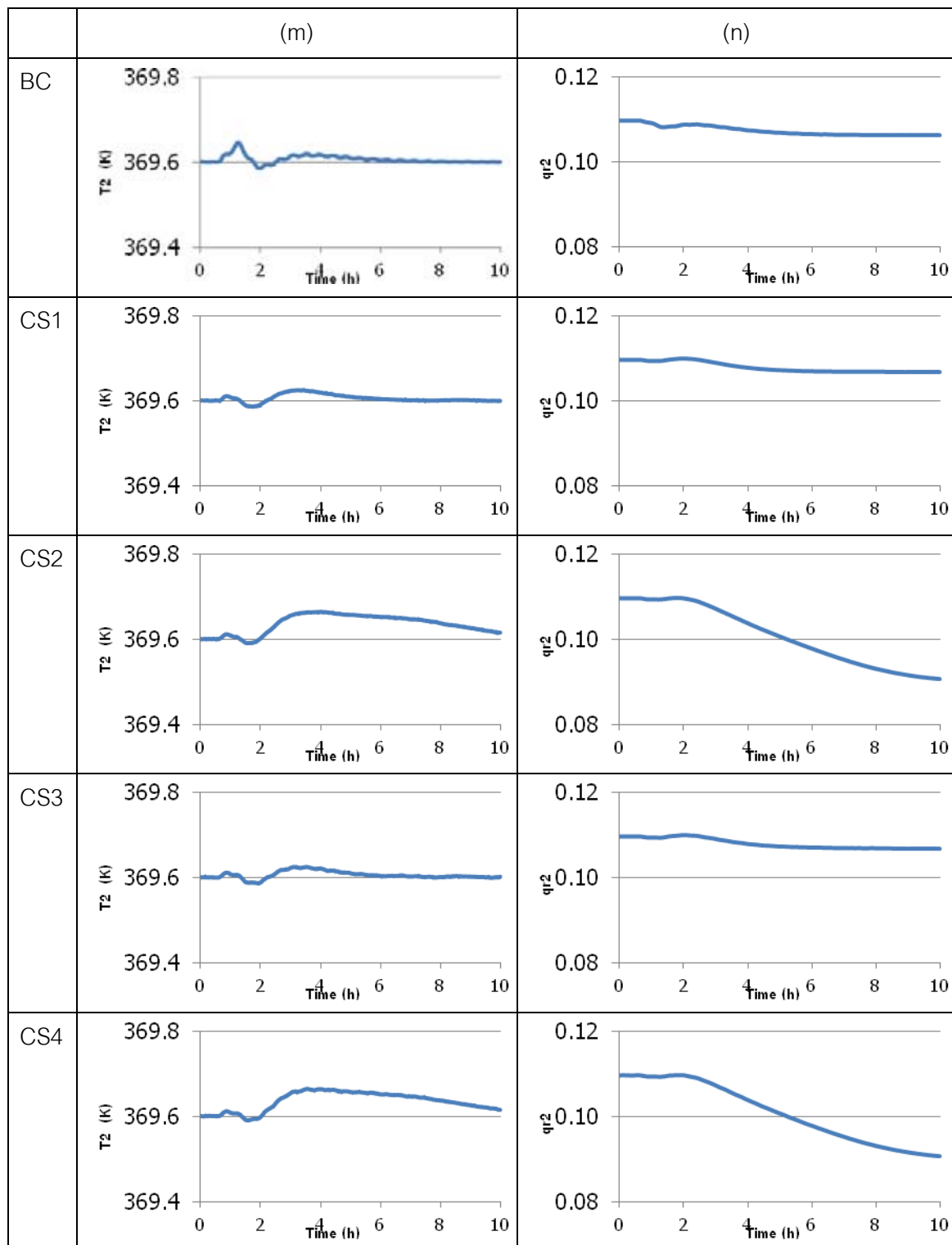


Table 5.15 Dynamic responses of the system to disturbance in fresh feed temperature for acetone process

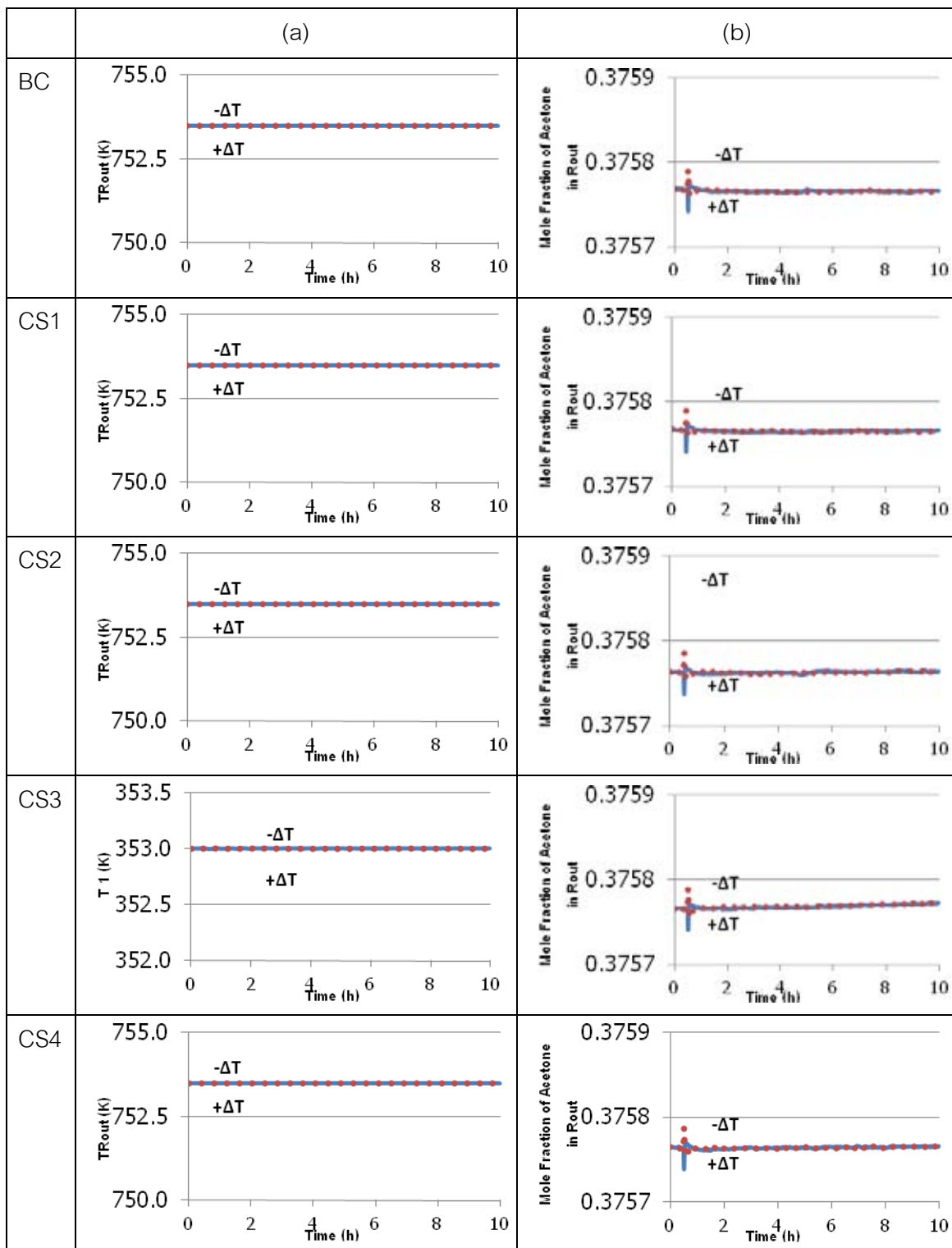


Table 5.15 (Continued) Dynamic responses of the system to disturbance in fresh feed temperature for acetone process

