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**AN INTEGRATED APPROACH FOR
SIMULTANEOUS OPERABILITY AND
SWITCHABILITY ANALYSIS OF
CHEMICAL PLANTS**

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Summary

Over the past decade, commercial pressures have encouraged more highly integrated plants, which are designed to perform at multiple operating conditions with varying throughput or product grades. In these modern plants, with small surge capacities between various processing units, it is important to completely eliminate disturbances that affect downstream processes, when propagating between interconnected units. Such plants demand safe operations, optimal switching policies, and efficient control schemes to satisfy strict product specifications, tough environment, and safety regulations. In this thesis another dimension has been added to the investigation of the operability in design or retrofit design of chemical processes thanks to the development of efficient nonlinear programming tools. The novelty is the expansion and incorporation of the switchability with the operability concept, which becomes a well-established strategy for the analysis. With much emphasis on the switching states, the thesis has developed a new integrated and systematic approach for simultaneous flexibility, switchability and controllability analysis. Due to possible disturbances and uncertainties, the procedure starts with the search for back-off states from nominal optimal operating conditions at the beginning and the end of a transition. Back-off trajectories from the nominal optimal trajectories, which connect the above states, are found next. Finally, the feasibility of the solution is tested against different combinations of possible disturbances. Controllability is included in the analysis since an appropriate control scheme usually brings the open loop back-off point closer to the nominal optimum and also provides a feasible policy for an efficient switch.

A framework within an optimization environment is proposed, leading to the uncertain dynamic nonlinear programming problems, which can be solved by two different mathematical approaches. The sequential optimization method tends to converge slowly and handle constraints on state variables with difficulty. However, it can be used to solve large-scale problems. The simultaneous optimization and integration method reduces the computational time but can only be used for small-scale problems. The closed-loop back-off problems are achieved first with traditional proportional plus integral controllers, then with linear and nonlinear model predictive

integration method reduces the computational time but can only be used for small-scale problems. The closed-loop back-off problems are achieved first with traditional proportional plus integral controllers, then with linear and nonlinear model predictive control techniques, since NLPC problems have a general mathematical formulation very similar to that of switchability problems.

The proposed procedure is finally applied to three examples of switching operations. The applications start from a simple pilot plant including two reactors in series to a complex distillation unit. In each example, the optimal operating conditions are found, and then the optimal trajectories for switching operations are considered. Possible improvements of the plant design, operation or control are proposed.

The applications have demonstrated the effectiveness of the procedure presented throughout the thesis. However, further development is needed for the efficient large-scale use of these tools. This is particularly true for the simultaneous flexibility, switchability and controllability study, since the analysis leads to dynamic optimization problems and on-line applications as well as design problems with complex models, which are being considered more frequently by industry.

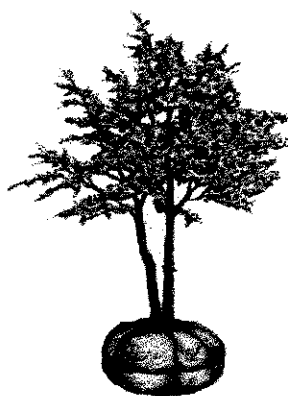


Table of Contents

ACKNOWLEDGEMENTS	i
SUMMARY	ii
TABLE OF CONTENTS	iv
LIST OF FIGURES	ix
LIST OF TABLES	xvi
1 INTRODUCTION	
1 Thesis objective	1.2
2 Thesis overview	1.3
Chapter 1: Introduction.....	1.3
Chapter 2: Steady state and dynamic flexibility analysis	1.3
Chapter 3: Switchability and operability assessment.....	1.4
Chapter 4: Switchability and controllability analysis.....	1.4
Chapter 5: Solution method for switchability analysis...	1.5
Chapter 6: Switchability analysis of real processes.....	1.5
Chapter 7: Conclusions and future works.....	1.6
3 Thesis format	1.6
4 References	1.7
2 STEADY STATE AND DYNAMIC FLEXIBILITY ANALYSIS OF CHEMICAL PROCESSES WITH FIXED DESIGN	
1 Introduction	2.1
2 Optimization of chemical processes	2.2
3 The effect of uncertainties on optimal operation	2.3
4 Deterministic flexibility analysis	2.4
5 Steady state open loop back-off calculation	2.5
5.1 Back-off concept.....	2.8
5.2 Problem formulation.....	2.8
5.3 Algorithm development.....	2.10
5.4 Modified algorithms.....	2.13

5.4.1	The KS modified algorithm.....	2.13
5.4.2	The KTC modified algorithm.....	2.14
5.5	Case studies.....	2.16
5.5.1	Case study 1: a single CSTR.....	2.16
5.5.2	Case study 2: two CSTRs in series.....	2.21
6	Dynamic closed-loop back-off calculation.....	2.27
7	Conclusion.....	2.29
8	Nomenclature.....	2.30
9	References.....	2.31
	Appendix 2A.....	2.32
	Appendix 2B.....	2.35
3	SWITCHABILITY AND OPERABILITY ASSESSMENT IN CHEMICAL PROCESSES	
1	Introduction.....	3.1
2	Switchability analysis.....	3.2
2.1	Process constraints and nonlinear feature.....	3.2
2.2	Model time delays, uncertainties and disturbances...	3.3
3	Switchability formulation.....	3.4
4	Solution methods for switchability problems.....	3.5
4.1	Sequential optimization.....	3.6
4.2	Simultaneous optimization and integration.....	3.8
5	Problem formulation.....	3.8
5.1	Problem formulation using sequential technique.....	3.11
5.2	Problem formulation using simultaneous technique.....	3.13
5.2.1	Global orthogonal collocation.....	3.14
5.2.1	Orthogonal collocation on finite elements.....	3.17
6	Case studies.....	3.21
6.1	Case study 1: a single CSTR.....	3.21
6.1.1	Dynamic closed-loop back-off problem.....	3.25
6.1.2	Switchability problem.....	3.29
6.1.3	Testing the feasibility of the solutions.....	3.40

6.2 Case study 2: two CSTRs in series.....	3.46
6.2.1 Dynamic closed-loop back-off problem.....	3.48
6.2.2 Switchability problem.....	3.49
6.2.3 Testing the feasibility of the solutions.....	3.57
6.2.4 Switching from startup operating conditions...	3.60
7 Conclusion.....	3.63
8 Nomenclature.....	3.66
9 References.....	3.67
Appendix 3A.....	3.69
4 SWITCHABILITY AND CONTROLABILITY ANALYSIS - PREDICTIVE CONTROL APPROACH	
1 Introduction.....	4.1
2 Model predictive control (MPC).....	4.2
2.1 Dynamic matrix control (DMC).....	4.2
2.2 Nonlinear predictive control (NLPC).....	4.5
3 Case studies.....	4.6
3.1 Case study 1: a single CSTR.....	4.7
3.1.1 Dynamic closed-loop back-off problem.....	4.8
3.1.2 Switchability problem with DMC.....	4.18
3.2 Case study 2: two CSTRs in series.....	4.26
3.2.1 Dynamic closed-loop back-off problem.....	4.30
3.2.2 Switchability problem with DMC.....	4.32
4 Conclusion.....	4.44
5 Nomenclature.....	4.49
6 References.....	4.49
Appendix 4A.....	4.50
Appendix 4B.....	4.53
5 SOLUTION METHOD FOR OPERABILITY AND SWITCHABILITY ANALYSIS	
1 Introduction.....	5.1
2 Open loop back-off calculations.....	5.2

2.1	Reactor problems.....	5.2
2.2	Distillation problems.....	5.7
3	Dynamic closed-loop back-off calculations.....	5.11
4	Switchability calculation.....	5.14
5	Nonlinear Model Predictive Control calculations.....	5.20
6	Conclusion.....	5.22
7	Nomenclature.....	5.25
8	References.....	5.25
	Appendix 5A.....	5.26
6	SWITCHABILITY AND OPERABILITY OF REAL PROCESSES	
1	Introduction.....	6.1
2	Application 1: Two CSTRs in series.....	6.2
2.1	Plant description and modeling.....	6.2
2.2	Result and discussion.....	6.5
2.3	Improvement of current design.....	6.14
3	Application 2: Binary distillation column.....	6.14
3.1	Plant description and modeling.....	6.14
3.2	Steady state ASPEN model.....	6.20
3.3	Optimal feed location using GAMS model.....	6.22
3.4	Steady state open loop back-off using SPEEDUP.....	6.24
3.5	Switching problem using sequential technique.....	6.26
4	Application 3: Multicomponent distillation column.....	6.42
4.1	Plant description.....	6.42
4.2	Steady state ASPEN model.....	6.44
4.3	Steady state open loop back-off using ASPEN.....	6.45
4.4	Dynamic problem using compartmental model.....	6.49
5	Conclusion.....	6.57
6	Nomenclature.....	6.57
7	References.....	6.58
	Appendix 6A.....	6.59
7	CONCLUSIONS AND FURTHER STUDIES	

1 Results and conclusions.....	7.1
1.1 A review of steady state and dynamic flexibility analysis of chemical processes with fixed design.....	7.1
1.2 Switchability and operability assessment in chemical processes.....	7.2
1.3 Switchability and controllability analysis - Predictive control approach.....	7.3
1.4 Solution method for switchability and operability analysis.....	7.4
1.5 Switchability and operability of real processes.....	7.4
2 Recommendations for further studies.....	7.5

List of Figures

Figure 2.1	Feasibility Test: Feasible Design and Infeasible Design (Feasible region in disturbance space)	2.5
Figure 2.2	Geometrical Interpretation of Flexibility Index F (Feasible region in disturbance space)	2.7
Figure 2.3	Movement of Nominal Optimal Point to Back-Off Point (Feasible region in decision variable space)	2.9
Figure 2.4	Case Study 1: Single CSTR	2.17
Figure 2.5a	Case Study 1: Nominal Feasible Region and Optimal Point	2.20
Figure 2.5b	Case Study 1: Permanent Feasible Region and Back-Off Point	2.20
Figure 2.6	Case Study 2: Two CSTRs in Series	2.22
Figure 2.7	Case Study 2: Nominal Operating Space and Nominal Optimal Point at Different Angles	2.25
Figure 2.8	Case Study 2: Permanent Feasible Space and Back-Off Point at Different Angles	2.26
Figure 3.1	Steps to Solve a Switching Problem	3.12
Figure 3.2	Logical Flow of Information Between Integrator and Optimizer	3.12
Figure 3.3a	Global Collocation (NCOL = 3)	3.19
Figure 3.3b	Finite Element Collocation (NCOL = 2, NFE = 3)	3.19
Figure 3.4	Single CSTR with Temperature and Level Controllers	3.23
Figure 3.5a	Inflow and Outflow Responses (Nominal Case)	3.33
Figure 3.5b	Concentration and Temperature Responses (Nominal Case)	3.34
Figure 3.6a	Concentration and Temperature Responses (Open Loop Back-Off Case)	3.36

Figure 3.6b	Inflow and Outflow Responses (Open Loop Back-Off Case)	3.37
Figure 3.6c	Temperature and Level Responses (Open Loop Back-Off Case)	3.38
Figure 3.6d	Inflow and Outflow Responses (Open Loop Back-Off Case)	3.39
Figure 3.7	Temperature Set Point Policies and Corresponding Inflow Profiles (Dynamic Closed-Loop Back-Off Case-Class I)	3.41
Figure 3.8	Inflow Profiles and Corresponding Temperature Responses (Dynamic Closed-Loop Back-Off Case)	3.42
Figure 3.9	Feed Flowrate Curve Fitting (Dynamic Closed-Loop Back-Off Case)	3.44
Figure 3.10	Manipulated and Controlled Variable Profiles (From SPEEDUP)	3.45
Figure 3.11	Two CSTRs in Series with Temperature and Level Controllers	3.47
Figure 3.12a	Effect of Level Controller Gain (Nominal Case)	3.52
Figure 3.12b	Effect of Level Controller Reset Time (Nominal Case)	3.52
Figure 3.13	Effect of Constraint on Inlet Valve (Open Loop Back-Off Case)	3.53
Figure 3.14a	Inflow Profiles (Open Loop Back-Off Case)	3.54
Figure 3.14b	Temperature Profiles (Open Loop Back-Off Case)	3.55
Figure 3.14c	Total Outflow Profiles (Open Loop Back-Off Case)	3.56
Figure 3.15	Inflow Profiles (Closed- Loop Back-Off Case)	3.58
Figure 3.16	Cooling and Corresponding Temperature Profiles (From SPEEDUP)	3.61
Figure 3.17	Profiles of Temperature in First Reactor (From SPEEDUP)	3.62

Figure 3.18a	Inflow Profiles (Open Loop Back-Off Case/Startup Problem)	3.64
Figure 3.18b	Concentration and Temperature Profiles (Open Loop Back-Off Case/Startup Problem)	3.65
Figure 4.1a	Temperature Response (First Operating Condition)	4.10
Figure 4.1b	Temperature Response (Final Operating Condition)	4.10
Figure 4.2a	Coolant Profile (Final Operating Condition)	4.12
Figure 4.2b	Coolant Profile (Final Operating Condition)	4.12
Figure 4.3a	Temperature and Corresponding Coolant Profiles (First Operating Condition)	4.13
Figure 4.3b	Temperature and Corresponding Coolant Profiles (Final Operating Condition)	4.14
Figure 4.4	Temperature and Corresponding Coolant Profiles (Final Operating Condition)	4.16
Figure 4.5	Temperature Difference Response to Unit Step Change in Coolant Flowrate	4.17
Figure 4.6	Optimal Feed Flowrate Profile and Corresponding Temperature Set Point Trajectory	4.21
Figure 4.7a, b	Temperature and Coolant Profiles (Controlled and Manipulated Variables)	4.22
Figure 4.7c	Cooling Profile	4.23
Figure 4.8a, b	Temperature and Coolant Profiles (Controlled and Manipulated Variables)	4.24
Figure 4.8c	Cooling Profile	4.25
Figure 4.9a, b	Temperature and Coolant Profiles (Controlled and Manipulated Variables)	4.27
Figure 4.9c	Cooling Profile	4.28
Figure 4.10	Coolant and Cooling Profiles	4.29