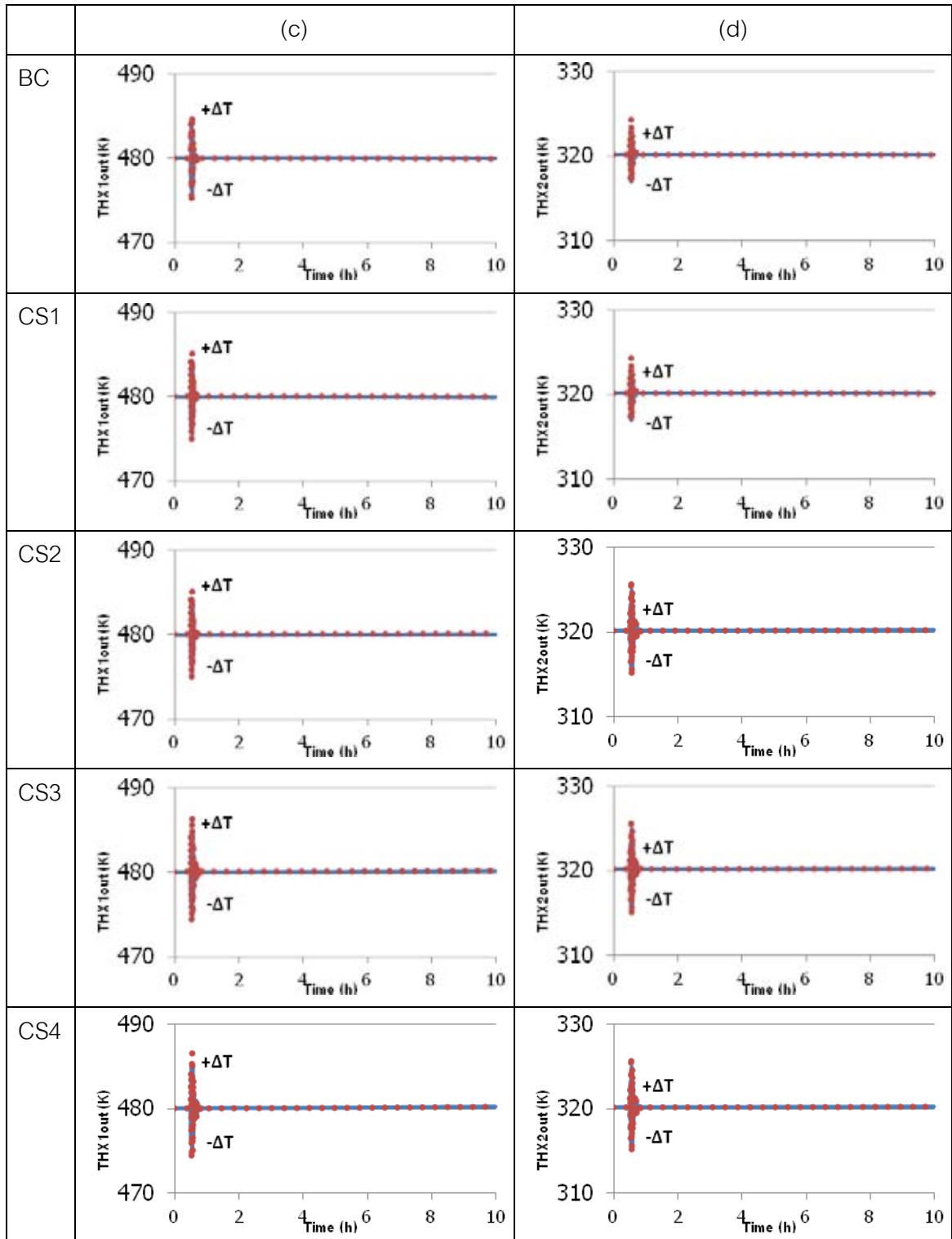
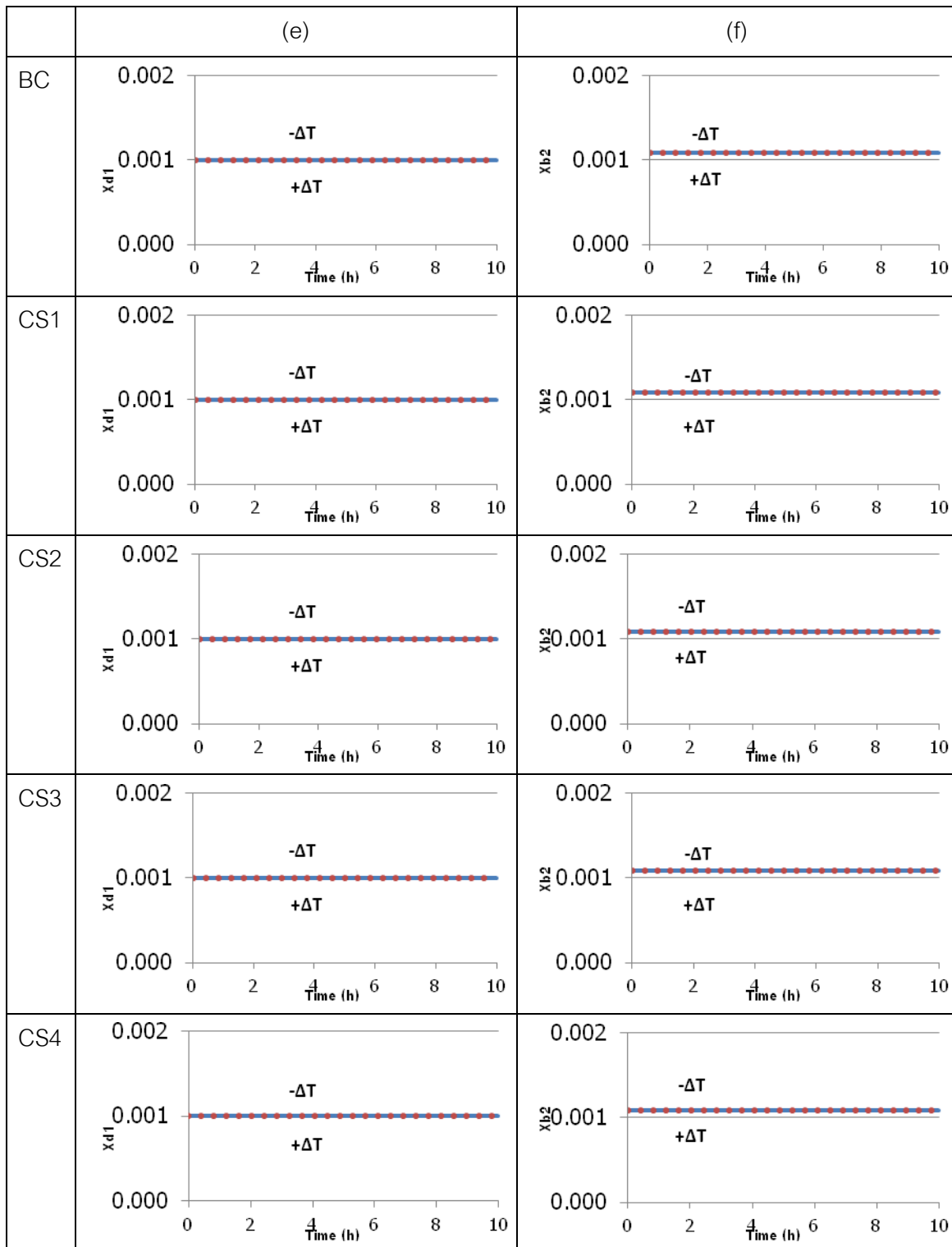


Table 5.15(Continued) Dynamic responses of the system to disturbance in fresh feed temperature for acetone process



5.4 Evaluation of the Dynamic Performance

In this research, integral absolute error (IAE) is used to evaluate the dynamic performance of the control structure of base case and designed control structures. The formulation of a dynamic performance as shown below:

$$IAE = \int |\boldsymbol{\varepsilon}(t)| dt$$

Note that $\boldsymbol{\varepsilon}(t) = y_{sp}(t) - y(t)$ is the deviation (error) of the response from the desired setpoint.

The IAE results are investigated from the safety loop control; temperature and pressure, and the composition of product control loop. The temperature and pressure control are taken into account because those control loop cause the operation smoothly and safely. The composition loops are also important because of requirement of the commercial product quality and maximizing the usage of raw material. The minimum IAE value indicates the best control structure handling the material and thermal disturbances which can operate smoothly and safely and also can keep the product quality at the specification value.

Table 5.16 IAE result for handling the disturbance in fresh feed flowrate

Control structure	Pressure	Temperature	Composition	IAE
Base case	0.00008	0.06661	0.09585	0.16255
CS1	0.00007	0.06254	0.20847	0.27108
CS2	0.00007	0.12501	0.08966	0.21474
CS3	0.00007	0.08116	0.16321	0.24444
CS4	0.00007	0.14941	0.04410	0.19358

Table 5.17 IAE result for handling the disturbance in fresh feed composition

Control structure	Pressure	Temperature	Composition	IAE
Base case	0.00002	0.02079	2.77252	2.79334
CS1	0.00002	0.02053	2.77968	2.80023
CS2	0.00003	1.32740	0.93383	2.26126
CS3	0.00002	0.02757	2.77382	2.80142
CS4	0.00003	1.33320	0.93747	2.27070

Table 5.18 IAE result for handling the disturbance in fresh feed temperature

Control structure	Pressure	Temperature	Composition	IAE
Base case	0.00004	0.05492	0.00423	0.05918
CS1	0.00003	0.05506	0.00488	0.06211
CS2	0.00004	0.06321	0.01026	0.07350
CS3	0.00004	0.07584	0.00311	0.07899
CS4	0.00004	0.08904	0.00613	0.09521

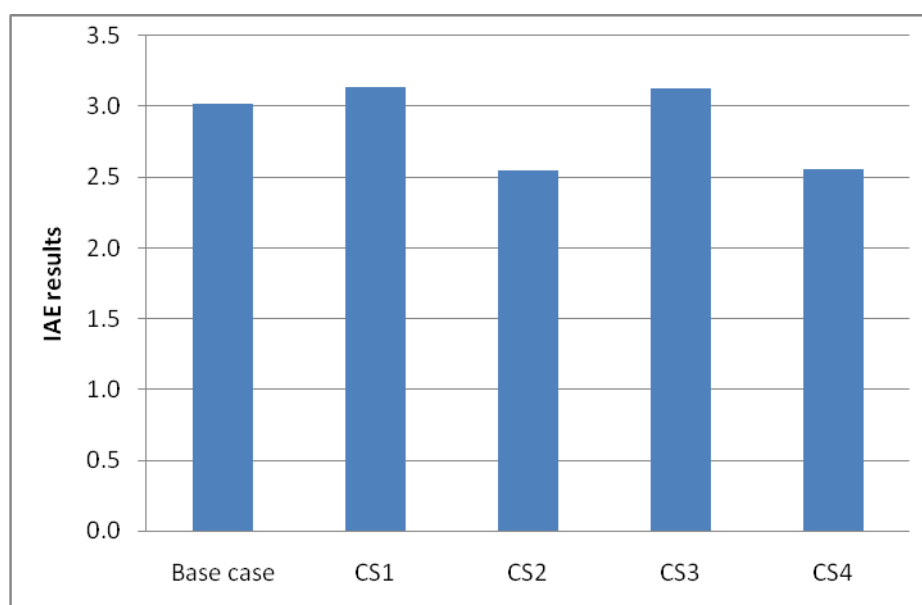
**Figure 5.23** Total IAE results for handling all the disturbances

Table 5.16-18 show the IAE results of the base case and designed control structure (CS1-4) when applied the disturbance though the process. For the CS2

and CS4, the IAE result of the temperature control loop is much larger than the base case, CS1 and CS3 because such control structures do not control the outlet temperature of the reactor. For the base case, CS2 and CS4, the IAE result of the composition loop is significantly less than the CS1 and CS3 because the composition control at the reactor and the C1. Although, the designed control structures; the CS1 and CS3 have total IAE value more than the CS2 and CS4. From the dynamic responses imply that when the outlet temperature of the reactor is no temperature control loop, the outlet temperature reaches up almost the constraint of catalyst activity limitation. So the CS1 and the CS3 are chosen. The comparison of total IAE value shows that the CS3 has the value smaller than the CS1 (Figure 5.23) which means the CS3 has more potential to handle the disturbances. Then the CS3 is evaluated the performance with heat-integrated plant for acetone process.