Figure 4.11	Temperature Difference Responses in First and Second CSTRs to Unit Step Change in Coolant Flowrate	4.31
Figure 4.12a	Cooling Profile in Reactors (First Operating Condition)	4.33
Figure 4.12b	Coolant Profile in Reactors (Final Operating Condition)	4.34
Figure 4.13a	Temperature Profiles at First and Final Operating Conditions (First Reactor)	4.35
Figure 4.13b	Coolant Profiles at First and Final Operating Conditions (First Reactor)	4.36
Figure 4.13c	Cooling Profiles at First and Final Operating Conditions (Second Reactor)	4.37
Figure 4.14	Optimal Flowrate Profile (Feed to First Reactor)	4.39
Figure 4.15	Temperature Difference Responses to Unit Step Change in Coolant Flowrate	4.40
Figure 4.16	Cooling Profile in Second Reactor (Constraint Violation)	4.42
Figure 4.17	Cooling Profile in Second Reactor (Constraint Satisfaction)	4.42
Figure 4.18a	Temperature Profiles in Reactors	4.45
Figure 4.18b	Corresponding Cooling Profiles in Reactors	4.46
Figure 4.19	Temperature Set Point Policies in First and Second Reactors	4.47
Figure 4.20a	Coolant Profile in First Reactor	4.47
Figure 4.20b, c	Cooling and Temperature Profiles in First Reactor	4.48
Figure 4a.1	Open-Loop Response Curve	4.51
Figure 5.1	Optimal Solution (Two Decision Variables & Two Active Constraints)	5.6
Figure 5.2	Optimal Solution (Three Decision Variables & Three Active Constraints)	5.6
Figure 5.3	Flowsheet of Purification Columns	5.9

Figure 5.4	Optimal Feed Profile	5.15
Figure 5.5	Responses from Second Tank	5.16
Figure 5.6	Optimal Feed Profile (SPEEDUP and sequential technique)	5.18
Figure 5.7	Corresponding Level Responses	5.18
Figure 5.8	Optimal Feed Profile (SPEEDUP and sequential technique)	5.19
Figure 5.9a	Temperature Response in First CSTR (Controlled Variable)	5.23
Figure 5.9b	Coolant Profile in First CSTR (Manipulated Variable)	5.23
Figure 5.10a	Temperature Response in Second CSTR (Controlled Variable)	5.24
Figure 5.10b	Coolant Profile in Second CSTR (Manipulated Variable)	5.24
Figure 6.1	Plant 1: Two CSTRs in Series	6.3
Figure 6.2a	Outflow Profile in First Reactor	6.7
Figure 6.2b	Outflow Profile in Second Reactor	6.7
Figure 6.3a	Level Profile in First Reactor	6.8
Figure 6.3b	Level Profile in Second Reactor	6.8
Figure 6.4a	Temperature Profile in First Reactor	6.9
Figure 6.4b	Temperature Profile in Second Reactor	6.9
Figure 6.5	Feed Policy	6.10
Figure 6.6	Outflow Response in Second Reactor	6.10
Figure 6.7	Optimal Feed Policy	6.12
Figure 6.8	Responses from MATLAB Dynamic Simulations	6.12
Figure 6.9a	Responses from SPEEDUP Dynamic Simulations	6.13

Figure 6.9b	Responses from SPEEDUP Dynamic Simulations	6.13
Figure 6.10a	Feed Profiles from Different Solving Techniques	6.15
Figure 6.10b	Feed Profiles from Simultaneous Technique with GAMS	6.15
Figure 6.11a	Total Conversion	6.16
Figure 6.11b	Level Profile in Second Reactor	6.16
Figure 6.12	Plant 2: Binary Distillation Column	6.18
Figure 6.13	Temperature and Composition Distributions	6.21
Figure 6.14a	Second Case: Nominal Feasible Region and Optimal Point	6.25
Figure 6.14b	Second Case: Permanent Feasible Region and Back-Off Point	6.25
Figure 6.15a	Optimal Feed Profile	6.29
Figure 6.15b	Reboiler Duty Profile	6.29
Figure 6.16	Distillate and Reflux Profiles	6.30
Figure 6.17	Profiles of Temperatures at Tray 4 and Tray 13	6.31
Figure 6.18a	Composition Profile of Ethanol in Distillate	6.32
Figure 6.18b	Composition Profile of Ethanol in Base Product	6.32
Figure 6.19	Feed and Reboiler Level Profiles	6.33
Figure 6.20	Ethanol Composition and Inferential Variable Profiles (Tray 4)	6.35
Figure 6.21	Ethanol Composition and Inferential Variable Profiles (Tray 13)	6.36
Figure 6.22	Profiles of Temperature (Tray 13) and Reboiler Duty	6.37
Figure 6.23a	Feed Profile (Data collected from the plant)	6.39
Figure 6.23b	Distillate Profile (Data collected from the plant)	6.39

Figure 6.24b	Steam Rate Profile (Data collected from the plant)	6.40
Figure 6.25	Profiles of Temperature (Tray 13) and Reboiler Duty	6.41
Figure 6.26	Plant 3: Purification Column	6.43
Figure 6.27	Flowsheet of Purification Column (Last Iteration)	6.48
Figure 6.28	Nominal Optimum Operating Regions at Different Angles (Decision Variable Space)	6.50
Figure 6.29	Permanent Feasible Operating Regions at Different Angles (Decision Variable Space)	6.51
Figure 6.30	Feed and Side Product Profiles	6.54
Figure 6.31	MA Composition in D and EA Composition in B	6.55
Figure 6.32	Different Setting of Base Level Control Loop	6.56
Figure 6.33	Additional Quality Control Loop	6.56

List of Tables

Table 2.1	Results from Mathematical Example (after three iterations)	2.13
Table 2.2	Results from Case Study 1 (after three iterations)	2.19
Table 2.3	Results from Case Study 2 (after four iterations)	2.23
Table 3.1	Two Common Approaches to Solve a Switching Problem	3.9
Table 3.2	Switchability Problem Formulation in Discrete Form	3.22
Table 3.3a	Optimal Operating Conditions ($C_{in} = 20$)	3.28
Table 3.3b	Optimal Operating Conditions ($C_{in} = 15$)	3.29
Table 3.4	Different Switching Cases	3.32
Table 3.5	Optimal Operating Conditions ($C_{in} = 20$)	3.49
Table 3.6	Different Shutdown Cases	3.50
Table 3.7	Sizes of Back-Off Problems and Limits in The Solver	3.57
Table 3.8	Switching Case from Startup Operating Conditions	3.63
Table 4.1	Dynamic Closed-Loop Back-Off Operating Conditions (A Single CSTR)	4.8
Table 4.2	Dynamic Closed-Loop Back-Off Operating Conditions (Two CSTRs)	4.30
Table 4.3	Two Step Switching Policy	4.38
Table 5.1	Results from First Iteration (Nominal Case, Single CSTR)	5.3
Table 5.2a	Results from First Iteration (Nominal Case, Two CSTRs)	5.5
Table 5.2b	Results from First Iteration (Two CSTRs, Four Decision Variables)	5.5

Table 5.3	Purification Column – Stream Section	5.10
Table 5.4	Results from Dynamic Closed-Loop Back-Off Calculations (A Single CSTR, Two Decision Variables)	5.12
Table 5.5	Results from Dynamic Closed-Loop Back-Off Calculations (A Single CSTR, Three Decision Variables)	5.13
Table 5.6	Execution Times of Dynamic Back-Off Calculations in GAMS	5.13
Table 5.7	Computational Time against KT Error (Sequential Technique – SPEEDUP)	5.17
Table 6.1	Nominal Optimal Operating Conditions	6.24
Table 6.2	Back-Off Conditions	6.26
Table 6.3	Simulation Result Compared to Laboratory Analysis	6.44
Table 6.4	Steady State Open Loop Back-Off Operating Conditions	6.47
Table 6.5	Results from ASPEN and Shortcut Models	6.52

Chapter 1

Introduction

1 Thesis objective.....	1.2
2 Thesis overview.....	1.3
Chapter 1: Introduction.....	1.3
Chapter 2: Steady state and dynamic flexibility analysis.....	1.3
Chapter 3: Switchability and operability assessment.....	1.4
Chapter 4: Switchability and controllability analysis.....	1.4
Chapter 5: Solution method for switchability analysis.....	1.5
Chapter 6: Switchability analysis of real processes.....	1.5
Chapter 7: Conclusions and future works.....	1.6
3 Thesis format.....	1.6
4 References.....	1.7

Optimization of flexible chemical processes in the face of uncertainties remains one of the most challenging problems in Process Systems Engineering over the last twenty years. The uncertainties commonly experienced in plant operation are due to changes in demand or product specification, fluctuations of feed or equipment failure. They might be the results of using uncertain technical parameters at the design state (e.g. transfer coefficients and efficiencies) or poor models to predict the performance of a plant. In view of these uncertainties, the common practice is to overdesign processes and verify the robustness or flexibility of a design (Grossmann, 1991). Over the last decade, most of the systematic design tools were directed towards the improvement of process economics, but they used to neglect the improvement of plant operability. Furthermore, if a plant is designed only on the basis of steady state economic considerations, unfavorable process dynamics might make the designed control system impossible. Finally, increased process integration and tight operating conditions demand a better control performance than any time in the past (Holt, 1985). Consequently, a good process design must show an optimal balance between capital and operating costs, and at the same time, exhibit operability characteristics, which allow the economic performance to be realizable in a practical operating environment. Different aspects of operability thus complicate process design objectives. They include flexibility, controllability, reliability and safety. Although these aspects may appear to be similar, they actually correspond to different technical concepts (Swaney, 1983).

- ❖ Flexibility allows the process to operate at other steady states without sacrificing efficiency or throughput. A flexible process has sufficient degrees of freedom and range of control to cope with all foreseeable changes in the steady state operating environment (Howell, 1984).
- ❖ Controllability is concerned with the quality and stability of the dynamic response of the process. It depends on how a deviation from the target is sensed. It also depends on the effectiveness of allowable corrective control actions. Such properties are independent of the control system itself, so may be used in the process design stages.
- ❖ On the other hand, reliability deals with the probability of normal operations given that mechanical and electrical failures can occur.
- ❖ Finally, safety deals with the hazards, which are consequences of these failures.

A strategy will be developed in the thesis to incorporate the switchability analysis with the first two concepts, which constitute one of the major aspects of process design known as “dynamic operability” or “dynamic resilience” (Morari, 1983).

- ❖ Switchability describes how readily a process moves between different operating states. It analyzes the dynamic behavior of the systems, in which the major disturbances often exceed the limits set for flexibility. The nonlinear feature of the system response is emphasized in the switching problem. Under these conditions, the range of control action will be constrained by physical and safety factors. These are essential differences between controllability and switchability.

In brief, the simultaneous operability and switchability analysis shows the ease of operating, switching between operating states and controlling the plant in a safe and optimal manner.

1. Thesis Objective

As discussed in this chapter, significant benefits can be achieved through the introduction of flexibility and controllability to design or retrofit design of a process. A systematic technique was developed to consider these problems at once, with the objective as a measure of the economic performance of the plant (Bahri, 1995). This integrated strategy is used as the starting platform, which results in economically desirable steady state conditions at the beginning and the end of a switch. A formulation is proposed to search for the optimal transition between these states, while dealing effectively with possible disturbances. The effect of conventional and advanced control techniques on the whole analysis is discussed afterwards. Basic problems to be solved in the thesis include:

- ❖ The **Flexibility** problem to ensure a feasible operation of the plant over a variety of operating conditions at two ends of the transition.
- ❖ The **Switchability** problem to ensure feasible and optimal trajectories in the face of disturbances, while changing operating states.
- ❖ The **Controllability** problem to ensure a feasible dynamic performance and efficient disturbance rejection.

Finally the proposed methodology is applied to some real plants to investigate the applicability of the procedures. Possible improvements of the plant design, operation or control are then proposed.

2. Thesis Overview

Various topics are presented through seven chapters.

Chapter 1 – Introduction

The first chapter presents the overview of the thesis with much emphasis on the concepts of operability and switchability. This will show the continuity of the subject in the thesis, while readers can follow the chapter independently.

Chapter 2 – Steady State and Dynamic Flexibility Analysis of Chemical Processes with Fixed Design

The second chapter reviews the concept of flexibility and the quantitative analysis of this property in a given model. The reviewed methodology analyzes the steady state open-loop (i.e. without control) flexibility of existing plants. This strategy can be used as a tool to find the economic loss associated with the open-loop operation of the plant, and also to justify the profit gained by the implementation of different sorts of controllers. An iterative algorithm was developed to quantitatively measure the movement of the optimum to a new position within the feasible region. This new position is referred to as the back-off position, and the amount of this backing off from the optimum represents the quantitative measure of the plant flexibility. The developed algorithm is an iterative dual level optimization. The primary level searches for the optimality of a process over the given set of disturbances. The sub-level tests the feasibility of the solution under different values of disturbances. The algorithm requires a number of iterations until it reaches the permanent feasible region providing a feasible solution. The iterative procedure for open loop cases can be extended to consider dynamic cases, when the dynamic plant is controlled. The formulation for dynamic closed-loop back-off calculations is the same as for steady state open loop cases except that dynamic models are used instead of steady state models and the control loops are closed. Consequently, some of the equality constraints are ordinary differential

equations, and different techniques are required to solve this type of problems. Three examples throughout the chapter demonstrate the methodology of implementing the algorithm.

Chapter 3 – Switchability and Operability Assessment in Chemical Processes

The third chapter studies the ability of a chemical plant to move safely and optimally from one operating condition to another. In order to cope with all likely disturbances throughout the transition, the switchability problem is simultaneously formulated with the flexibility and controllability problems. This formulation leads to an uncertain dynamic nonlinear programming (NLP) problem, which can be solved by two different approaches. The integrated strategy reviewed in Chapter 2 for operability analysis has been used as the starting platform that results in economically desirable steady state conditions at the beginning and the end of the transition. Although switchability is a part of controllability, there are also some characteristics, which distinguish one aspect from the other. Switchability problems take into account the process limitations and other restrictions under the form of path constraints to ensure a safe and feasible changeover. Thus the control actions are constrained by physical and safety factors. Switchability analysis employs the solution method based on nonlinear models. State delays can be included in model equations or in a discrete formulation. Minimizing the integral squared deviation of the state and control variables drives them to their new target values in a short period of time. Due to possible disturbances entering the plant during the transition, closed-loop back off from nominal trajectories of control variables should also be considered. The effectiveness of the proposed strategy is tested against two case studies. Different optimization problems generated in this chapter are solved using the software packages SPEEDUP and GAMS with MINOS 5.2 optimizer.

Chapter 4 – Switchability and Controllability Analysis – Predictive Control Approach

A good control strategy can partially or completely recover the profit loss due to disturbances and uncertainties in the process. It can also give feasible and optimal policies for an efficient switch. Linear systems have dominated the control scheme for many years. However, during the last two decades progresses in nonlinear control theory, combined with computer software and hardware advances have allowed

advanced nonlinear control strategies to be successfully implemented on chemical processes. The fourth chapter considers the predictive control approaches: linear and nonlinear model predictive control, because their formulations are very similar to the switchability formulation. Dynamic matrix control (DMC) is the most cited linear model predictive control. It is based on a linear convolution model and can successfully handle process constraints by using on-line measurements to adjust controller settings. Nonlinear predictive control, which is a direct extension of the LMPC method, uses the nonlinear dynamic process model. The application of MPC to replace PI controllers is thoroughly discussed through many case studies.

Chapter 5 – *Solution Method for Switchability and Operability Analysis*

The fifth chapter discusses the application of three packages: SPEEDUP, GAMS and MATLAB in solving optimization problems generated by the flexibility, switchability and controllability analysis. Each package has its own advantages and disadvantages. The algorithm developed for the steady-state flexibility study finds solutions of standard optimization problems. In both levels, these problems aim to different objectives but share a similar mathematical structure, in which an appropriate objective function is optimized and subject to a set of algebraic equality and inequality constraints. The standard optimization problems can be solved easily by any optimizer. The algorithm developed for the dynamic flexibility, switchability and controllability study requires the minimum of a cost or an integral error objective function, subject to a set of mixed algebraic and differential equations. These optimal control problems can be solved by two sophisticated mathematical techniques: sequential optimization and simultaneous integration and optimization approaches. The selection of software and technique to approach the dynamic optimization problems affects the computational time, convergence and accuracy. These factors are considered in the case studies solved throughout the thesis.

Chapter 6 – *Switchability and Operability Analysis of Real Processes*

Theories on simultaneous flexibility, switchability and controllability analysis are applied to improve the performance of real chemical processes. The applications start from a simple pilot plant to a more complicated industrial distillation column. The first essential key in the exercise is a good model, which can predict well the process

behavior. Some special systems face the problems of large time delay and inverse response. An appropriate control strategy should be applied to these systems to achieve a better control performance. Other processes involving physical and thermodynamic properties such as distillation processes require models, which are formulated to calculate these properties or can extract them from some internal and external sources. Some properties of these chemical processes in real time cannot be measured fast enough so that the control action can be calculated, based on their measurements. An inferential control scheme is applied to solve the problem. The sixth chapter considers these problems through three applications: two Continuous-Stirred Tank Reactors in series, the binary distillation column and the multicomponent distillation column.

Chapter 7 – *Conclusions and Future Works*

The last chapter summarizes the major issues discussed throughout the thesis and draws the general conclusions. Some highlights for the future research are presented.

3. Thesis Format

Five main chapters in the thesis share the same format. Each starts with a brief introduction to its theme. The conclusion at the end summarizes the discussion and solution of each problem. Nomenclatures, references and appendices are presented for each chapter instead of the whole thesis. The references are referred to by last names of the authors, years of publication, titles, names of publishers or journals (*italic*), volumes (**bold**) and numbers of pages. Broken lines in all graphs represent constraints or targets to reach.

4. References

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Chapter 2

Steady State and Dynamic Flexibility Analysis of Chemical Processes with Fixed Design

1 Introduction.....	2.1
2 Optimization of chemical processes.....	2.2
3 The effect of uncertainties on optimal operation.....	2.3
4 Deterministic flexibility analysis.....	2.4
5 Steady state open loop back-off calculation.....	2.5
5.1 Back-off concept.....	2.8
5.2 Problem formulation.....	2.8
5.3 Algorithm development.....	2.10
5.4 Modified algorithms.....	2.13
5.4.1 The KS modified algorithm.....	2.13
5.4.2 The KTC modified algorithm.....	2.14
5.5 Case studies.....	2.16
5.5.1 Case study 1: a single CSTR.....	2.16
5.5.2 Case study 2: two CSTRs in series.....	2.21
6 Dynamic closed-loop back-off calculation.....	2.27
7 Conclusion.....	2.29
8 Nomenclature.....	2.30
9 References.....	2.31
Appendix 2A.....	2.32
Appendix 2B.....	2.35

Chapter 2 reviews the main concept of flexibility and the quantitative analysis of this property in a given model. Effects of disturbances and uncertainties on the open loop and closed-loop operations of chemical plants can be measured by the amount of backing off from nominal operations. With special emphasis, the methodology of implementing the iterative algorithm approach is introduced and demonstrated through two case studies.

1. Introduction

Flexibility represents the ability of a process to permit a feasible steady state operation over a range of operating conditions. For three decades, many famous authors have dealt with flexibility problems using various solution strategies. Two principal approaches described by Bahri (1995) are the deterministic and stochastic cases. The first approach simply requires an average (or best-known) value, within an estimated range of variation for each single parameter, subject to uncertainty. The second approach is based on the assumption of some kind of probabilistic distribution of parametric uncertainties. The deterministic flexibility has shown to be very practical in real applications, since it requires less information of uncertainties than the other case. Therefore, it will be reviewed in detail later.

The stochastic flexibility (SF) measures the probability of a feasible operation, when uncertain parameters described by probability distribution functions are continuous. These continuous uncertainties propagate through the process and result in variations in the output variables. The constraints that restrict the values of the output variables define the feasibility of the operation. The output distribution that lies within the constraints defines the stochastic flexibility. Straub and Grossmann (1990) proposed the expected stochastic flexibility (ESF) as an extension of the SF, when there were discrete uncertainties associated with the process. In the above cases, it is assumed that the vector describing the availability and unavailability of the corresponding design variables is fixed. Thus the problems solved are those of flexibility in operation. Other works in literature also deal with parameter uncertainties in process design (Grossmann (1978), Halemane (1983), Floudas (1987), Pistikopoulos (1988)).

In most design problems, if the plant itself does not exist, the main focus is finding a feasible design with the minimum capital cost, subject to uncertainties, by adjusting design and control variables. Other design problems attempt to improve the operation and profitability of existing plants through structural or design changes. On the other hand, problems of flexibility in operation involve optimal operating condition of a plant or optimal control of a process. Despite the distinct difference between flexibility in design and in operation, the mathematical formulations of these problems are closely related. Thus the solution strategies developed for the flexibility in design can be extended and applied for the flexibility in operation.

Through the review of the deterministic approach, a measure of flexibility, namely the back-off index, is discussed in the following sections. The iterative algorithm is tested for open loop and closed-loop operations through two case studies. Since the flexibility analysis is mainly based on an optimization model of the process, it is important to go through the concept of optimal operations of chemical plants under uncertainty first.

2. Optimization of Chemical Processes

The aim of optimization is to find the values of the variables that yield the best value of the performance criterion in the process. The best performance might be a reduction in energy consumption, in yield of contaminants or a growth in profit and processing rates. Optimization problems can take place at many levels in an industrial plant, but those engaged in process design and operation generate a fundamental formulation in the flexibility analysis. A wide variety of optimization problems may represent simple or complex processes that have different applications in the real world, but they all share an amazing similar mathematical structure. The essential features of an optimization problem includes an appropriate objective function to be optimized, subject to a set of equality constraints describing the process model, and a set of inequality constraints describing the process limitations. The typical optimization problem (P0) is formulated as:

$$\text{Minimize (or maximize):} \quad F(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) \quad (\text{P0})$$

Subject to:

$$\mathbf{c}_i(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) = 0 \quad i \in E$$

$$g_j(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) \leq 0 \quad j \in I$$

$$\mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U$$

The objective function $\mathbf{F}$ is most commonly a cost function to be minimized or a profit function to be maximized. $\mathbf{x}(t)$ and $\mathbf{u}(t)$ represent the state (dependent) and the control (independent) variables, respectively. The vector $\mathbf{p}$, independent of time, is the process constants, and $\mathbf{d}^n$ is a vector of process inputs that is exposed to uncertainties. $\mathbf{c}_i$, the equality constraints, describe the process model such as mass and energy balances, equipment performance relationship, etc. $\mathbf{g}_j$, the inequality constraints, describe the system limitations in terms of raw material, unit capacities, product qualities, etc.

A feasible solution is a set of variables that satisfy $\mathbf{c}_i$ and $\mathbf{g}_j$ for the given set $\mathbf{d}^n$. The feasible region contains all feasible solutions and is defined by $\mathbf{c}_i$ and $\mathbf{g}_j$. However, in the real world, the plant operating parameters and environs are not always static, and variations commonly occur in $\mathbf{d}^n$. Such variations are sometimes referred to as parametric uncertainties and disturbances, and the corresponding problem becomes the optimization problem under uncertainties.

3. The Effect of Uncertainties on Optimal Operation

Most of the time, a process is subject to disturbances or some sorts of uncertainties in the mathematical model or the data used in the model. Disturbances might be caused by variations in the input of the plant (e.g. feed rate, temperature) and/or in the performance of the plant itself (e.g. catalyst degradation, fouling factor, heat transfer coefficients). Based on how fast they change, disturbances are classified into slow and fast categories. The slow category, such as catalyst degradation, occurs on a time scale much slower than the dominant time constants of the system and can be handled by an on-line or even an off-line optimizer. The fast disturbances may lead to a constraint violation that produces a change in the feasible region. Their effects on the process depend on the magnitude, the frequency of occurrence and the control strategies implemented as well. Thus solving an optimization problem under uncertainties is dealing with flexibility and controllability. As mentioned in the introduction, the following optimization problems will be posed as deterministic models.

4. Deterministic Flexibility Analysis

In a deterministic flexibility case, the process inputs have the nominal values $\mathbf{d}^n$ with expected deviations in the positive and negative directions $\Delta \mathbf{d}^+$, $\Delta \mathbf{d}^-$. Including design variables, problem (P0) can be stated as:

$$\text{Minimize (or maximize):} \quad \mathbf{F}(\mathbf{x}, \mathbf{u}, \theta, \mathbf{p}, \mathbf{d}^n) \quad (\text{P0d})$$

Subject to:

$$\mathbf{c}_i(\mathbf{x}, \mathbf{u}, \theta, \mathbf{p}, \mathbf{d}^n) = 0 \quad i \in E$$

$$\mathbf{g}_j(\mathbf{x}, \mathbf{u}, \theta, \mathbf{p}, \mathbf{d}^n) \leq 0 \quad j \in I$$

$$\mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U$$

$$\theta = \mathbf{D}\mathbf{y}$$

θ is the vector of design variables that defines the structure and equipment sizes of a process. $\mathbf{D}$ is a diagonal matrix whose elements in the diagonal correspond to θ . $\mathbf{y}$ describes the availability (1) or unavailability (0) of the corresponding design variables. For the problems described below, $\mathbf{y}$ is fixed.

The feasibility test developed by Halemane and Grossmann (1983) was one of the first attempts to measure the process flexibility. The test determines the feasibility of a fixed design θ for every point $\mathbf{d} \in \mathbf{T}$, where: $\mathbf{T} = \{\mathbf{d}: (\mathbf{d}^n - \Delta \mathbf{d}^-) \leq \mathbf{d} \leq (\mathbf{d}^n + \Delta \mathbf{d}^+)\}$. A function is defined as:

$$\psi(\mathbf{d}, \theta) = \min_{\mathbf{u}, \varepsilon} \varepsilon \quad (2.1)$$

Subject to:

$$\mathbf{h}_j(\mathbf{u}, \mathbf{d}, \theta) \leq \varepsilon \quad j \in I$$

If $\psi \leq 0$, the design is feasible. The set of $\mathbf{d}$ for which $\psi \leq 0$ lies within the feasible region $\mathbf{R}$ is shown in Figure 2.1.

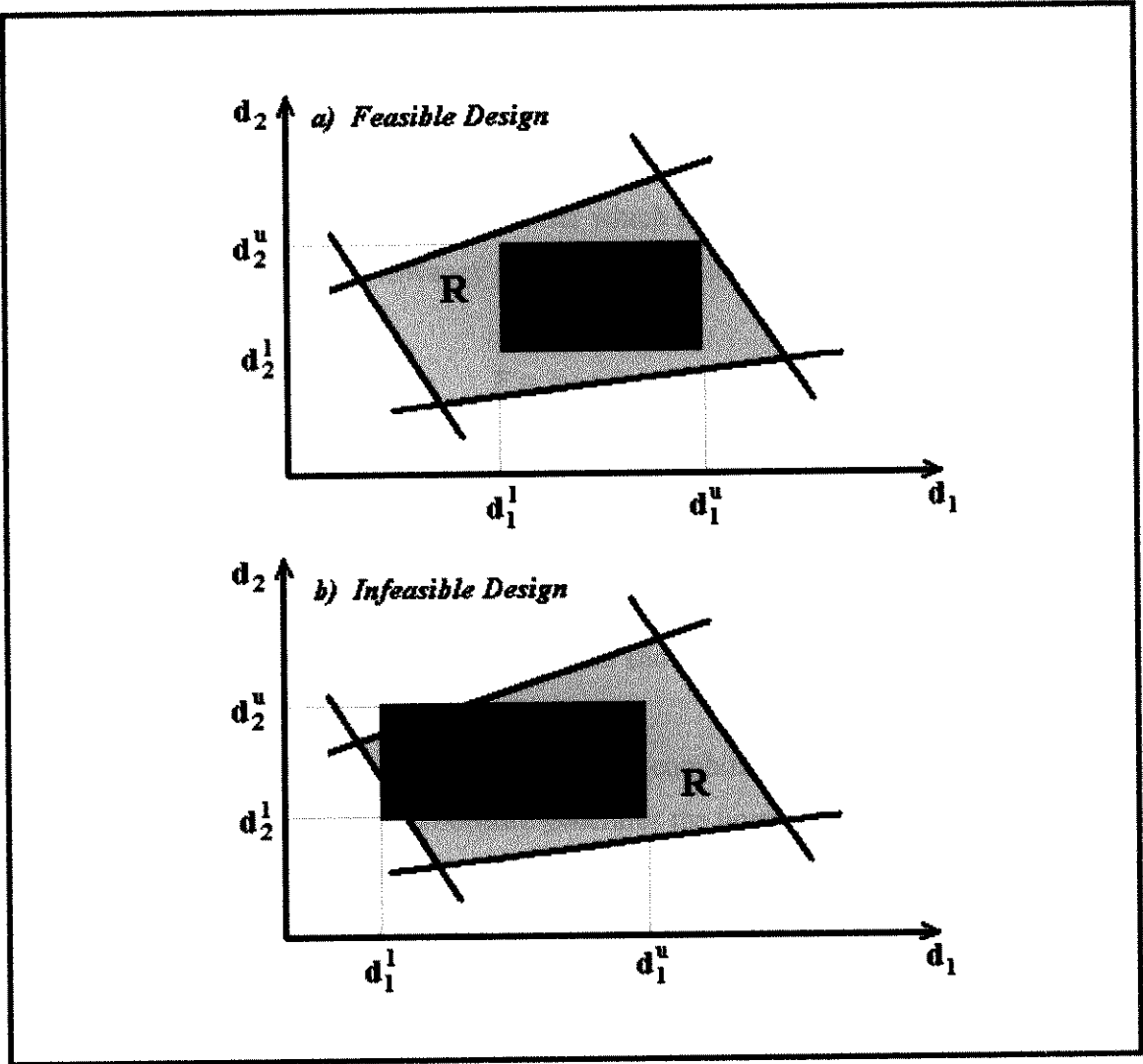


Figure 2.1 Feasibility Test : Feasible Design and Infeasible Design
(Feasible region in disturbance space)

The feasibility test cannot indicate to what degree the design is infeasible. Therefore, Swaney and Grossmann (1985) proposed the index of flexibility as a remedy to measure the size of the feasible operational region. It may be assumed that the uncertain parameters vary independently of each other. The maximum ranges, over which the parameters may vary while still remaining inside the feasible region, form a hyper-rectangle. The lengths of the sides of this hyper-rectangle will characterize the size of the feasible region. The flexibility index F is defined as the largest scaled deviation δ of the expected deviations that the design can handle for a feasible operation. Another result of the analysis is the identification of the critical points, or worst case operations, which accompanies the solution. Sufficient conditions are established for the constraint functions under which the solution is guaranteed to lie at a vertex of the feasible region. Swaney presented the following formulation:

$$F = \max \delta \quad (2.2)$$

Subject to:

$$\begin{aligned} \forall d \in T(\delta) \quad \{ \exists u \mid h_j(u, d, \theta) \leq 0 \} \quad j \in I \\ T(\delta) = \{ d \mid (d^n - \delta \Delta d^-) \leq d \leq (d^n + \delta \Delta d^+) \} \end{aligned}$$

The geometrical interpretation of the problem is shown in Figure 2.2.