5.5 Evaluation of cost

The operation cost of energy includes the cost energy of vaporizer, reactor, coolers and reboilers and condensers. The calculated utility costs for each control structure indicates the performance of using the energy when the disturbances occurring. Table 5.19-21 show energy consumption and cost for each disturbance test. By the result, the CS4 is using the minimum of energy cost for all disturbances as shown in Figure 5.24.

Table 5.19 Energy consumption and cost when fresh feed flowrate changed

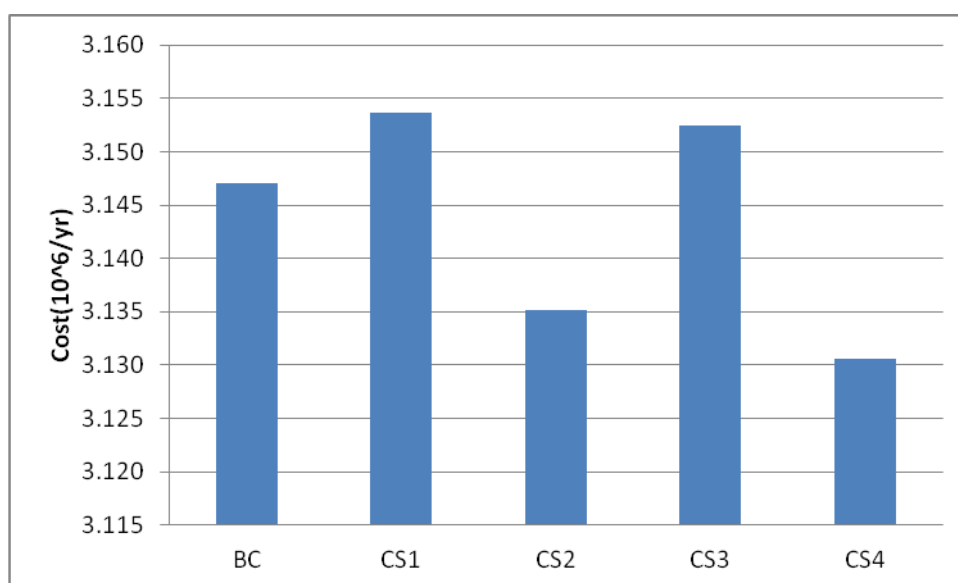
CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
BC	1.6807	1.7096	1.9975	0.0188	0.4194	0.6192	5.3878	1.0574
CS1	1.6757	1.7112	1.9999	0.0187	0.4199	0.6200	5.3868	1.0585
CS2	1.6731	1.7114	1.9991	0.0187	0.4199	0.6197	5.3836	1.0583
CS3	1.6758	1.7111	1.9992	0.0187	0.4198	0.6198	5.3862	1.0583
CS4	1.6731	1.7110	1.9937	0.0187	0.4198	0.6181	5.3778	1.0565

Table 5.20 Energy consumption and costs fresh feed composition changed

CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
BC	1.5679	1.6586	1.9580	0.0175	0.4069	0.6070	5.1844	1.0314
CS1	1.5809	1.6684	1.9678	0.0176	0.4093	0.6100	5.2171	1.0370
CS2	1.6116	1.6869	1.8977	0.0180	0.4139	0.5883	5.1963	1.0202
CS3	1.5795	1.6676	1.9669	0.0176	0.4091	0.6097	5.2140	1.0365
CS4	1.6130	1.6878	1.8900	0.0180	0.4141	0.5859	5.1908	1.0180

Table 5.21 Energy consumption and costs fresh feed temperature changed

CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
BC	1.6480	1.7112	2.0001	0.0184	0.4199	0.6200	5.3594	1.0583
CS1	1.6473	1.7107	2.0001	0.0184	0.4197	0.6200	5.3581	1.0581
CS2	1.5452	1.7107	1.9993	0.0173	0.4197	0.6198	5.2552	1.0567
CS3	1.6475	1.7108	1.9988	0.0184	0.4197	0.6196	5.3570	1.0577
CS4	1.6476	1.7108	1.9935	0.0184	0.4198	0.6180	5.3519	1.0561

**Figure 5.24** The summation of utility costs for each control structure when test all disturbances.

Form the IAE result, the CS3 is used to evaluate the dynamic performance compare with the base case. Table 5.22-24 show the dynamic response of all disturbances; fresh feed flowrate, fresh feed composition and fresh feed temperature, respectively.

Table 5.22 Dynamic responses of the system to disturbance in fresh feed flowrate for heat-integrated process of acetone

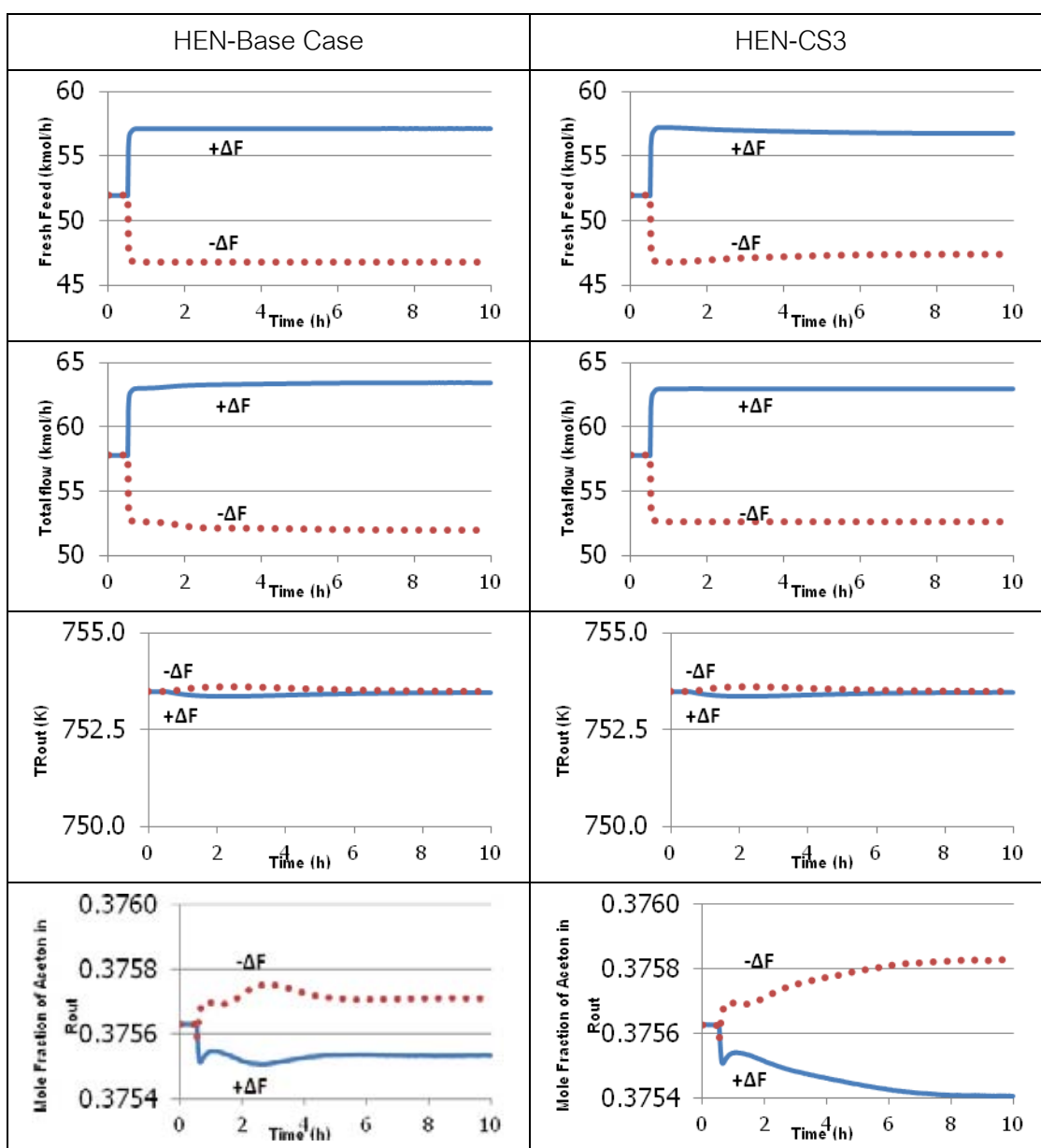


Table 5.22 (Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for heat-integrated process of acetone