Bahri developed an algorithm for the combination of feasibility test and flexibility index. The iterative procedure generates the nominal feasible region over the nominal set of uncertain parameters first. Then it searches for the permanent feasible region (PFR) that guarantees feasible operations despite the effect of all disturbances. The movement of the optimal solution due to variations of uncertain parameters is referred to as the amount of back-off.

5. Steady State Open Loop Back-Off Calculation

Using the concept of backing-off from the economic optimum point, the open loop operation of a plant with a fixed design will be considered.

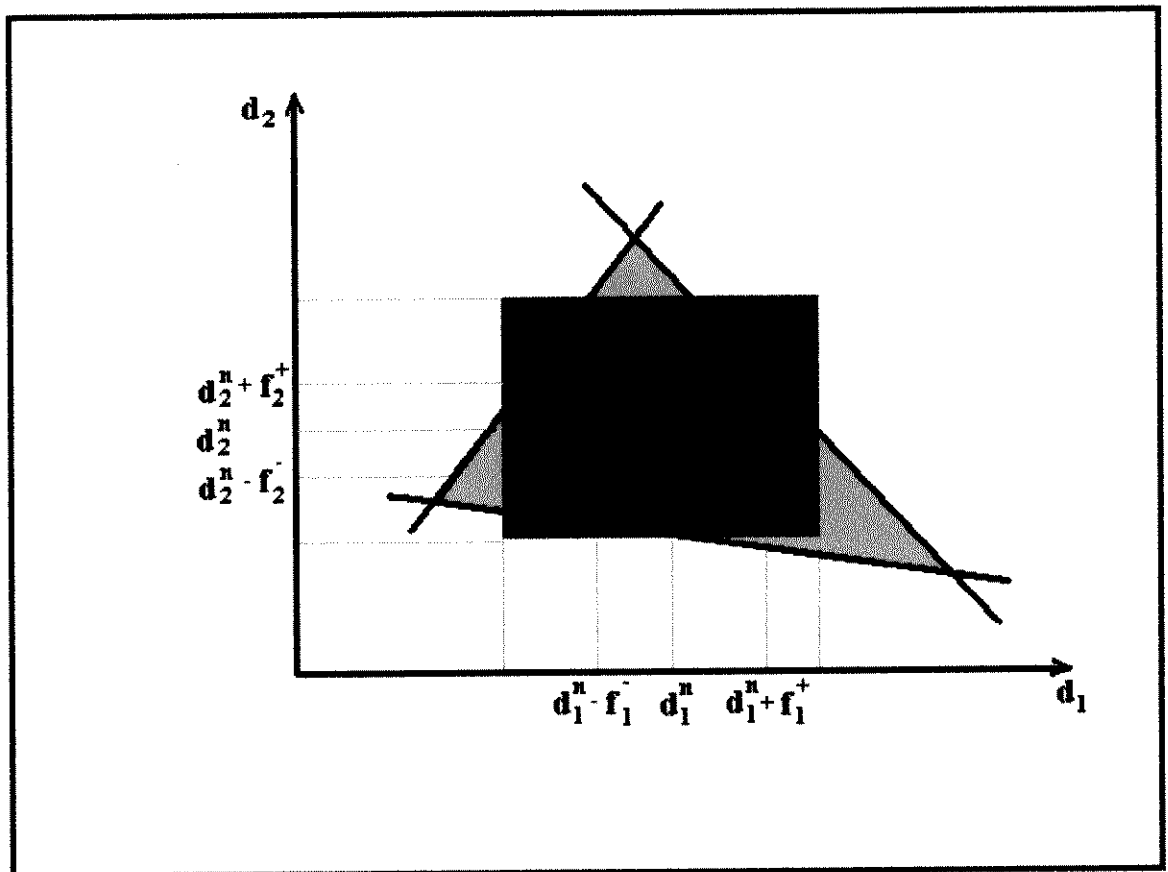


Figure 2.2 Geometrical Interpretation of Flexibility Index F

(Feasible region in disturbance space)

$$(f_i^+ = F^* \Delta d_i^+; f_i^- = F^* \Delta d_i^-)$$

5.1. Back-Off Concept

As discussed in the above sections, an optimal solution is a set of control (decision) variables that satisfies the equality and inequality constraints. This set also provides the best value of the objective function. The optimal solution is usually located at one or more active constraints. However, due to variations in operating conditions and uncertainties in the process model, the current operating point (i.e. nominal optimal point) might cause some constraint violations. This can result in an undesirable or unsafe operation of the process. To maintain permanent feasibility regardless of possible uncertainties and disturbances, the operating point should move to a new position referred to as the back-off position. Figure 2.3 shows the change of the feasible region and the movement of the operating point to the back-off position. It is possible to determine in advance how large this movement should be, and if any movement is actually required to avoid constraint violations. A study of the effect of disturbances on the process at steady state will be established next.

5.2. Problem Formulation

Throughout this work, the region of variation for disturbances and uncertainties is defined as: $\Gamma = \{\mathbf{d}: \mathbf{d}^L \leq \mathbf{d} \leq \mathbf{d}^U\}$. Each $\mathbf{d} \in \Gamma$ will provide a different set of constraints that generates a different feasible region $\mathbf{R}$. The nominal feasible region $\mathbf{R}^n$ is the original one defined by the nominal set $\mathbf{d}^n$. Problem (P1) is expanded from (P0) including the uncertainties.

$$\text{Minimize (or maximize):} \quad F(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) \quad (\text{P1})$$

Subject to:

$$c_i(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) = 0 \quad i \in E$$

$$\max_{\mathbf{k} \in \Gamma} \max_j g_j(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^n) \leq 0 \quad j \in I$$

$$\mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U$$

$$\mathbf{d}^k \in \Gamma$$

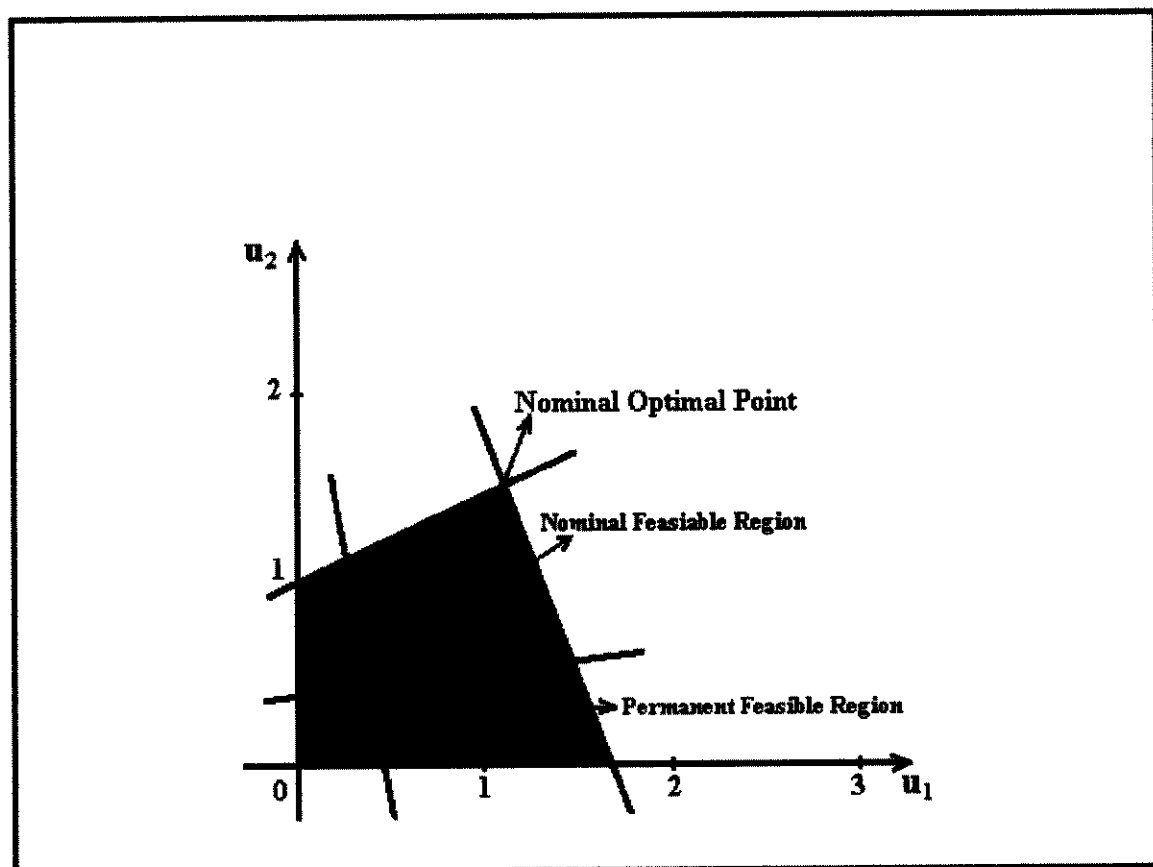


Figure 2.3 Movement of Nominal Optimal Point to Back-Off Point
(Feasible region in decision variable space)

Since it is very difficult to solve (P1) directly, the problem is decomposed into two levels of optimization.

5.3. Algorithm Development

The algorithm developed by Bahri is an iterative dual level optimization. The primary level (outer level, OL) searches for the optimality of problem (P1) over the fixed set $\mathbf{d}^k$. The sub-level (inner level, IL) tests the feasibility of the solution under different values of disturbances. If the solution is not feasible, the sub-level then searches for the worst case of disturbances, which produces the maximum violation. The algorithm requires a number of iterations until it reaches the permanent feasible region providing a feasible solution.

Let $\mathbf{u}^n \in \mathbf{R}^n$ be the solution of (P0) after the first iteration ($k=0$) of the OL optimization, then $\mathbf{u}^{*k} = \mathbf{u}^{*0} = \mathbf{u}^n$. The set $\mathbf{u}^{*k}$ is passed to the IL optimization to search for the worst case of disturbances that produces the maximum violation.

$$\text{Maximize:} \quad g_j(\mathbf{x}, \mathbf{u}^{*k}, \mathbf{p}, \mathbf{d}) \quad (\text{P2})$$

Subject to:

$$c_i(\mathbf{x}, \mathbf{u}^{*k}, \mathbf{p}, \mathbf{d}) = 0 \quad i \in E$$

$$\mathbf{d}^k \in \Gamma$$

Let $\mathbf{d}^{*k}$ be the solution of (P2), in the first iteration, $\mathbf{d}^{*k} = \mathbf{d}^{*0}$. For any $j \in I$, the vector $\mathbf{d}^{*k}$, which causes $g_j(\mathbf{x}, \mathbf{u}^{*k}, \mathbf{p}, \mathbf{d}^{*k}) > 0$, must be added to the vector of uncertain parameters. The second iteration ($k = 1$) of the OL optimization solves problem (P3) similar to (P0), but the matrix $\mathbf{d}^k$ now includes $\mathbf{d}^n$ and $\mathbf{d}^{*k}$. The feasible region $\mathbf{R}^k$ is the intersection of $\mathbf{R}^n$ and $\mathbf{R}^{*k}$.

$$\text{Minimize (or maximize):} \quad F(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^k) \quad (\text{P3})$$

Subject to:

$$c_i(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^k) = 0 \quad i \in E$$

$$g_j(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}^k) \leq 0 \quad j \in I$$

$$\mathbf{d}^k = \mathbf{d}^n + \mathbf{d}^{*1} + \dots + \mathbf{d}^{*k}$$

$$\mathbf{u} \in \mathbf{R}^k \quad \mathbf{R}^k = \mathbf{R}^n \cap \mathbf{R}^{*k}$$

The new solution $\mathbf{u}^k = \mathbf{u}^{*1}$ is passed to the IL optimization that solves (P2) and (P3). At each IL optimization, if there is a constraint violation, the size of $\mathbf{d}^k$ increases, but the size of the feasible region reduces.

$$\mathbf{d}^k = \mathbf{d}^n + \mathbf{d}^{*1} + \mathbf{d}^{*2} + \mathbf{d}^{*3} \quad \mathbf{R}^k = \mathbf{R}^n \cap \mathbf{R}^{*1} \cap \mathbf{R}^{*2} \cap \mathbf{R}^{*3}$$

The whole procedure can be summarized in the following steps:

- **Step 1** solves (P0) for $\mathbf{u}^n$. “ n ” denotes the value of a variable when all elements of $\mathbf{d}^n$ are fixed at nominal values.
- **Step 2** sets the iteration counter $L = 1$, $\mathbf{u}^{*L} = \mathbf{u}^{*1} = \mathbf{u}^n$.
- **Step 3** solves (P2) for $\mathbf{d}^{*L}$.
- **Step 4** updates $\mathbf{d}^k$ and $\mathbf{R}^k$.
- **Step 5** solves (P3) for $\mathbf{u}^{*L}$, checks the feasibility of $\mathbf{u}^{*L}$ with possible combinations of maximum, minimum and nominal values of $\mathbf{d}$, continues **step 6**, if there is a violation. If all constraints are satisfied, the algorithm stops.
- **Step 6** sets $L = L+1$, and then goes back to step 3.

Let's take the mathematical example from Landers (1997) to follow the steps of the whole procedure. This example is selected because it can be easily solved using the software package MATLAB (1997). Although the equality constraints are nonlinear, the inequality constraints are linear and hence the IL problems are also linear. Samples of some input files are shown in Appendix 2A. Results of this example were plotted before, in Figure 2.3. The example is formulated as:

$$\text{Max } F = u_1 + 3 u_2$$

st

$$\text{c1...} \quad x_1 = (-4d_1^2 + 3d_2^2 + 3.25)u_1 + (d_1 + 2d_2 - 1.75)u_2$$

$$\text{c2...} \quad x_2 = (d_2 - 6)u_1 + (-3d_1^2 + 4d_2^2 + 4d_1d_2 - d_1 - 1.0)u_2$$

$$\text{g1...} \quad x_1 - 3d_1 - d_2 - 5.5 \leq 0$$

$$\text{g2...} \quad x_2 - 10 \leq 0$$

$$0.0 \leq (u_1, u_2) \leq 2.0$$

$$0.5 \leq (d_1, d_2) \leq 2.5$$

The nominal values of the uncertain parameters are $d^n = [1.0, 1.5]$. The initial guess for the first OL optimization is $u = [0.9, 1.1]$.

- In **step 1** the first OL optimization is solved. The solution is $u^n = [1.1052, 1.4973]$, which is also the nominal optimal operating point shown in Figure 2.3. The blue area is the nominal feasible region. At this stage it is not necessary to perform the feasibility test, however, for demonstration purposes, the input file “band1.m” (see Appendix 2.A) also includes the test. It is found that for $u^n = [1.1052, 1.4973]$, many sets of disturbances will cause constraint violations.
- **Step 2** starts the iteration by setting the counter equal 1.
- In **step 3** the IL optimization is solved (see “band2.m”). It is shown that the set $d_7 = [1, 2.5]$ causes the maximum violation of constraint g_2 . Therefore, in **step 4** the nominal set d^n is updated to include d_7 .

$$d^1 = \begin{bmatrix} 1 & 1.5 \\ 1 & 2.5 \end{bmatrix}$$

- In **step 5** for the fixed set d^1 , the OL optimization is solved again. The new solution is tested for feasibility (see “band3.m”). The new solution $u^1 = [0.8091, 0.4173]$ is not feasible so in **step 6** the counter is added by one and another iteration begins with **step 3**. The algorithm continues until a feasible solution is found. This point is shown as the back-off point in Figure 2.3. The magenta area is the permanent feasible region. Table 2.1 summarizes the results after three iterations.

The above example has two inequality constraints; therefore, in step 3 of the algorithm two different optimization problems must be solved (see “band2.m”). If the original problem (P0) has a large number of inequality constraints (for example, n inequality constraints), then the job of solving n different optimization problem in step 3 will be very tedious. The attempts to reduce computational time and simplify the programming job are discussed next.

Iteration N°	Input File	Uncertain Parameters	Decision Variables
L = 0 (Nominal)	Band1.m	$d^n = [1, 1.5]$	$u^n = [1.1052, 1.4973]$
L = 1	Band2.m Band3.m	$d^1 = \begin{bmatrix} 1 & 1.5 \\ 1 & 2.5 \end{bmatrix}$	$u^1 = [0.8091, 0.4173]$
L = 2	Band2.m Band3.m	$d^2 = \begin{bmatrix} 1.0 & 1.5 \\ 1.0 & 2.5 \\ 0.5 & 2.5 \end{bmatrix}$	$u^2 = [0.3865, 0.3692]$
Stop	Optimal solution found		

Table 2.1 Results from Mathematical Example (after three iterations)

5.4. Modified Algorithms

In order to improve the computational efficiency of the basic algorithm, Landers (1997) identified two possibilities: using the KS function and adding the KTC conditions in the original problem. Based on previous works done by Daichendt and Grossmann (1994), Ovstrosky et al. (1994), Landers presented these possibilities in detail through several examples. The aim of this section is to briefly review the modified algorithms but focusing on the application of the algorithms in chemical processes.

5.4.1. The KS modified algorithm

The main idea of the modified algorithm is to approximate n inequality constraints using one function. Thus the n different optimization problems in the IL will reduce to one problem. The KS function was originally developed by Kreisselmeier and Steinhauser (1979) and later named after them.

For the set of constraints $g_j(\mathbf{x}, \mathbf{u}, \mathbf{p}, \mathbf{d}) \leq 0$, it is defined:

$$ks(g) = \left(\frac{1}{\rho}\right) \ln \left\{ \sum_{j=1}^n \exp[\rho g_j(x, u, p, d)] \right\} \quad (2.3)$$

ρ is a parameter set by the user. It can take a value between 5 and 20. In the KS modified algorithm problem (P2) now becomes:

Maximize: (P2k)

$$ks(g) = \frac{1}{\rho} \ln \left\{ \sum_{j=1}^n \exp[\rho g_j(x, u^k, p, d)] \right\}$$

Subject to: $i \in E$

$$c_i(x, u^k, p, d) = 0$$

$$d^k \in \Gamma$$

The KS modified algorithm was tested in the mathematical example presented before. The file “bks1.m” was used instead of “band2.m”(see Appendix 2A), which was shorter, because only one optimization problem was required. The algorithm terminated after three iterations. Since there are only two inequality constraints in this example, the efficiency of the KS modified algorithm is not easily seen. A larger problem such as the second case study might show its advantage.

5.4.2. The KTC modified algorithm

This approach transforms the dual level problem into a single level by formulating the Kuhn-Tucker optimality conditions of the IL and including them as constraints into the OL. The optimality conditions of a general nonlinear programming problem with the complementary conditions are shown as follows:

$$\lambda_u g_j(x) = 0$$

$$\lambda_j \geq 0, \quad g_j(x) \leq 0 \quad (2.4)$$

λ_j are the Lagrange multipliers for g_j .

The single level problem has the form:

$$\begin{aligned}
 \text{Minimize:} \quad & F(x, u, d^n) & (P4) \\
 \text{Subject to:} \quad & c_i(x, u, d^n) = 0 & i \in E \\
 & c_i^j(x, u, d^j) = 0 & i \in E, j \in I \\
 & g_k^j(x, u, d^j) \leq 0 & k \in I, j \in I \\
 & -\nabla_d g_j + \sum_i \mu_i^j \nabla_d c_i^j + \sum_u \lambda_u^j \nabla_d q_u^j(d^j) = 0 & u \in U \\
 & -\nabla_x g_j + \sum_i \mu_i^j \nabla_x c_i^j = 0 \\
 & \lambda_u^j - (\lambda_u^j + q_u^j(d^j))_+ = 0
 \end{aligned}$$

λ_u are the Lagrange multipliers for q_u . μ_i are the Lagrange multipliers for c_i . q_u is the whole set of inequality constraints for the whole set of d .

By applying the KS modified algorithm, the problem becomes:

$$\begin{aligned}
 \text{Minimize:} \quad & F(x, u, d^n) & (P5) \\
 \text{Subject to:} \quad & c_i(x, u, d^n) = 0 & i \in E \\
 & c_i^j(x, u, d^j) = 0 & i \in E, j \in I \\
 & g_k^j(x, u, d^j) \leq 0 & k \in I, j \in I \\
 & -\nabla_d k_s + \sum_i \mu_i^j \nabla_d c_i^j + \sum_u \lambda_u^j \nabla_d q_u^j(d^j) = 0 & u \in U \\
 & -\nabla_x k_s + \sum_i \mu_i^j \nabla_x c_i^j = 0 \\
 & \lambda_u^j - (\lambda_u^j + q_u^j(d^j))_+ = 0
 \end{aligned}$$

The single level algorithm requires the partial derivatives of the Lagrangian with respect to the uncertain parameters and the Lagrange multipliers for the constraints. This is not a simple task even for a small model. For a set of three uncertain parameters, the number of possible combinations of these three parameters becomes 3^3 , making the problem more sophisticated. Therefore, the single algorithm is included for reference. No implementation of this will be made in the case studies.

The dual level KS modified algorithm will be used in the following case studies, since in an industrial problem the number of equality constraints is commonly much larger than the inequality constraints. As the structure of the IL problem remains the same but only the objective function changes, the dual level algorithm normally converges in a few iterations.

5.5. Case Studies

The examples used as the case studies should be able to evaluate the validity of the algorithm and clarify the steps of the whole procedure. To illustrate how the iterative algorithm works, the first example is solved in MATLAB. For more complicated models, two software packages: GAMS (1992) and SPEEDUP (1996) are used.

5.5.1. Case study 1: a single CSTR

The first case study is a simple problem of a single continuous-stirred tank reactor (CSTR) as shown in Figure 2.4. Component B is formed from A by the single, irreversible, exothermic and first order reaction $A \rightarrow B$. Heat is removed from the system by a cooling jacket surrounding the reactor. Assuming that the density and heat capacity of the mixtures are constant and independent of temperature and concentration of the solutions, the equality constraints describing the model include:

$$\text{Rate of consuming A:} \quad \text{Rate} = -k_0 e^{(-E/R_s T)} V C \quad (2.5)$$

$$\text{Mass balance for A} \quad \{d(V C)/dt\} = \text{Rate} + Q_{in} C_{in} - Q_o C_o \quad (2.6)$$

$$\text{Rate of heat removal} \quad \text{Cool} = U a (T - T_{co}) = m (T_{ci} - T_{co}) \quad (2.7)$$

$$\text{Energy balance} \quad \{d(V T)/dt\} = D H * \text{Rate} + Q_{in} T_{in} - Q_o T_o - \text{Cool} \quad (2.8)$$

$$\text{where} \quad D H = -\{\Delta H_r / (\rho_r C_p)\} \quad (2.9)$$

$$\text{Perfect mixing} \quad C = C_o; T = T_o \quad (2.10)$$

$$\text{Overall mass balance} \quad Q_{in} = Q_o \quad (2.11)$$

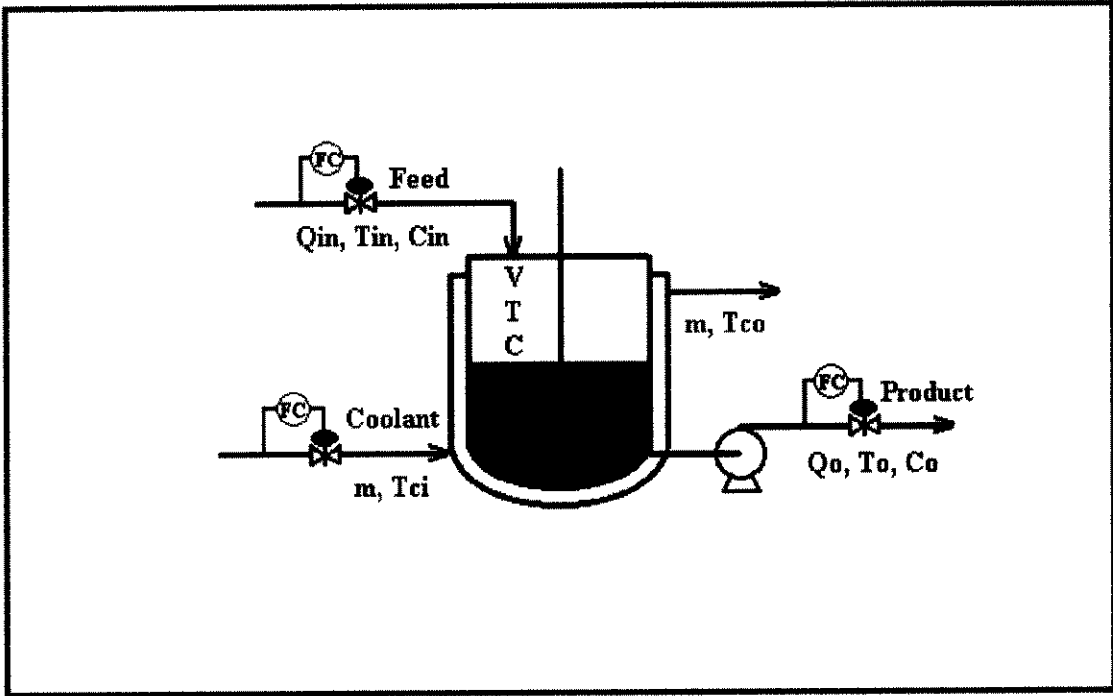


Figure 2.4 Case Study 1: Single CSTR

Optimal Operating Condition

$Q_{in} =$	0.286 L s^{-1}
$T_{in} =$	300 K
$C_{in} =$	20 mol.l^{-1}
$T_{ci} =$	283 K
$V =$	373 l
$m =$	1.04 L s^{-1}

The inequality constraints describing the limitations of the process under consideration are:

<i>Safety restriction</i>	$T \leq 350 \text{ K}$	Constraint 1
	$100 \leq V \leq 500 \text{ l}$	Constraint 2
<i>Process limitation</i>	$\text{Cool} \leq 20 \text{ l.K.s}^{-1}$	Constraint 3
<i>Maximum, minimum Throughput</i>	$0.05 \leq Q_{\text{in}} \leq 0.8 \text{ l.s}^{-1}$	Constraint 4
	$C_o \leq 0.3 \text{ mol.l}^{-1}$	Constraint 5

The set of uncertain parameters contains three elements that have upper and lower bounds as:

	Lower Bound	Nominal Value	Upper Bound
$T_{\text{in}}(\text{K})$	295	300	305
$T_{\text{ci}}(\text{K})$	278	283	288
$Ua(\text{l/s})$	0.33	0.35	0.37

The net profit is selected as the objective function:

$$\text{Profit} = \text{product value} - \text{raw material cost} - \text{cost of cooling}$$

$$\text{Obj (\$/time)} = p_v * Q_{\text{in}} * (C_{\text{in}} - C_o) - m_c * Q_{\text{in}} * C_{\text{in}} - c_c * \text{Cool}$$

The optimization problem is solved for two decision variables: feed flowrate Q_{in} and inventory V . The latter variable is not explicitly seen in the objective function, but it is related to the outlet concentration. If the inventory is increased, the residence time goes up, and the outlet concentration becomes smaller. However, a larger inventory requires a bigger reactor, which means the fixed cost is increased. Constraint 2 puts the limits on the reactor size.

SPEEDUP is selected to solve this case study. In step 3 of the algorithm, depending on the size of the uncertain vector, problem (P0) recurs many times and each time the set of equality constraints must be duplicated or triplicated, etc. SPEEDUP can handle well this situation. The OL problems using SPEEDUP have the same model

section but different flowsheet and operation sections (see Appendix 2B). In the IL optimization, the KS modified algorithm is used to reduce the set of inequality constraints to one equation so only one optimization problem must be solved.