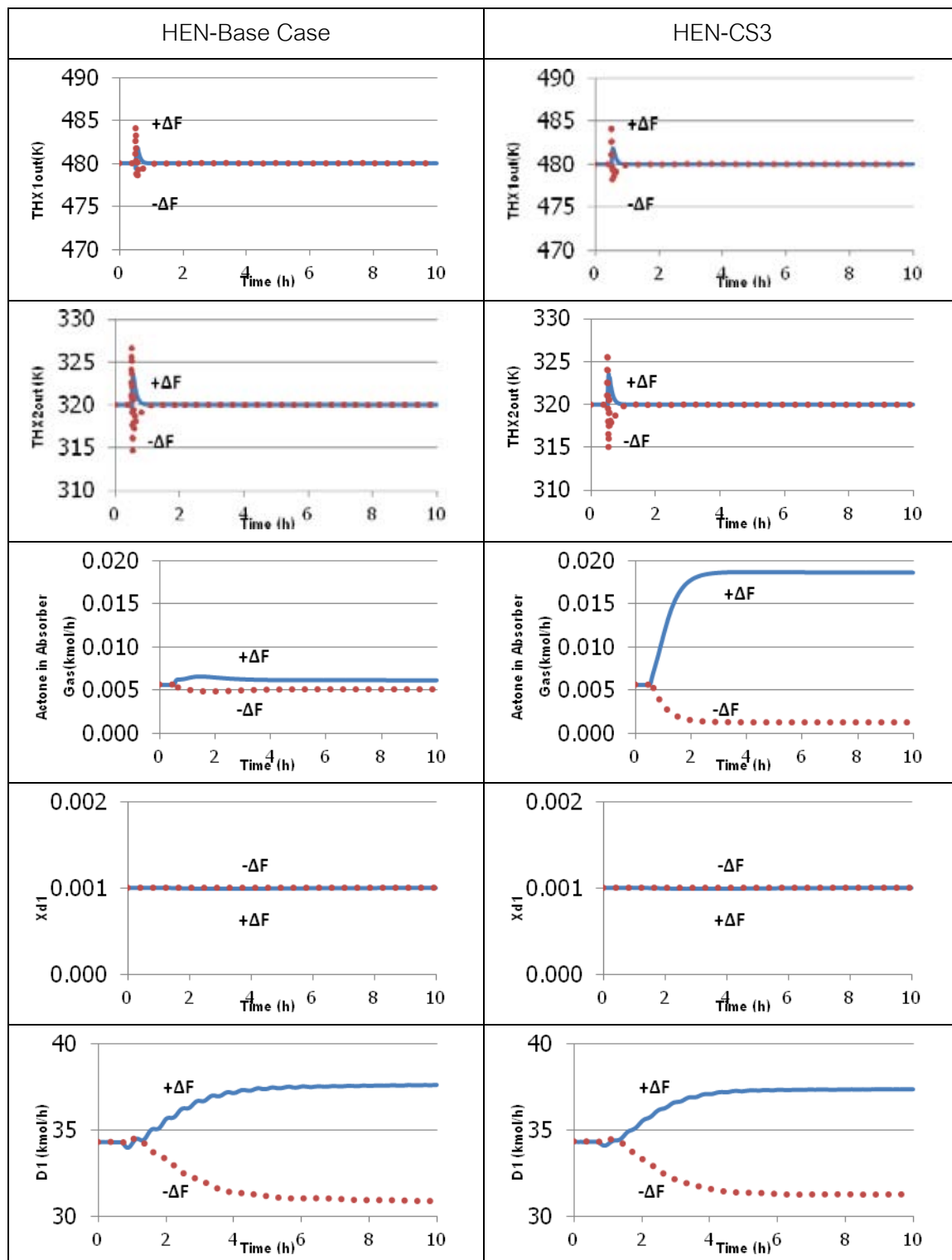


Table 5.22 (Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for heat-integrated process of acetone

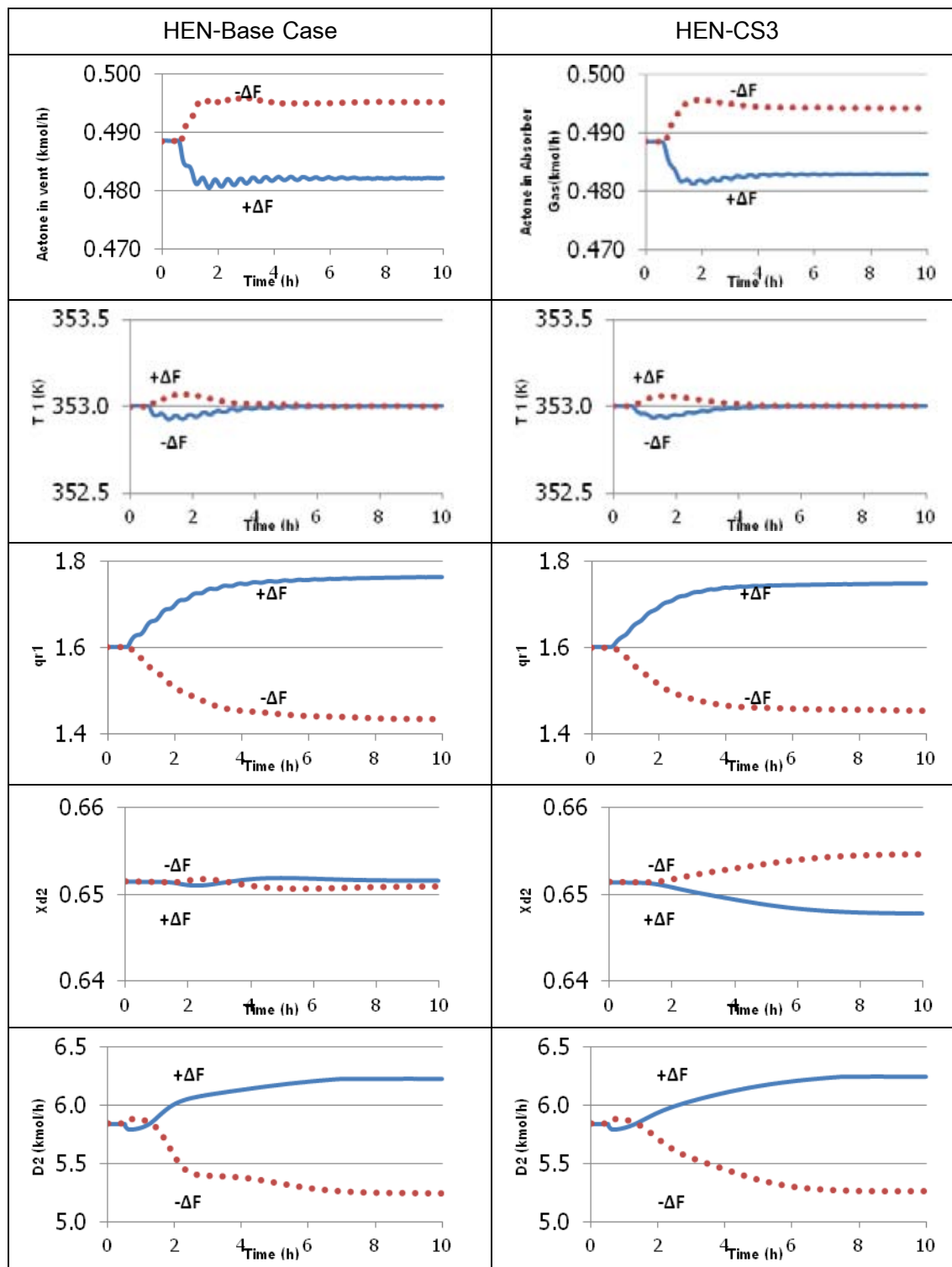


Table 5.22 (Continued) Dynamic responses of the system to disturbance in fresh feed flowrate for heat-integrated process of acetone

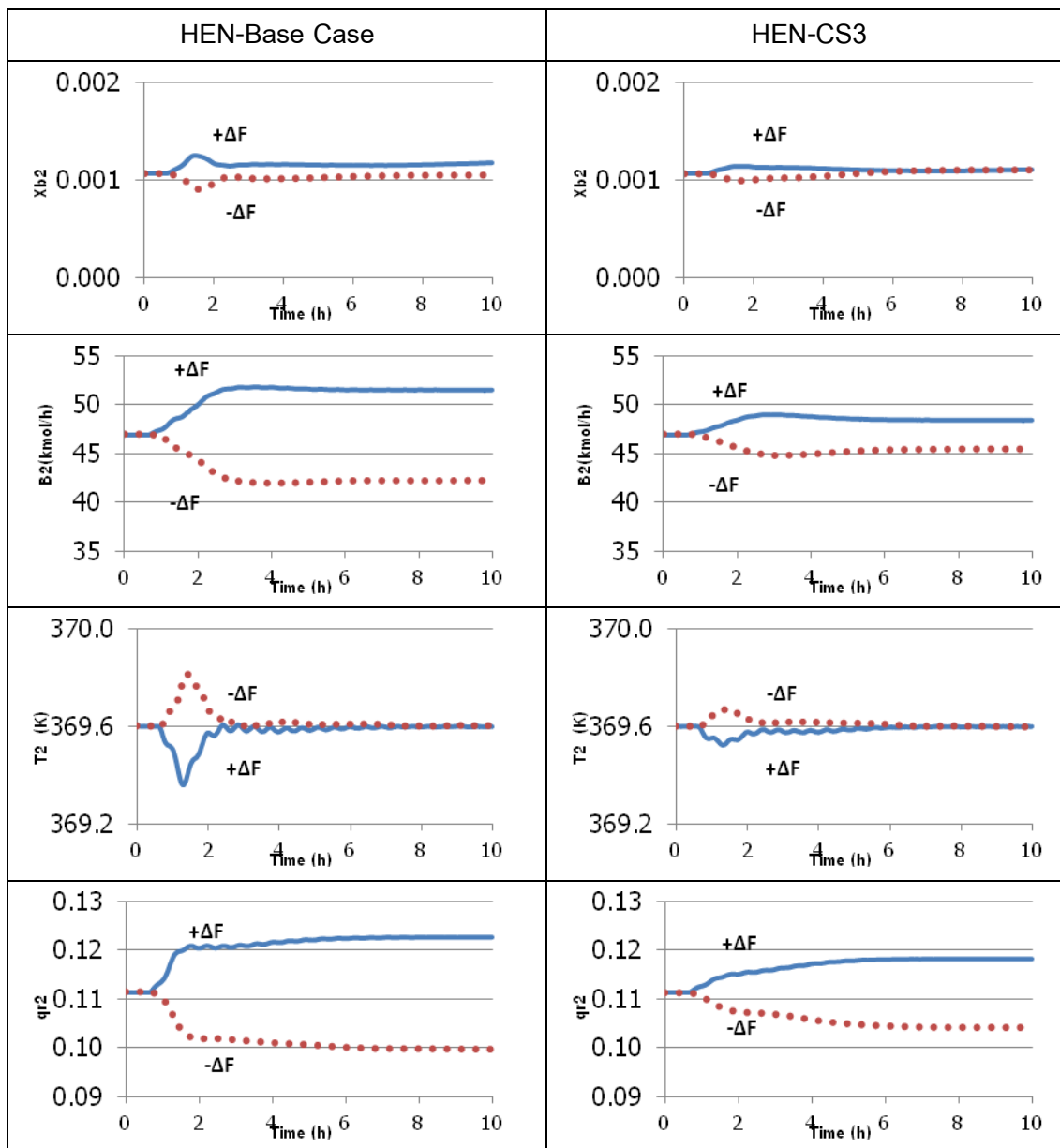


Table 5.23 Dynamic responses of the system to disturbance in fresh feed composition for heat-integrated process of acetone

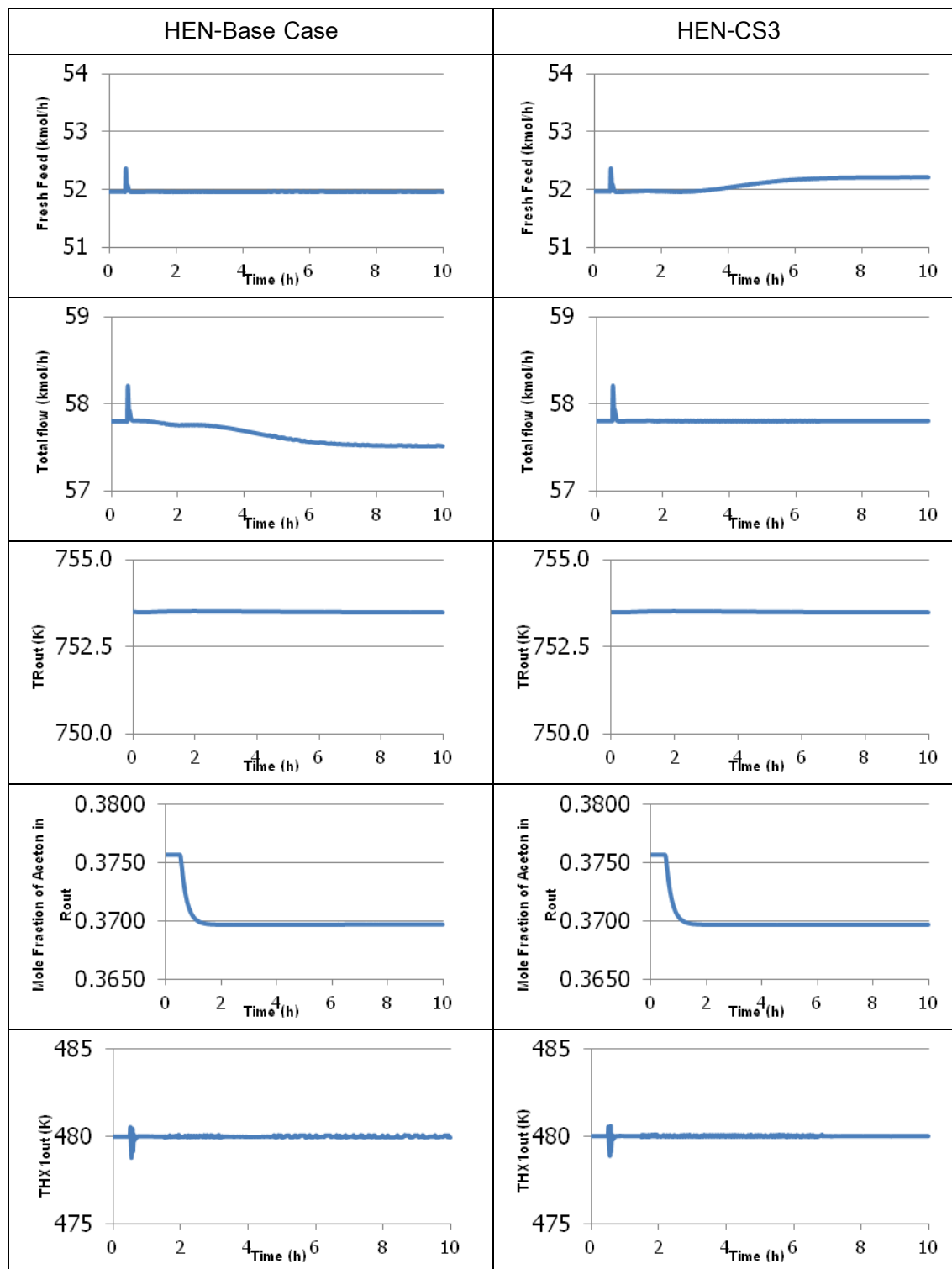


Table 5.23 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for heat-integrated process of acetone

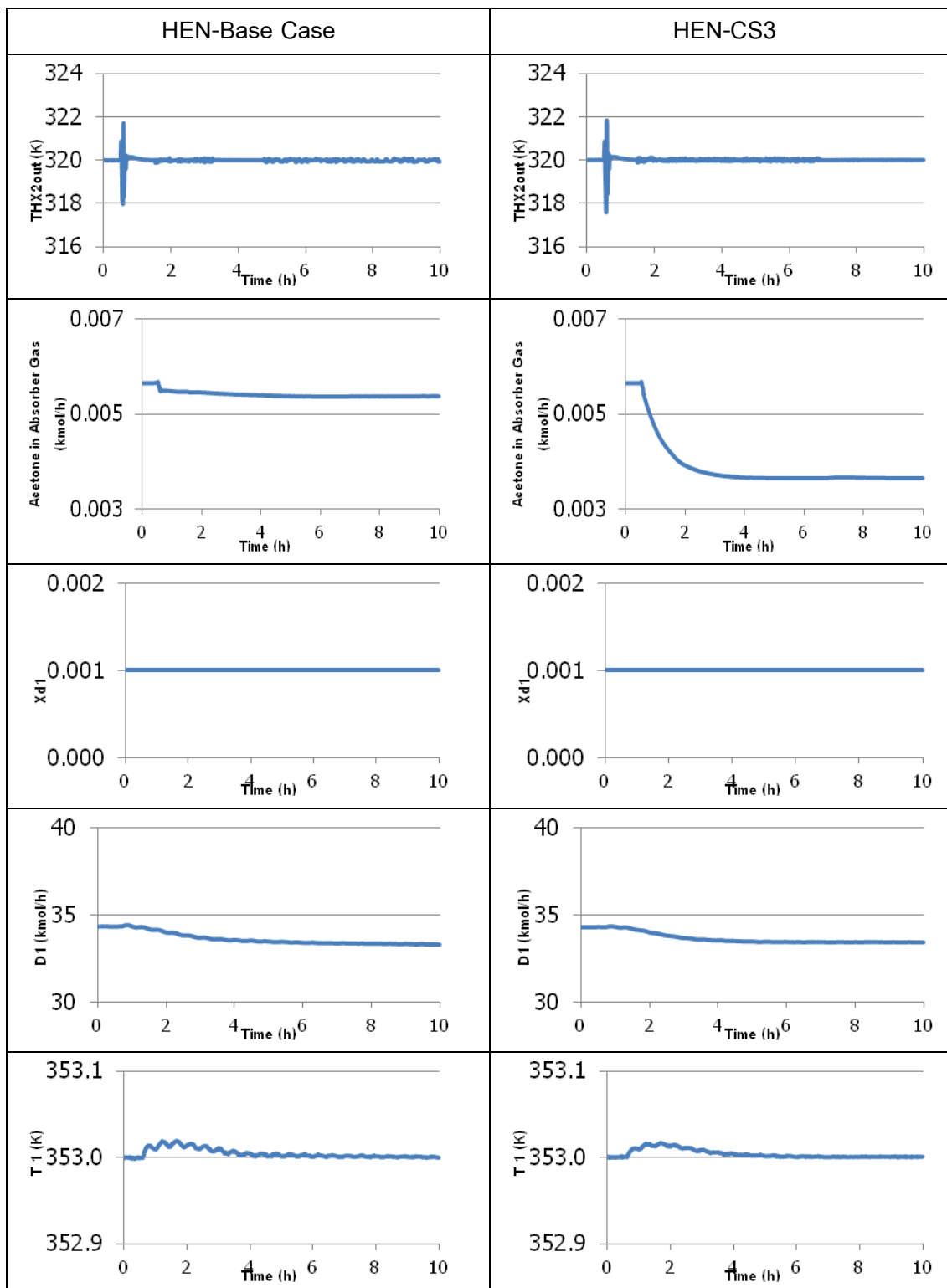


Table 5.23 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for heat-integrated process of acetone