Iteration N°	Input File	Objective Function	Uncertain Parameters $D = [T_{in}, Ua, T_{ci}]$	Decision Var. $u = [Q_{in}, V]$
L = 0 (Nominal)	c2c1.spe	71.0	$d^n = [300, 0.35, 283]$	$u = [0.362, 245]$
L = 1	c2c1a.spe c2c1b.spe	56.6	$d^n = [300, 0.35, 283;$ $305, 0.33, 288]$	$u = [0.288, 270]$
L = 2	c2c1a.spe c2c1b.spe	56.5	$d^n = [300, 0.35, 283;$ $305, 0.33, 288;$ $295, 0.37, 278]$	$u = [0.286, 373]$
Stop	Optimal solution found			

Table 2.2 Results from Case Study 1 (after three iterations)

The above table summarizes the results after three iterations. In the first iteration, constraint 5 is violated. Therefore, a larger inventory is required (from 270 l to 373 l). However, this increase in the reactor size does not affect the operating cost (profit reduces from \$56.6 to \$56.5). The optimal solution is located at the intersection of two active constraints: constraint 1 and constraint 5.

Figure 2.5 shows the movement of the optimal point. Two lines representing constraint 1 ($T = 350$) and constraint 5 ($C = 0.3$) form the feasible regions. The feasible region after two iterations (Figure 2.5a) is the intersection of the nominal feasible region (area bounded by magenta curves) and the intermediate region (area bounded by green curves). $R^1 = R^n \cap R^{*1}$. Two yellow curves represent the objective contours: profit = 50 and profit = 70. In Figure 2.5b the permanent feasible region with the corresponding permanent optimal point (back-off point) is the intersection area of the NFR and two intermediate regions. $R^2 = R^n \cap R^{*1} \cap R^{*2}$.

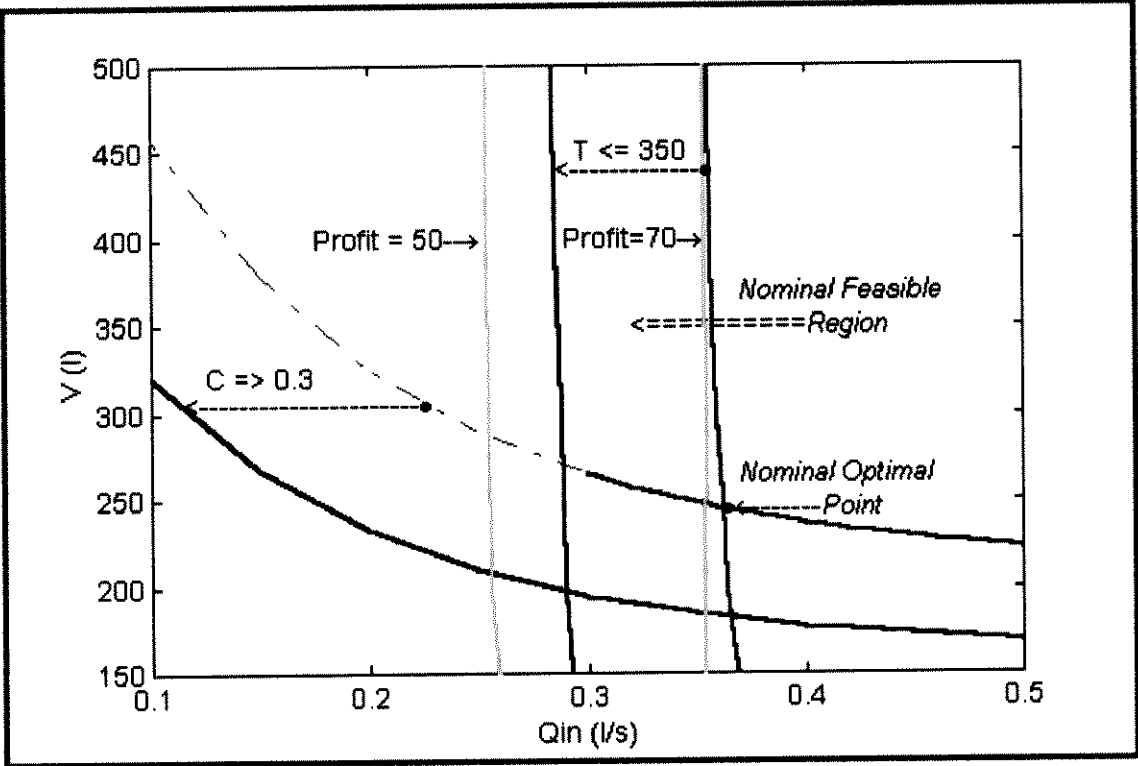


Figure 2.5a Case Study 1: Nominal Feasible Region and Optimal Point

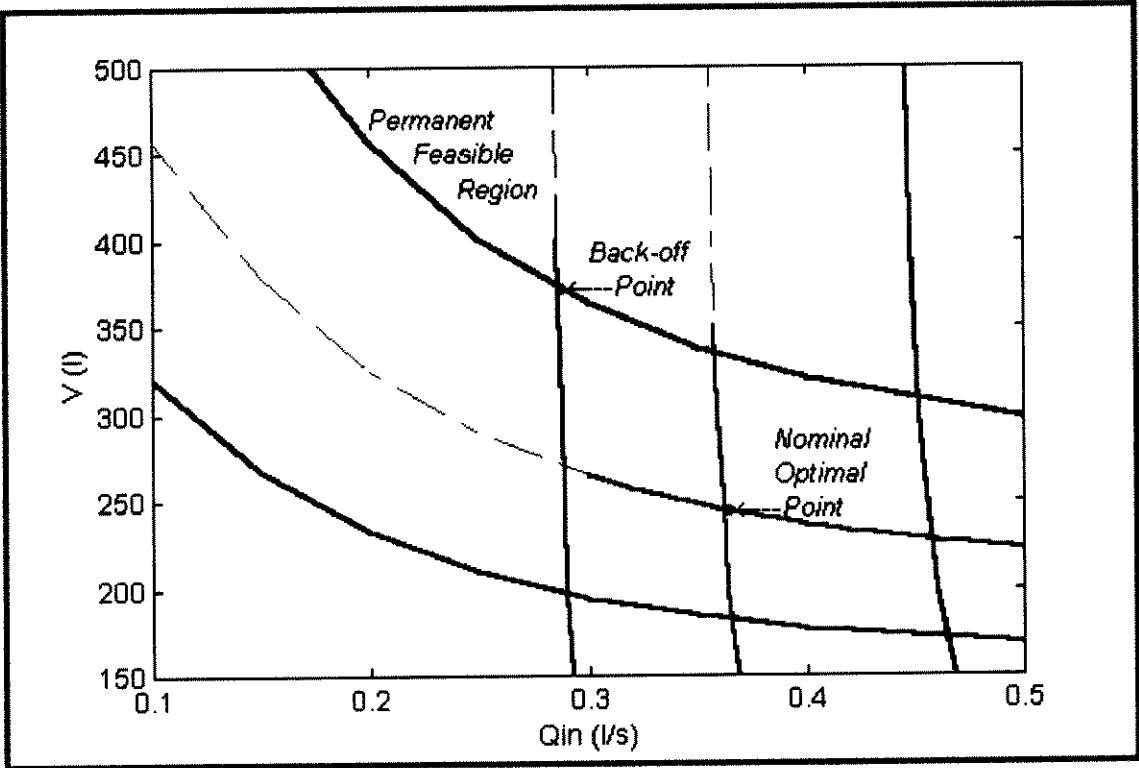


Figure 2.5b Case Study 1: Permanent Feasible Region and Back-Off Point

5.5.2. Case study 2: two CSTRs in series

The second case study is a system of two CSTRs in series with an intermediate mixer as shown in Figure 2.6. The problem was originally taken from de Hennin (1991) and modified by Bahri. Some details are changed to suit the aims of the following chapter. The model equations are similar to those in the first case study but more equations are required for the intermediate mixer.

$$\text{Overall mass balance} \quad Q^2_{in} = Q^1_o + Q^2 \quad (2.12)$$

$$\text{Mass balance for A} \quad C^2_{in} Q^2_{in} = C_1 Q^1_o + C_f Q^2 \quad (2.13)$$

$$\text{Energy balance} \quad T^2_{in} Q^2_{in} = T_1 Q^1_o + T_f Q^2 \quad (2.14)$$

The inequality constraints on the systems are:

<i>Safety restriction</i>	$T_1 \leq 350 \text{ K}$	Constraint 2.1
	$T_2 \leq 350 \text{ K}$	Constraint 2.2
	$100 \leq V_1, V_2 \leq 500 \text{ l}$	Constraint 2.3
<i>Process limitation</i>	$\text{Cool}_1 \leq 20 \text{ l.K.s}^{-1}$	Constraint 2.4
	$\text{Cool}_2 \leq 15 \text{ l.K.s}^{-1}$	Constraint 2.5
<i>Maximum, minimum Throughput</i>	$0.1 \leq Q_f \leq 0.8 \text{ l.s}^{-1}$	Constraint 2.6
	$0.05 \leq Q^1_{in}, Q^1_o, Q^2_o \leq 0.8 \text{ l.s}^{-1}$	Constraint 2.7
	$C^2_o \leq 0.3 \text{ mol.l}^{-1}$	Constraint 2.8

The set of uncertain parameters contains two elements that have upper and lower bounds as:

	Lower Bound	Nominal Value	Upper Bound
$T_{in}(K)$	298	300	305
$T_{ci}(K)$	280	283	286

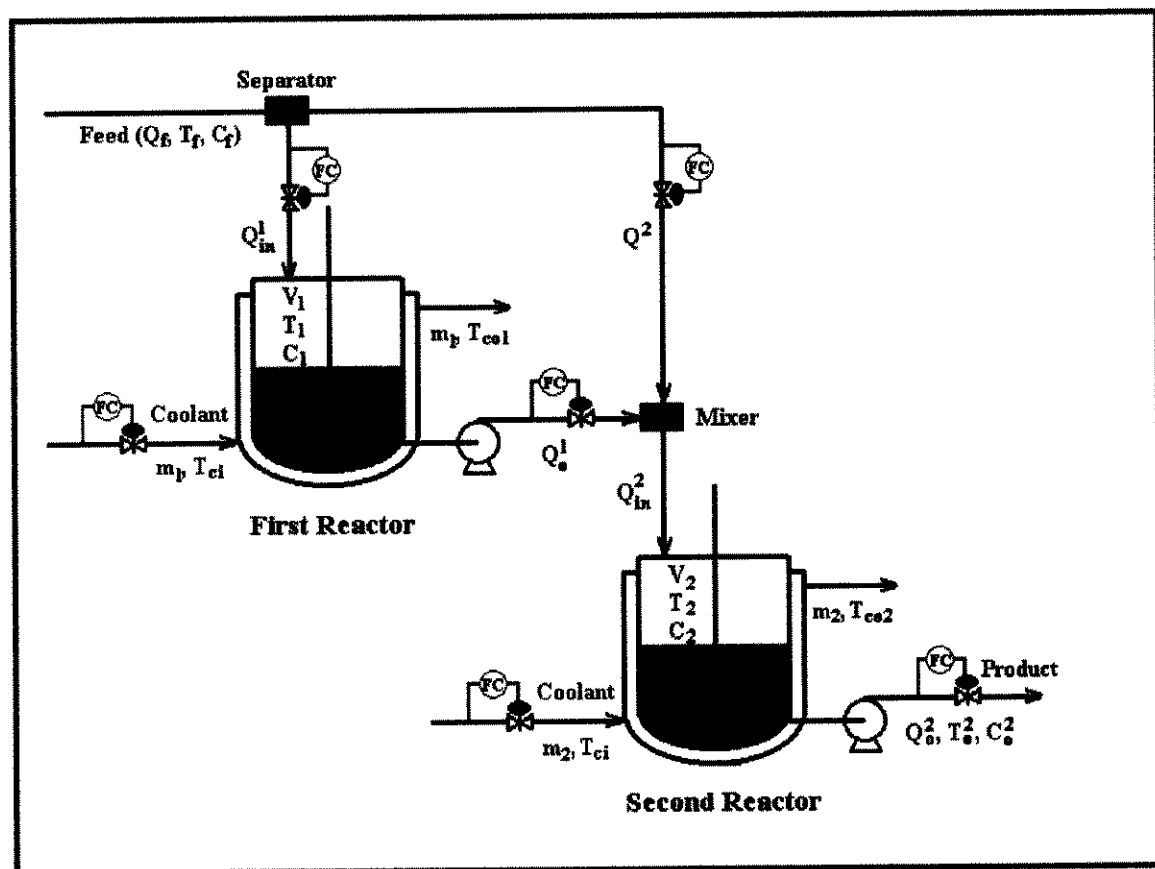


Figure 2.6 Case Study 2: Two CSTRs in Series

The net profit is selected as the objective function:

Obj (\$/time) = pv*Q_f*(C_f - C²_o) - mc* Q_f*C_f - cc₁*Cool¹ - cc₂*Cool²

The optimization problem is solved for three decision variables: feed flowrates Q¹_{in}, Q² and inventory (V = V₁ = V₂). The problem becomes complicated, although only two uncertain parameters are considered. The optimal operating conditions of the plant are:

Q¹_{in} = 0.439 l.s⁻¹
Q² = 0.220 l.s⁻¹
T_{in} = 300 K
C_{in} = 20 mol.l⁻¹
T_{ci} = 283 K
V = 354 l
m₁ = 0.70 l.s⁻¹
m₂ = 1.04 l.s⁻¹

Iteration N°	Input File	Objective Function	Uncertain Parameters	Decision Variables
L = 0 (Nominal)	EX2OL	141.4	d ⁿ = [300, 283]	u = [0.551,0.244, 273.4]
L = 1	EX2IL EX2FIN1	129.8	d ⁿ = [300, 283; 305, 286]	u = [0.440,0.295, 349.5]
L = 2	EX2IL EX2FIN2	116.2	d ⁿ = [300, 283; 305, 286; 305, 280]	u = [0.441,0.220, 309.4]
L = 3	EX2IL EX2FIN3	116.1	d ⁿ = [300, 283; 305, 286; 305, 280; 298, 280]	u = [0.439,0.220, 353.9]
Stop	Optimal solution found			

Table 2.3 Results from Case Study 2 (after four iterations)

The nominal optimal conditions found in Table 2.3 are defined by three active constraints: constraint 2.1, constraint 2.5 and constraint 2.8. The nominal problem is fully constrained, since the number of active constraints is equal to the number of decision variables. It is also shown in Table 2.3 that a larger inventory is required in the last iteration (from 309 l to 354 l). This does not affect the operating cost (profit remains at \$116), but it does have the effect on constraint 2.8. For this case study, the final OL optimization problem (EX2FIN3) must be solved for four systems of two CSTRs in series. Each system is subject to a different situation described by a corresponding row of the uncertain matrix:

$$d^n = \begin{vmatrix} T_{in} & T_{ci} \\ 300 & 283 \\ 305 & 286 \\ 305 & 280 \\ 298 & 280 \end{vmatrix}$$

The number of equality and inequality constraints is three times more than in the original optimization problem. SPEEDUP is more favorable to handle this case than MATLAB and GAMS. The KS modified algorithm also shows more efficiency than the original algorithm, since only one instead of eight optimization problems in the IL is solved.