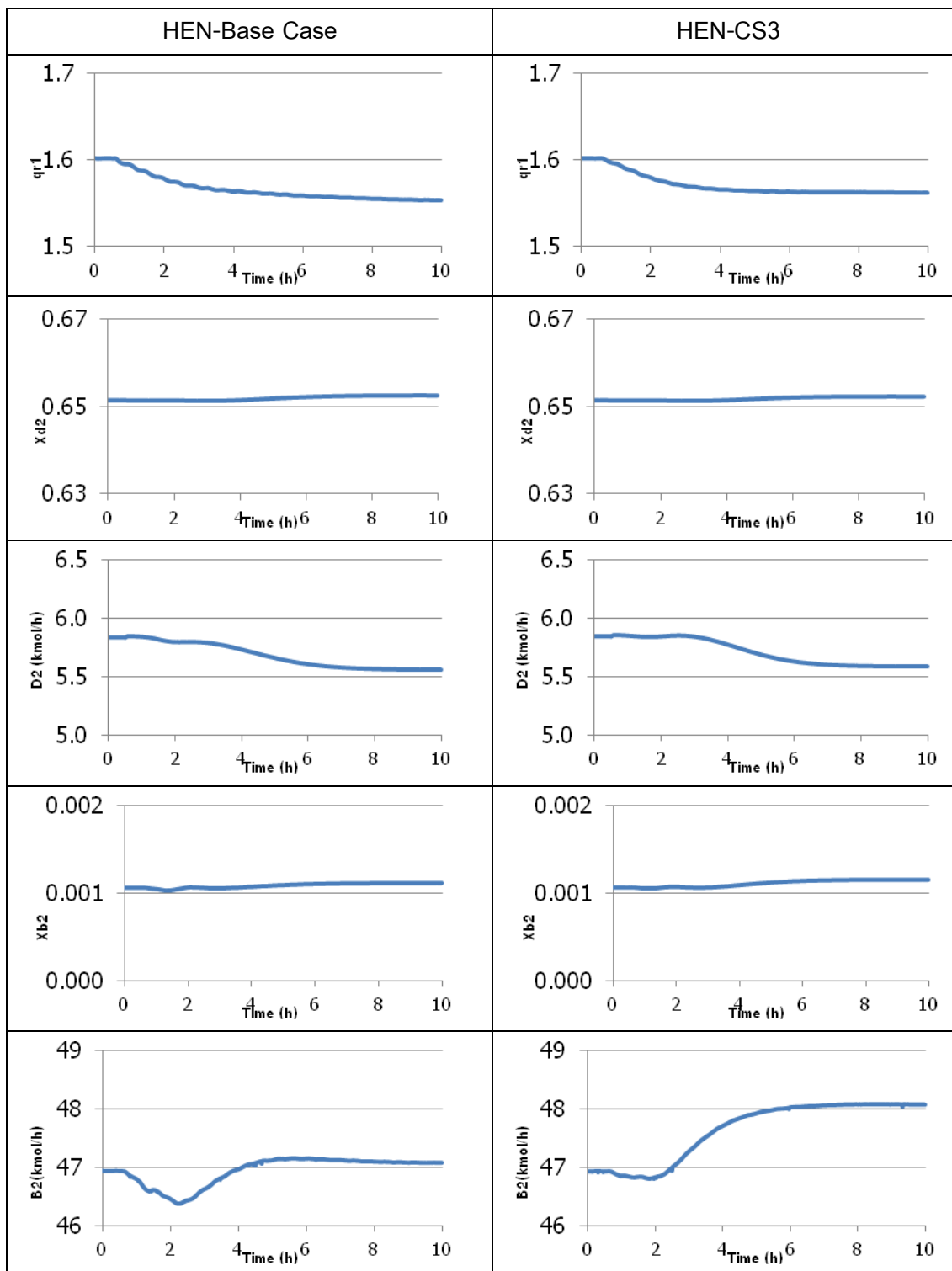


Table 5.23 (Continued) Dynamic responses of the system to disturbance in fresh feed composition for heat-integrated process of acetone

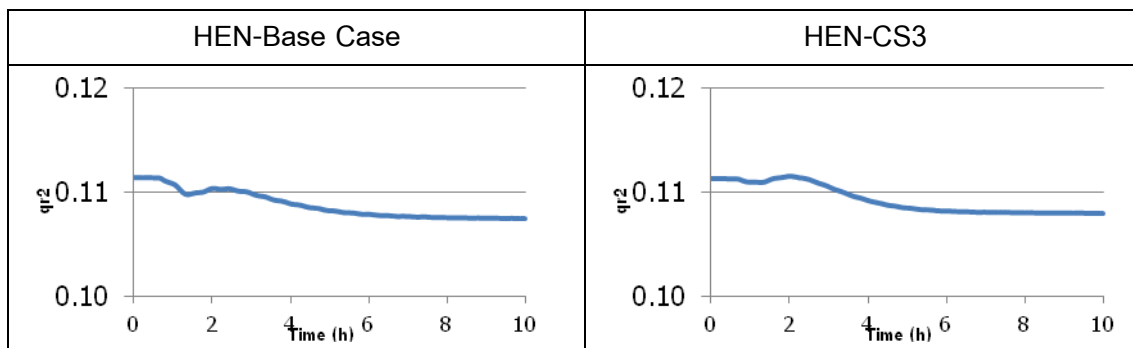


Table 5.24 Dynamic responses of the system to disturbance in fresh feed temperature for heat-integrated process of acetone

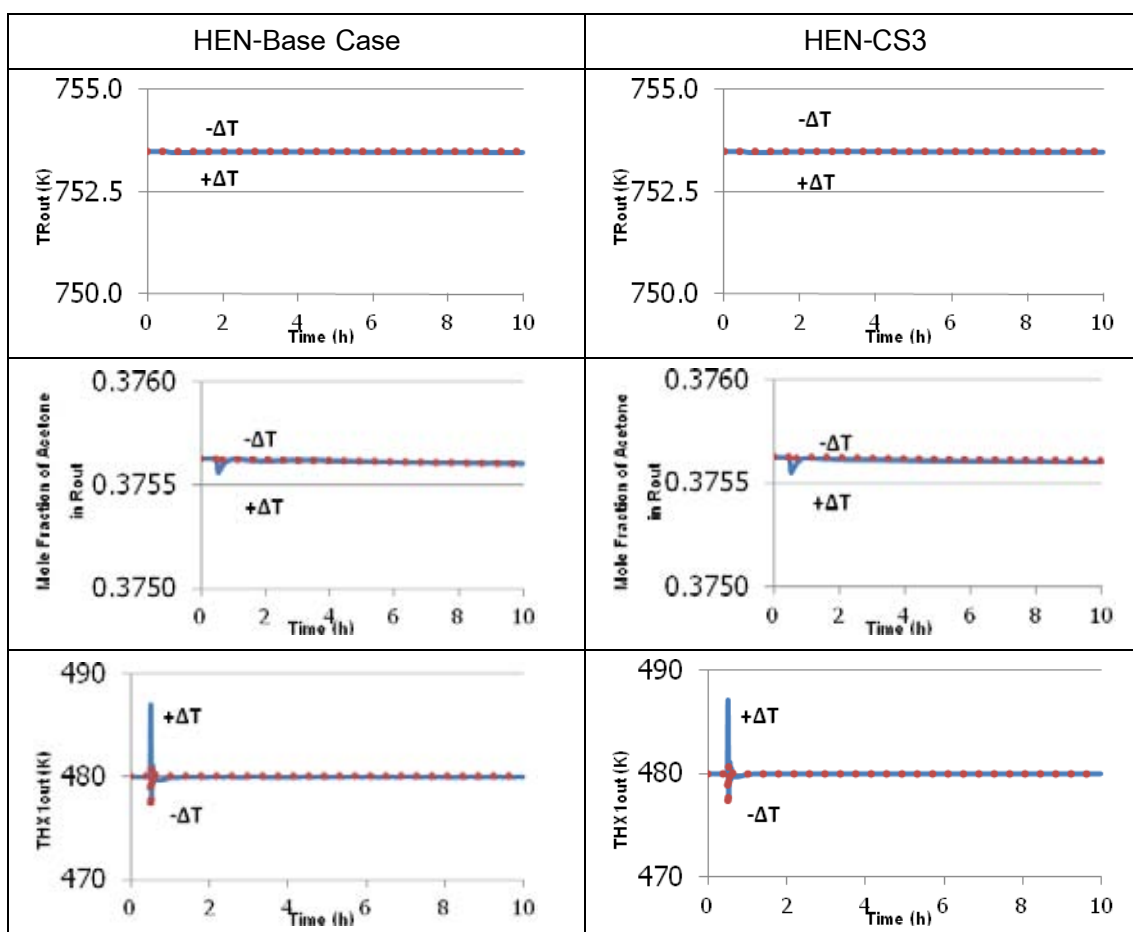


Table 5.24 (Continued) Dynamic responses of the system to disturbance in fresh feed temperature for heat-integrated process of acetone