The movement of the nominal optimal point to its back-off position is plotted against three decision variables in 3-D figures (Figures 2.7 and 2.8). The green, blue and magenta surfaces represent three active constraints: constraint 2.1 ($T_1 = 350$), constraint 2.5 ($Cool_2 = 15$) and constraint 2.8 ($C_o^2 = 0.3$), respectively. These surfaces intersect at the nominal optimal point viewed at different angles in Figure 2.7a and 2.7b. The feasible operating regions in this case study are rather space than area, bounded by three active and other constraint surfaces. Figure 2.8 plots the final positions of the active constraints and the back-off point. This point is no longer the intersection of three active constraints.

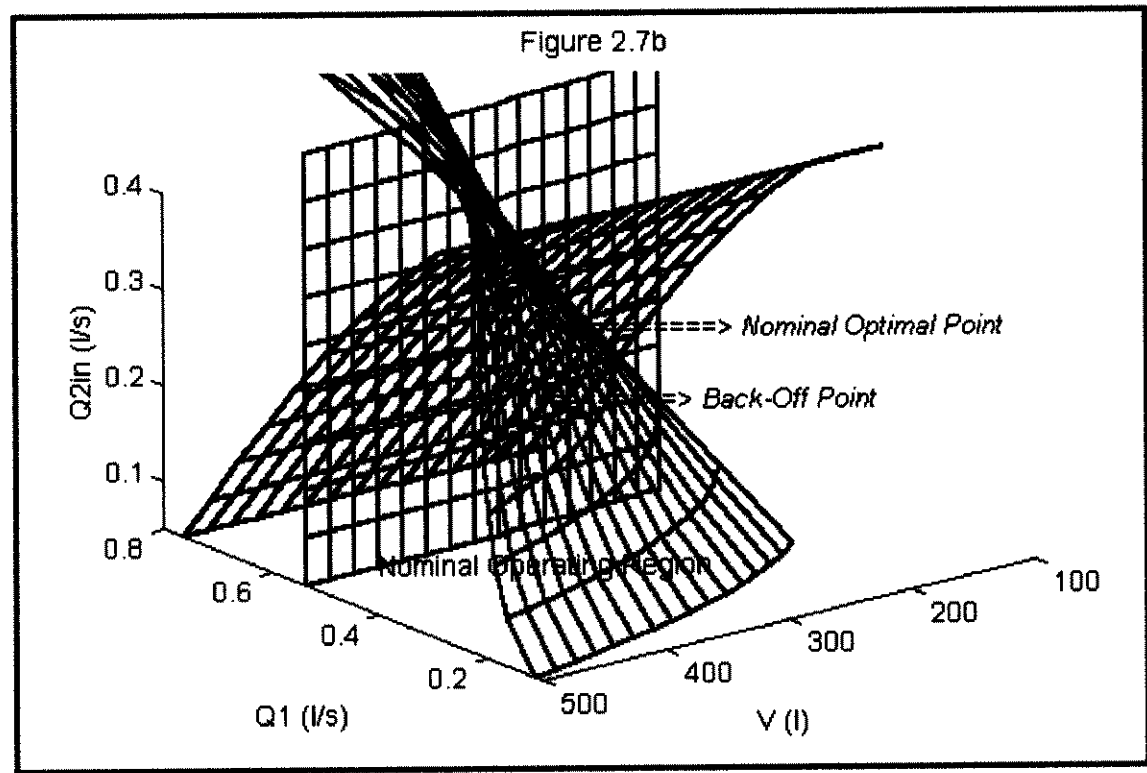
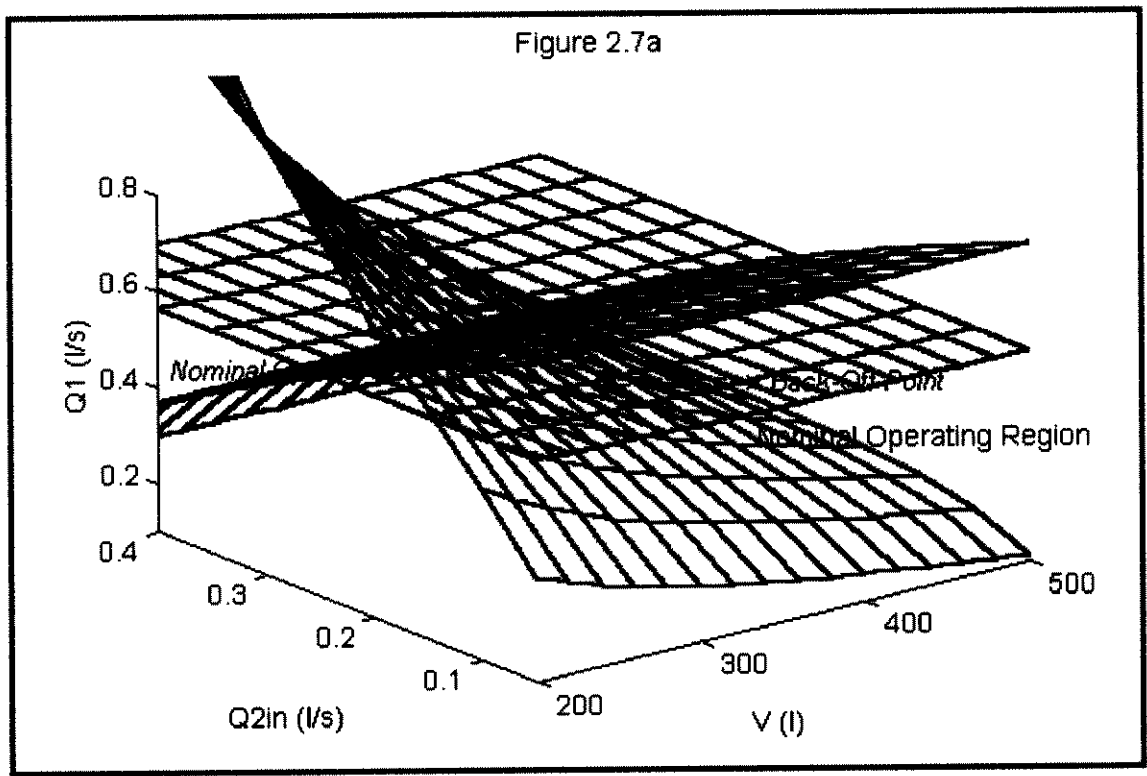


Figure 2.7 Case Study 2:

Nominal Operating Space and Nominal Optimal Point at Different Angles

(Blue surfaces: $Cool_2 = 15$)

(Green surfaces: $T_1 = 350 \text{ K}$)

(Magenta surfaces: $C^2_o = 0.3$)

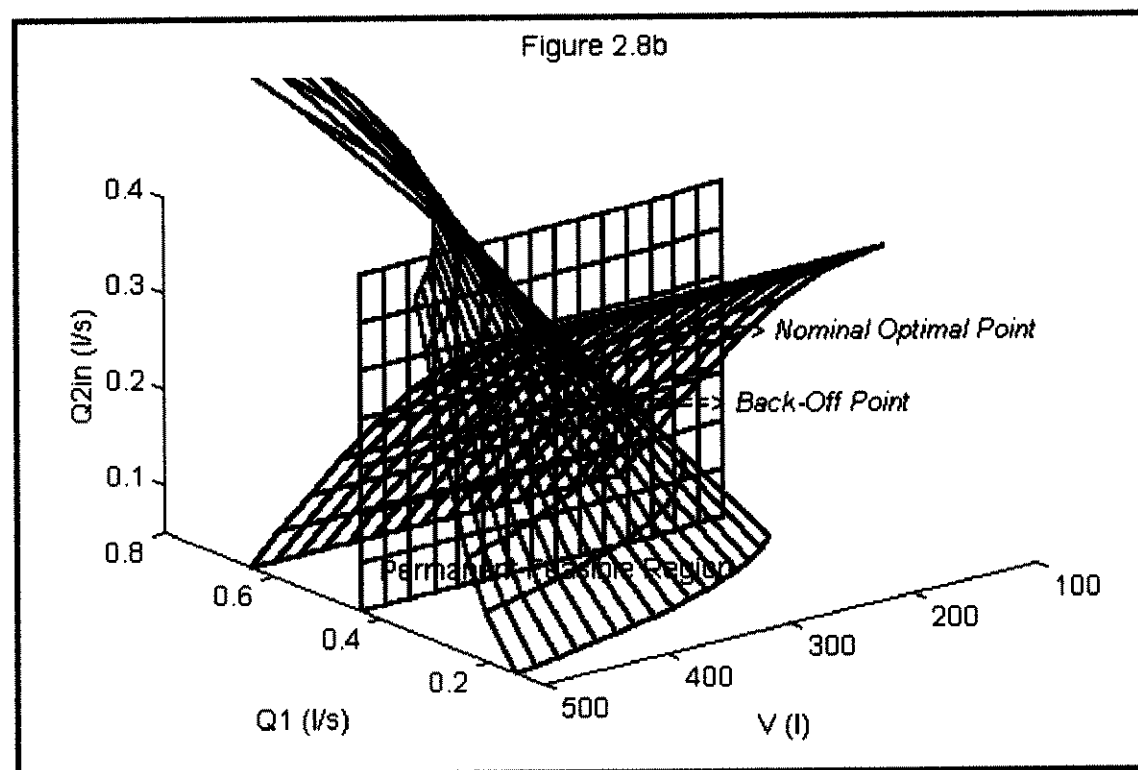
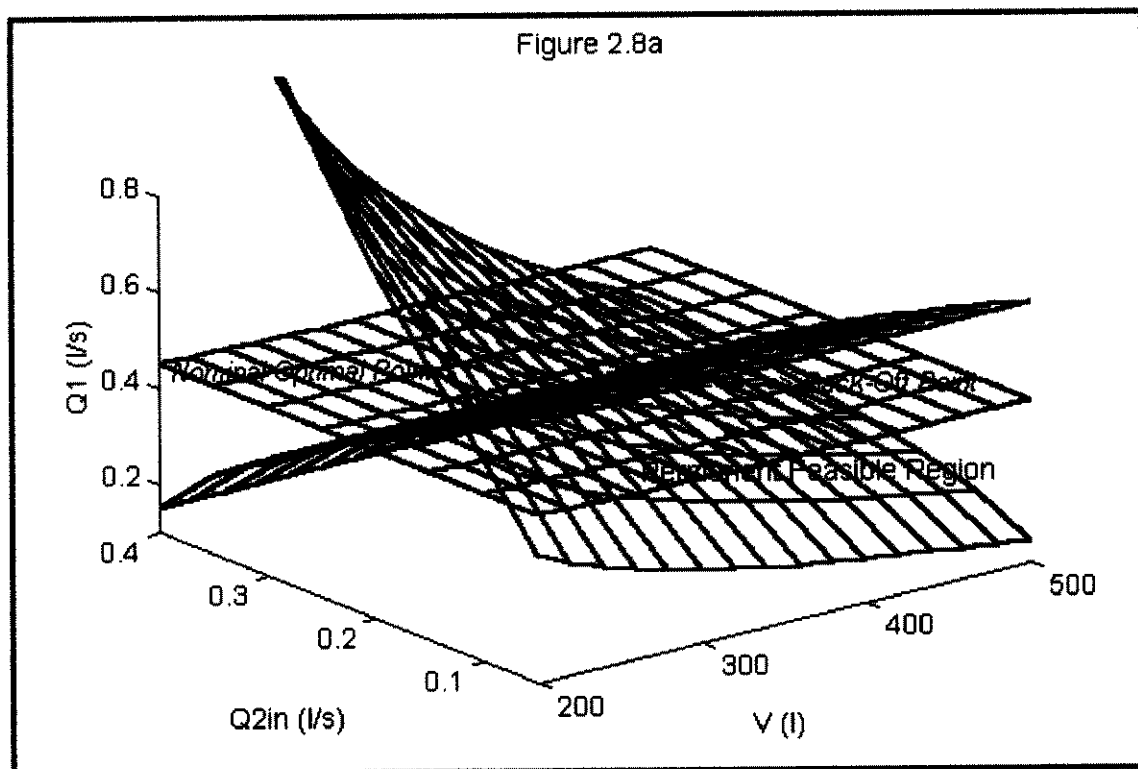


Figure 2.8 Case Study 2:

Permanent Feasible Space and Back-Off Point at Different Angles

(Blue surfaces: $Cool_2 = 15$)

(Green surfaces: $T_1 = 350$ K)

(Magenta surfaces: $C^2_o = 0.3$)

The above case studies have proved that due to uncertain parameters and disturbances, the plants have to operate at the back-off conditions instead of the nominal optimal conditions to guarantee safe operations. However, a further backing-off from the optimum means a greater loss in profit. A good control strategy may totally or partially recover this loss, and the steady state flexibility analysis can estimate the upper bound on the cost of any type of controller applied in the plant. The following section briefly discusses the flexibility analysis in the dynamic situation.

6. Dynamic Closed-Loop Back-Off Calculation

Section 5 has established a procedure to measure a loss in profit due to the effect of uncertainties for open loop plants. This section estimates the potential recovery that a control system can provide. The recovery may be perfect or nearly perfect, and the economical loss can be completely recovered. In that situation, the plant can operate at the nominal optimal condition, when the control loops are applied. However, in many cases the recovery is poor because of the imperfect control or the limitation of the process. The closed-loop back-off calculation measures the loss, when the dynamic plant is controlled. The formulation of a dynamic optimization problem for closed-loop back-off calculation is exactly the same as the formulation of a steady state open loop case, but dynamic models are used. Consequently, some of the equality constraints are ordinary differential equations (ODEs), and the involving problems are referred to as optimal control problems, which will be discussed in Chapter 3. Problem (P6) can be written as:

$$\text{Minimize (or maximize):} \quad F[x(t), u, m(t), p, cp, d^n, t]_{t=\bar{t}} \quad (P6)$$

Subject to:

$$c_i[x(t), u, m(t), p, cp, d^n, t] = 0 \quad i \in E$$

$$\max_{\theta^k \in \Gamma} \max_j g_j[x(t), u, m(t), p, cp, d^n, t] \leq 0 \quad j \in I$$

$$(dx/dt) = h[x(t), u, m(t), p, cp, d^n, t]$$

$$u^L \leq u \leq u^U$$

$$d^k \in \Gamma$$

Vector $\mathbf{m}$ represents the set of manipulated variables. Vector $\mathbf{cp}$, independent of time, is the set of controller parameters.

The six-step iterative procedure for open loop back-off calculation can be extended to consider dynamic situations.