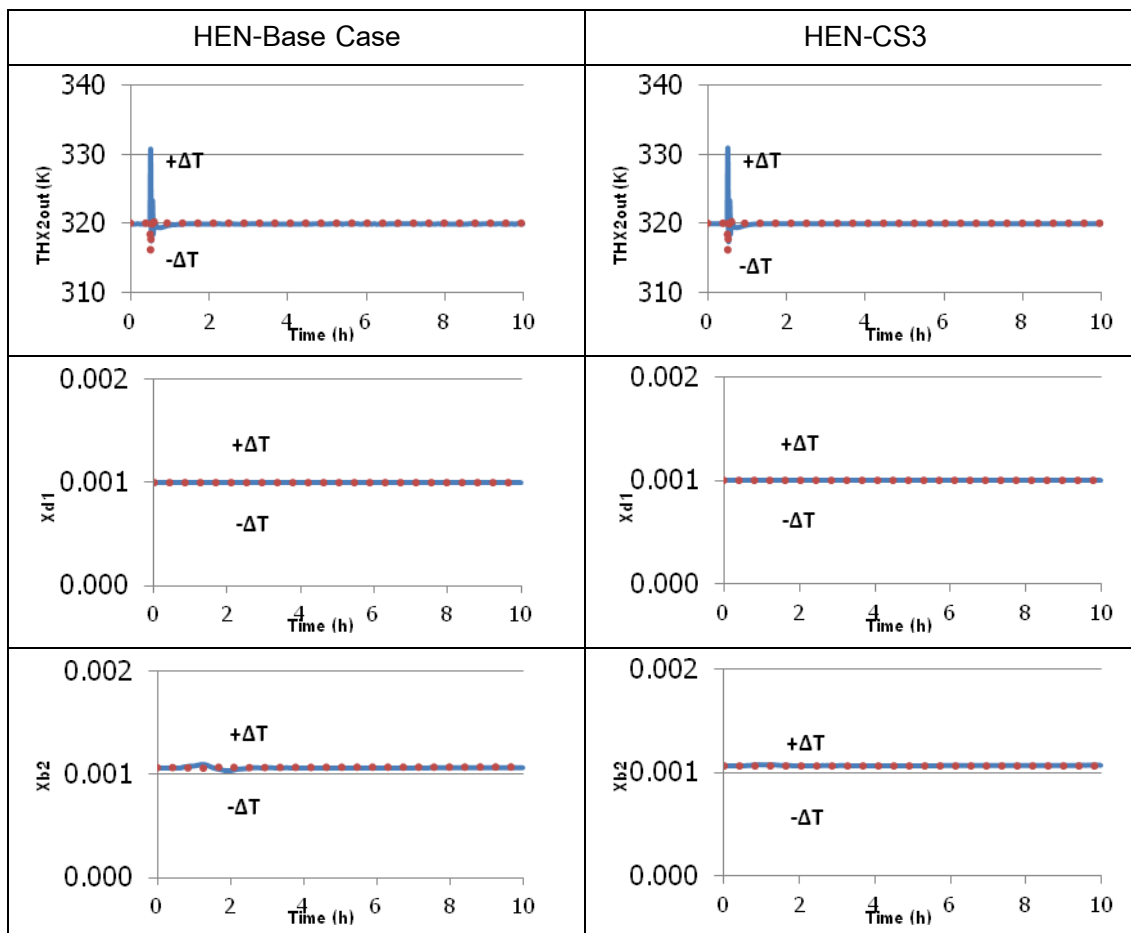


Table 5.25-27 show the IAE result for all disturbances; fresh feed flowrate, fresh feed composition and fresh feed temperature, respectively. Furthermore, the utility costs is investigated to compare the performance of using the energy when the disturbances applying.

Table 5.25 IAE result for handling the disturbance in fresh feed flowrate

Control structure	Pressure	Temperature	Composition	IAE
HEN-BC	0.05189	0.03733	0.02881	0.11803
HEN-CS3	0.04756	0.03602	0.02607	0.10965

Table 5.26 IAE result for handling the disturbance in fresh feed composition

Control structure	Pressure	Temperature	Composition	IAE
HEN-BC	0.00565	0.01083	0.00419	0.02067
HEN-CS3	0.00546	0.00846	0.00367	0.01759

Table 5.27 IAE result for handling the disturbance in fresh feed temperature

Control structure	Pressure	Temperature	Composition	IAE
HEN-BC	0.00350	0.02102	0.00104	0.02555
HEN-CS3	0.00151	0.01675	0.00095	0.01921

The IAE result for the CS3 is less than the base case for all disturbances. Figure 5.25 shows the cost value of the base case and the CS3 used to handle the disturbances. The utility cost of both control structure is similar.

Table 5.28 Energy consumption and cost when fresh feed flowrate changed

CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
HEN-BC	2.4750	1.8598	1.5718	0.0276	0.4563	0.4872	5.9066	0.9712
HEN-CS3	2.4726	1.8635	1.5839	0.0276	0.4572	0.4910	5.9200	0.9758

Table 5.29 Energy consumption and cost fresh feed composition changed

CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
HEN-BC	2.3499	1.8025	1.5358	0.0262	0.4422	0.4761	5.6882	0.9446
HEN-CS3	2.3657	1.8135	1.5537	0.0264	0.4449	0.4816	5.7329	0.9530

Table 5.30 Energy consumption and cost fresh feed temperature changed

CS	Energy(MW)			Cost(\$)			Total	
	CW	LPS	HPS	CW	LPS	HPS	Energy(MW)	Cost(\$)
HEN-BC	2.4349	1.8627	1.5739	0.0272	0.4570	0.4879	5.8716	0.9721
HEN-CS3	2.4347	1.8627	1.5825	0.0272	0.4570	0.4906	5.8800	0.9748

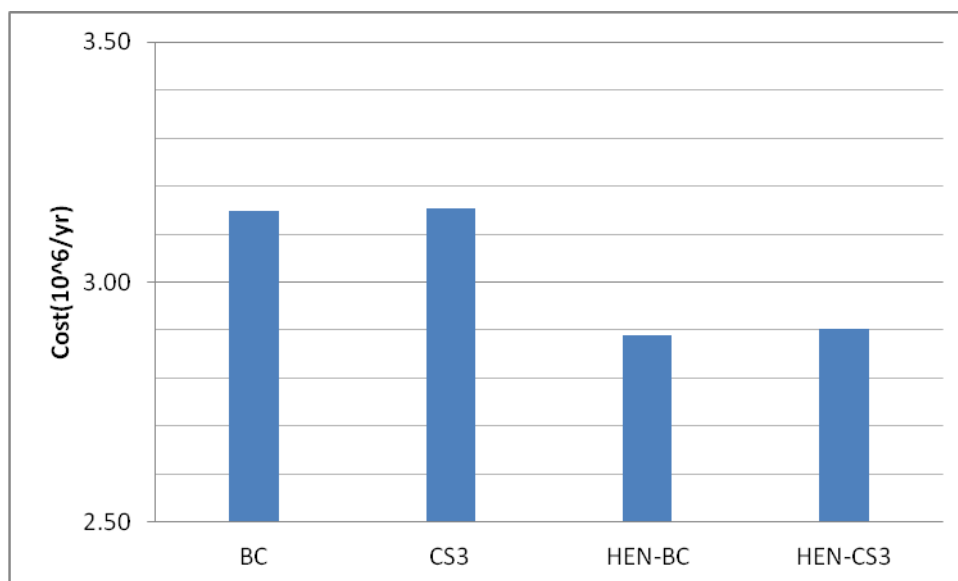


Figure 5.25 The summation of utility costs for the base case and CS3 handling the disturbances for acetone process and heat-integrated of acetone process.

CHAPTER VI

CONCLUSION AND RECOMMENDATIONS

6.1 Conclusion

The new design procedure of Wongsri (2012) provides a simple methodology to design plantwide control structures. The total IAE results show that the designed control structures, the CS1 and CS3, are able to handle the material and thermal disturbances nearby the base case and the CS3 is the best designed control structure. These results indicate that temperature control loop is better than composition control loop at the reactor effluent. Furthermore, the fixing reflux ratio is another alternative to maintain the product specification without investment on the composition analyzer at the acetone column.

The heat-integrated process is also used to evaluate the dynamic performance with the best designed control structure. The comparison of the IAE result shows that the CS3 is less than the base case which means the designed control structure is able to use with more complex process.

6.2 Recommendation

Study and apply the new design procedure of Wongsri (2012) to the other process. Furthermore, the by-pass control is an alternative to study and evaluate the dynamic performance.

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APPENDICES

APPENDIX A

PROCESS STREAM AND EQUIPMENT DATA

Table A.1 Flow summary for the acetone process shown in Figure 4.2

Stream name	Fresh feed in	Rin	Rout	HX1out	HX2out	Gas	Liquid	Water in
Temperature (K)	320.0	450.1	753.5	480.0	320.0	320.0	320.0	320.0
Pressure (atm)	17.50	17.50	17.33	17.20	17.06	17.06	17.06	17.00
Vapor fraction	0.0000	1.000	1.000	1.000	0.3881	1.0000	0.0000	0.0000
Mass flow (kg/h)	2401	2664	2664	2664	2664	138.9	2525	540.8
Molar flow (kmol/h)	51.96	57.76	92.52	92.52	92.52	35.90	56.61	30.00
Component mole fraction								
2-Propanol	0.6700	0.6680	0.0413	0.0413	0.0413	0.0013	0.0667	0.0000
Water	0.3300	0.3319	0.2072	0.2072	0.2072	0.0046	0.3357	1.0000
Acetone	0.0000	0.0001	0.3758	0.3758	0.3758	0.0304	0.5948	0.0000
Hydrogen	0.0000	0.0000	0.3757	0.3757	0.3757	0.9637	0.0028	0.0000

Table A.1 (Continued) Flow summary for the acetone process shown in figure 4.2

Stream name	Absorber gas	Absorber bottom	F1	Vent product	Acetone product	B1	Recycle	Water product
Temperature (K)	321.3	332.6	323.1	321.0	321.1	367.5	354.1	373.3
Pressure (atm)	17.00	15.95	1.349	1.000	1.000	1.000	17.50	1.000
Vapor fraction	1.0000	0.0000	0.0004	1.0000	0.0000	0.0000	0.0000	0.0000
Mass flow (kg/h)	74.17	605.5	605.5	28.71	1991	1112	263.4	847.9
Molar flow (kmol/h)	34.83	31.10	31.10	0.6540	34.31	52.76	5.799	46.95
Component mole fraction								
2-Propanol	0.0000	0.0015	0.0436	0.0000	0.0000	0.0725	0.6504	0.0011
Water	0.0065	0.9633	0.5582	0.0005	0.0010	0.9274	0.3487	0.9989
Acetone	0.0002	0.0350	0.3963	0.7470	0.9989	0.0001	0.0009	0.0000
Hydrogen	0.9933	0.0003	0.0019	0.2525	0.0001	0.0000	0.0000	0.0000

Table A.2 Equipment summary for the acetone process

Unit operations	Properties	Size
Vaporizer	Length (m)	1.497
	Diameter (m)	0.9977
Reactor	Length (m)	6.096
	Diameter (m)	0.0504
	Number of tubes	200
	U (kW/m ³ .K)	0.06
HX1	Area (m ²)	20.60
HX2	Area (m ²)	14.72
Flash tank	Length (m)	2.197
	Diameter (m)	1.464
Absorber	Length (m)	3.048
	Diameter (m)	0.7106
Reflux drum C1	Length (m)	1.888
	Diameter (m)	1.259

Table A.2 (Continued) Equipment summary for the acetone process

Unit operations	Properties	Size
Reflux drum C2	Length (m)	0.8019
	Diameter (m)	0.5346
Reboiler C1	Length (m)	1.581
	Diameter (m)	1.054
Reboiler C2	Length (m)	1.127
	Diameter (m)	0.7515

APPENDIX B

TUNING PARAMETER OF CONTROL STRUCTURES

The relay-feedback testing is a simple method to find the dynamic parameters. The results of the test are the ultimate gain and the ultimate frequency. This information is sufficient to calculate tuning parameters of controllers as shown in Table B.1.

Table B.1 Tyreus-Luyben rule

Controller type	Tuning parameters		
	K_c	t_i	t_d
PI	$0.31K_{cu}$	$2.2P_u$	-
PID	$0.45K_{cu}$	$2.2P_u$	$P_u/6.3$

Table B.2 Type of controllers and tuning parameters of base case

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Fresh feed	FC	Feed Forward	Fresh feed flow rate	Fresh feed flow rate	Reverse	51.96kmol/h	0-100	0.50	0.30	-
Water feed	FC	Ratio	Water flow rate	Water flow rate	Reverse	30kmol/h	0-60	0.50	0.30	-
Vaporizer	LC	Feed Back	Level	Duty flow rate	Direct	50%	0-100	3.00	-	-
Reactor	TC	Feed Back	Outlet temperature	Duty flow rate	Reverse	753.5K	700-800	27.8	191	13.8
Exchanger(HX1)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	480K	430-530	2.05	2.20	-
Exchanger(HX2)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	320K	273-373	1.24	2.93	-
Flash tank	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
Absorber	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Back	Vessel pressure of condenser	Absorber gas out flow rate	Direct	17atm	12.5-21.5	5.83	0.0234	-
Acetone	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
column(C1)	LC	Feed Back	Reflux drum level	Reflux flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	24.9	0.214	-
	TC	Feed Back	Stage Temp tray80	Reboiler duty	Reverse	353K	300-400	10.7	19.8	1.43

Table B.2 (Continued) Type of controllers and tuning parameters of base case

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Acetone column(C1)	CC	Cascade_ Primary	Water composition in distillate	Distillate to reflux SP	Reverse	0.001	0-0.002	6.44	117	8.41
		Cascade_ Secondary	Distillate flow rate	Distillate flow rate	Reverse	34.31kmol/h	0-70	0.50	0.30	-
Water column(C2)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Distillate flow rate	Direct	50%	0-100	4.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	17.1	0.112	-
	TC	Feed Back	Stage Temp tray17	Roboiler duty	Reverse	369.6K	320-420	7.41	18.30	1.32
	FC	Ratio	Reflux to feed ratio	Reflux flow rate	Reverse	3.57kmol/h	0-7	0.50	0.30	-

Table B.3 Type of controllers and tuning parameters of CS1

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Fresh feed	FC	Feed Back	Total flow rate	Fresh feed flow rate	Reverse	51.96kmol/h	0-100	0.50	0.30	-
Water feed	FC	Feed Back	Water flow rate	Water flow rate	Reverse	30kmol/h	0-60	0.50	0.30	-
Vaporizer	LC	Feed Back	Level	Duty flow rate	Direct	50%	0-100	3.00	-	-
Reactor	TC	Feed Back	Outlet temperature	Duty flow rate	Reverse	753.5K	700-800	27.8	191	13.8
Exchanger(HX1)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	480K	430-530	2.05	2.20	-
Exchanger(HX2)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	320K	273-373	1.24	2.93	-
Flash tank	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
Absorber	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Back	Vessel pressure of condenser	Absorber gas out flow rate	Direct	17atm	12.5-21.5	5.83	0.0234	-
Acetone	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
column(C1)	LC	Feed Back	Reflux drum level	Reflux flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	24.9	0.214	-
	TC	Feed Back	Stage Temp tray80	Reboiler duty	Reverse	353K	300-400	10.7	19.8	1.43

Table B.3 (Continued) Type of controllers and tuning parameters of CS1

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Acetone column(C1)	FC	Ratio	Distillate to reflux ratio	Distillate flow rate	Reverse	34.31kmol/h	0-70	0.50	0.30	-
Water column(C2)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Distillate flow rate	Direct	50%	0-100	4.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	17.1	0.112	-
	TC	Feed Back	Stage Temp tray17	Roboiler duty	Reverse	369.6K	320-420	7.41	18.30	1.32

Table B.4 Type of controllers and tuning parameters of CS2

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Fresh feed	FC	Feed Back	Total flow rate	Fresh feed flow rate	Reverse	51.96kmol/h	0-100	0.50	0.30	-
Water feed	FC	Feed Back	Water flow rate	Water flow rate	Reverse	30kmol/h	0-60	0.50	0.30	-
Vaporizer	LC	Feed Back	Level	Duty flow rate	Direct	50%	0-100	3.00	-	-
Reactor	CC	Feed Back	Outlet composition of acetone	Duty flow rate	Reverse	0.3758	0.3658-0.3858	16.28	126	-
Exchanger(HX1)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	480K	430-530	2.05	2.20	-
Exchanger(HX2)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	320K	273-373	1.24	2.93	-
Flash tank	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
Absorber	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Back	Vessel pressure of condenser	Absorber gas out flow rate	Direct	17atm	12.5-21.5	5.83	0.0234	-
Acetone column(C1)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Reflux flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	24.9	0.214	-
	TC	Feed Back	Stage Temp tray80	Reboiler duty	Reverse	353K	300-400	10.7	19.8	1.43

Table B.4 (Continued) Type of controllers and tuning parameters of CS2

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Acetone column(C1)	FC	Ratio	Distillate to reflux ratio	Distillate flow rate	Reverse	34.31kmol/h	0-70	0.50	0.30	-
Water column(C2)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Distillate flow rate	Direct	50%	0-100	4.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	17.1	0.112	-
	TC	Feed Back	Stage Temp tray17	Roboiler duty	Reverse	369.6K	320-420	7.41	18.30	1.32

Table B.5 Type of controllers and tuning parameters of CS3

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Fresh feed	FC	Feed Back	Total flow rate	Fresh feed flow rate	Reverse	51.96kmol/h	0-100	0.50	0.30	-
Water feed	FC	Feed Back	Water flow rate	Water flow rate	Reverse	30kmol/h	0-60	0.50	0.30	-
Vaporizer	LC	Feed Back	Level	Duty flow rate	Direct	50%	0-100	3.00	-	-
Reactor	TC	Feed Back	Outlet temperature	Duty flow rate	Reverse	753.5K	700-800	27.8	191	13.8
Exchanger(HX1)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	480K	430-530	2.05	2.20	-
Exchanger(HX2)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	320K	273-373	1.24	2.93	-
Flash tank	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
Absorber	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Back	Vessel pressure of condenser	Absorber gas out flow rate	Direct	17atm	12.5-21.5	5.83	0.0234	-
Acetone	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
column(C1)	LC	Feed Back	Reflux drum level	Reflux flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	24.9	0.214	-
	TC	Feed Back	Stage Temp tray80	Reboiler duty	Reverse	353K	300-400	10.7	19.8	1.43

Table B.5 (Continued) Type of controllers and tuning parameters of CS3

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Acetone column(C1)	CC	Cascade_ Primary	Water composition in distillate	Distillate to reflux SP	Reverse	0.001	0-0.002	6.44	117	8.41
		Cascade_ Secondary	Distillate flow rate	Distillate flow rate	Reverse	34.31kmol/h	0-70	0.50	0.30	-
Water column(C2)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Distillate flow rate	Direct	50%	0-100	4.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	17.1	0.112	-
	TC	Feed Back	Stage Temp tray17	Roboiler duty	Reverse	369.6K	320-420	7.41	18.30	1.32

Table B.6 Type of controllers and tuning parameters of CS4

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Fresh feed	FC	Feed Back	Total flow rate	Fresh feed flow rate	Reverse	51.96kmol/h	0-100	0.50	0.30	-
Water feed	FC	Feed Back	Water flow rate	Water flow rate	Reverse	30kmol/h	0-60	0.50	0.30	-
Vaporizer	LC	Feed Back	Level	Duty flow rate	Direct	50%	0-100	3.00	-	-
Reactor	CC	Feed Back	Outlet composition of acetone	Duty flow rate	Reverse	0.3758	0.3658-0.3858	16.28	126	-
Exchanger(HX1)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	480K	430-530	2.05	2.20	-
Exchanger(HX2)	TC	Feed Back	Outlet temperature	Duty flow rate	Direct	320K	273-373	1.24	2.93	-
Flash tank	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
Absorber	LC	Feed Back	Level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Back	Vessel pressure of condenser	Absorber gas out flow rate	Direct	17atm	12.5-21.5	5.83	0.0234	-
Acetone	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
column(C1)	LC	Feed Back	Reflux drum level	Reflux flow rate	Direct	50%	0-100	2.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	24.9	0.214	-
	TC	Feed Back	Stage Temp tray80	Reboiler duty	Reverse	353K	300-400	10.7	19.8	1.43

Table B.6 (Continued) Type of controllers and tuning parameters of CS4

Equipment	Controller	Type of Controller	Controlled Variables	Manipulated Variables	Controller Action	Set Point	Transmitter Range	Tuning Parameters		
								K_c	t_i	t_d
Acetone column(C1)	CC	Cascade_ Primary	Water composition in distillate	Distillate to reflux SP	Reverse	0.001	0-0.002	6.44	117	8.41
	FC	Cascade_ Secondary	Distillate flow rate	Distillate flow rate	Reverse	34.31kmol/h	0-70	0.50	0.30	-
Water column(C2)	LC	Feed Back	Reboiler level	Bottom flow rate	Direct	50%	0-100	2.00	-	-
	LC	Feed Back	Reflux drum level	Distillate flow rate	Direct	50%	0-100	4.00	-	-
	PC	Feed Forward	Top stage pressure	Condenser duty	Direct	1atm	0-2	17.1	0.112	-
	TC	Feed Back	Stage Temp tray17	Roboiler duty	Reverse	369.6K	320-420	7.41	18.30	1.32

VITAE

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