- **Step 1** solves the steady state optimization problem (P0) for the control variables $\mathbf{u}^n$, when all elements of $\mathbf{d}^n$ are set at nominal values as in the open loop back-off calculation. Since the system is at steady state, the variables and equations related to controllers are removed.
- **Step 2** sets the iteration counter $L = 1$.
- **Step 3** solves the IL dynamic optimization problem to recognize the worst case that produces the maximum constraint violation over the time. However, the results obtained from solving the IL steady state optimization shown in section 5 can be used in the following step to save the computational time.
- **Step 4** updates $\mathbf{d}^k$ and $\mathbf{R}^k$.
- **Step 5** solves the following dynamic optimization problem and tests the feasibility of the solution with possible combinations of disturbances.

$$\text{Minimize (or maximize):} \quad \mathbf{F}[\mathbf{x}(t), \mathbf{u}, \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^n, t]_t = \bar{\tau} \quad (\text{P7})$$

Subject to:

$$\mathbf{c}_i[\mathbf{x}(t), \mathbf{u}, \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^n, t] = 0 \quad i \in E$$

$$\mathbf{g}_j[\mathbf{x}(t), \mathbf{u}, \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^n, t] \leq 0 \quad j \in I$$

$$(\mathbf{dx}/\mathbf{dt}) = \mathbf{h}[\mathbf{x}(t), \mathbf{u}, \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^n, t]$$

The objective function in (P7) is evaluated at a specific time such as $t = 0$. The decision variables may include the control variables as well as the controller parameters. If the solution is not feasible, steps 3, 4 and 5 are repeated until all constraints are satisfied. Problem (P7) also includes a set of ordinary differential equality constraints ($\mathbf{dx}/\mathbf{dt}$). Different techniques are required to solve this type of optimal control problems. Since the recovery of the profit loss (due to disturbances) greatly depends on the control strategies, different types of controllers should be examined to minimize the amount of dynamic closed-loop back off. Those jobs will be discussed through the case studies in the following chapters.

7. Conclusion

This chapter is mainly based on the works done by Bahri and Landers. The basic algorithm and its KS modified form for the open loop back-off calculation are demonstrated in a mathematical example and two case studies. The extension of the algorithm to handle the dynamic situations is also introduced in the previous section. The case studies for dynamic closed-loop back-off calculation will be discussed in the following chapters, as special techniques are required to solve the dynamic optimization problems. To implement the algorithmic approach within an optimization framework, different packages can be used giving the same result. In this chapter MATLAB and SPEEDUP are introduced first, GAMS is reserved for the dynamic cases later.

By calculating the back-off index, the iterative procedure can be used as a straightforward methodology to systematically analyze the performance of the plant, under the effect of disturbances or uncertainties and under different operating conditions. It can predict at the same time the combination of disturbances that will produce the maximum constraint violation. The extension of the algorithm to dynamic cases can be used for controllability analysis of the plant, to provide the best control scheme, together with the best structure and configuration. All these features lead to the main theme in Chapter 3, the analysis of the plant transition from one operating condition to another.

8. Nomenclature

c_i	: Set of equality constraints
cc	: Cost of cooling, $\$.(l.K)^{-1}$
C	: Concentration, $mol.l^{-1}$
$cool$	: Removal heat from the reactor to the cooling jacket, $l.K.s^{-1}$
cp	: Vector of controller parameters
C_{pc}	: Coolant heat capacity, $kJ.(kg.K)^{-1}$
d	: Vector of disturbances or uncertain parameters.
D	: Diagonal matrix
E	: Activation energy, $l.atm.mol^{-1}$
F	: Objective function or flexibility index
g_j	: Set of inequality constraints
ko	: Arrhenius constant, s^{-1}
ks	: KS function
L	: Iteration counter
m	: Coolant flowrate = $(m_c C_{pc} / \rho_r C_{pr}), l.s^{-1}$
m_c	: Coolant flowrate, $kg.mol^{-1}$
mc	: Material cost, $\$.hr^{-1}$

p	: Vector of process constants
p_v	: Product price, $\$/\text{mol}$
q	: Whole set of inequality constraints for the whole set d
Q	: Flowrate, l.s^{-1}
R	: Feasible region
R_a	: Universal gas constant, $\text{l.atm.}(\text{K.mol})^{-1}$
Rate	: Rate of reaction, mol.s^{-1}
T	: Temperature, K
u	: Vector of control (independent) variables
U_a	: Overall heat transfer coefficient/ $(\rho_r C_{pr})$, l.s^{-1}
V	: Volume, l
x	: Vector of state (dependent) variables
y	: Availability or unavailability

Greek Letters

Γ	: Disturbance region
$\Delta d^+, \Delta d^-$	: Deviation of d in the positive and negative directions, respectively
ΔH_r	: Heat of reaction, kJ.mol^{-1}
θ	: Vector of design variables
ρ	: Parameter set by users for the KS function
ρ_r	: Density, kg.l^{-1}
λ	: Lagrange multipliers for g and q
μ	: Lagrange multipliers for c
Ψ	: Operational region

Superscripts

1	: First CSTR
2	: Second CSTR
L	: Lower bound
n	: Nominal value
U	: Upper bound
*	: Optimal solution

Subscripts

c	: Coolant
f	: Feed

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Appendix 2A: MATLAB Input Files

A sample of MATLAB files illustrates how the iterative algorithm for open loop back-off calculation works. The following m-file “band.m” automatically calls other files to solve the OL and the IL optimization problems.

band.m

```
% first iteration for nominal case
band1
% algorithm starts
for i = 1 :6
    if i <= 6
        band2
        band3
    end
end
end
```

File “band1.m” solves the OL optimization problem for the nominal case. The feasibility test is also included in this file, although it is not necessary to check the feasibility of the solutions at this stage.

band1.m

```
clear
% initial guess
u0 = [0.9, 1.1];
options = [];
vlb = [0, 0];
vub = [2.0, 2.0];
u = constr('fun1',u0,options,vlb,vub);
[f,g] = fun1(u)
save bd1 u
% feasibility test
d1=[1, 1.5];d2=[0.5, 0.5];d3=[0.5, 2.5];d4=[2.5, 2.5];d5=[2.5, 0.5];
d6=[1, 0.5];d7=[1, 2.5];d8=[0.5, 1.5];d9=[2.5, 1.5];
dd=[d1 d2 d3 d4 d5 d6 d7 d8 d9];
sd=size(dd);
m=sd(2)
for i = 1: 2: m
    x(i)=(-4*dd(i)^2+3*dd(i+1)^2+3.25)*u(1) + (dd(i)+2*dd(i+1)-1.75)*u(2);
    x(i+1)=(dd(i+1)-6)*u(1) + (-3*dd(i)^2+4*dd(i+1)^2+4*dd(i)*dd(i+1)...
        -dd(i) 1.0)*u(2);
    g(i)=x(i) - 3*dd(i) - dd(i+1) - 5.5;    % constraints
    g(i+1)=x(i+1) - 10;                    %constraints
end
gmax=max(g);
```

```

if gmax <= 1e-6
load bd
d
u
display('program terminates')
pause
bdpl
pause
quit
end

```

When the program terminates, file “bdpl.m” is called to plot the feasible regions. The algorithm starts with the IL optimization problem in file “band2.m” and the OL problem in file “band3.m”:

band2.m

```

%initial guess
d0 = [0.9, 1.1];
options = [];
vlb = [0.5, 0.5]; vub = [2.5, 2.5];
d = constr('cst1',d0,options,vlb,vub);
d1 = d;
[g1,const] = cst1(d)
d0 = [0.9, 1.1];
options = [];
vlb = [0.5, 0.5];
vub = [2.5, 2.5];
d = constr('cst2',d0,options,vlb,vub);
d2 = d;
[g2,const] = cst2(d);
if g2<=g1
    dis = d2;
else
    dis = d1;
end
load bd
d = [d dis];
save bd d

```

band3.m

```

clear
% initial guess
u0 = [0.9, 1.1];
options = [];
vlb = [0, 0];
vub = [2.0, 2.0];

```

```

u = constr('fun2',u0,options,vlb,vub);
[f,g] = fun2(u);
save bdl u
% feasibility test
d1=[1, 1.5];d2=[0.5, 0.5];d3=[0.5, 2.5];d4=[2.5, 2.5];d5=[2.5, 0.5];
d6=[1, 0.5];d7=[1, 2.5];d8=[0.5, 1.5];d9=[2.5, 1.5];
dd=[d1 d2 d3 d4 d5 d6 d7 d8 d9];
sd=size(dd);
m=sd(2)
for i = 1: 2 :m
x(i)=(-4*dd(i)^2+3*dd(i+1)^2+3.25)*u(1) + (dd(i)+2*dd(i+1)-1.75)*u(2);
x(i+1)=(dd(i+1)-6)*u(1) + (-3*dd(i)^2+4*dd(i+1)^2+4*dd(i)*dd(i+1)...
-dd(i)-1.0)*u(2);
g(i)=x(i) - 3*dd(i) - dd(i+1) - 5.5;    % constraints
g(i+1)=x(i+1) - 10;                    % constraints
end
gmax=max(g);
if gmax <= 1e-6
load bd
d
u
display('program terminates')
pause
bdpl
pause
quit
end

```

The file “band2.m” optimizes two functions in “cst1.m” and “cst2.m”. The file “band3.m” optimizes a function in “fun2.m”.

cst1.m

```

function [g1,const] = cst1(d)
load bdl
x(1) = (-4*d(1)^2+3*d(2)^2+3.25)*u(1) + (d(1)+2*d(2)-1.75)*u(2);
g1=-x(1) + 3*d(1) + d(2) + 5.5;
%constraint
const(1)=0.5-d(1);
const(2)=d(1)-2.5;

```

fun2.m

```

function [f,g] = fun2(u)
f = -u(1) - 3*u(2);
load bd
s=size(d);
n=s(2);
for i=1: 2: n
x(i) = (-4*d(i)^2+3*d(i+1)^2+3.25)*u(1) + (d(i)+2*d(i+1)-1.75)*u(2);
x(i+1) = (d(i+1)-6)*u(1) + (-3*d(i)^2+4*d(i+1)^2+4*d(i)*d(i+1)...

```

```

-d(i)-1.0)*u(2);
g(i)= x(i) - 3*d(i) - d(i+1) - 5.5; % constraints
g(i+1)= x(i+1) - 10;
end

```

The KS modified algorithm calls the file “bks1.m” to optimize a function in “bks.m” instead of two functions in “cst1.m” and “cst2.m”.

bks.m

```

function [ks,const] = bks(d)
load bd1 % value of u
x(1) = (-4*d(1)^2+3*d(2)^2+3.25)*u(1) + (d(1)+2*d(2)-1.75)*u(2);
x(2) = (d(2)-6)*u(1) + (-3*d(1)^2+4*d(2)^2+4*d(1)*d(2)-d(1)-1.0)*u(2);
g(1)=x(1) - 3*d(1) - d(2) - 5.5;
g(2)= x(2) - 10;
rho = 2;
ks=-(1/rho)*log(exp(rho*g(1)) + exp(rho*g(2)));
%constraint
const(1)=0.5-d(1);
const(2)=d(1)-2.5;
const(3)=0.5-d(2);
const(4)=d(2)-2.5;

```

Appendix 2B: SPEEDUP Input Files

A sample of SPEEDUP input file shows that only one set of equality constraints is required for four systems of two CSTRs.

EX2FIN3.SPE

```

MODEL      CSTR
      TYPE
      TEMP, TC, TCI, T_IN, T_OUT      AS      TEMPERATURE
      FLOW_IN, FLOW_OUT                AS      FLOWRATE
      C_IN, C_OUT, C                   AS      CONCENTRATION
      V                                 AS      VOLUME
      RATE                             AS      RATE
      COOL                             AS      HEAT
      Ua, E, K0, DH, M                 AS      PARAMETER

      STREAM
      INPUT      T_IN, FLOW_IN, C_IN
      OUTPUT     T_OUT, FLOW_OUT, C_OUT

```

EQUATION

```

#      CALCULATION OF PARAMETERS
      COOL=Ua*(TEMP-TC);
      COOL=M*(TC-TCI);
      RATE=K0*EXP(-E/TEMP)*C*V;

#      OVERALL MATERIAL BALANCE
      0=FLOW_IN - FLOW_OUT;

#      COMPONENT MATERIAL BALANCE
      $C=(-RATE+FLOW_IN*C_IN-FLOW_OUT*C_OUT)/V;

#      PERFECT MIXING
      C=C_OUT;

#      ENERGY BALANCE
      $TEMP=(DH*RATE+FLOW_IN*T_IN-FLOW_OUT*T_OUT-COOL)/V;

#      PERFECT MIXING
      TEMP=T_OUT;
****
MODEL      MIXER
      TYPE
      T_IN_1,T_IN_2,T_OUT      AS      TEMPERATURE
      FLOW_IN_1,FLOW_IN_2,FLOW_OUT      AS      FLOWRATE
      C_IN_1,C_IN_2,C_OUT      AS      CONCENTRATION
      STREAM
      INPUT      1      T_IN_1,FLOW_IN_1,C_IN_1
      INPUT      2      T_IN_2,FLOW_IN_2,C_IN_2
      OUTPUT      T_OUT,FLOW_OUT,C_OUT

EQUATION
#      OVERALL MATERIAL BALANCE
      FLOW_OUT=FLOW_IN_1+FLOW_IN_2;

#      COMPONENT MATERIAL BALANCE
      FLOW_OUT*C_OUT=FLOW_IN_1*C_IN_1+FLOW_IN_2*C_IN_2;

#      ENERGY BALANCE
      FLOW_OUT*T_OUT=FLOW_IN_1*T_IN_1+FLOW_IN_2*T_IN_2;

****
MODEL      MIXR
      TYPE
      T_IN_1,T_IN_2,T_IN_3,T_IN_4,T_OUT      AS      TEMPERATURE
      FLOW_IN_1,FLOW_IN_2,FLOW_IN_3      AS      FLOWRATE
      FLOW_IN_4,FLOW_OUT      AS      FLOWRATE
      C_IN_1,C_IN_2,C_IN_3,C_IN_4,C_OUT      AS      CONCENTRATION
      STREAM
      INPUT      1      T_IN_1,FLOW_IN_1,C_IN_1
      INPUT      2      T_IN_2,FLOW_IN_2,C_IN_2
      INPUT      3      T_IN_3,FLOW_IN_3,C_IN_3
      INPUT      4      T_IN_4,FLOW_IN_4,C_IN_4

```

OUTPUT

T_OUT, FLOW_OUT, C_OUT

EQUATION

OVERALL MATERIAL BALANCE

 $FLOW_OUT = FLOW_IN_1 + FLOW_IN_2 + FLOW_IN_3 + FLOW_IN_4;$

COMPONENT MATERIAL BALANCE

 $FLOW_OUT * C_OUT = FLOW_IN_1 * C_IN_1 + FLOW_IN_2 * C_IN_2 +$
 $FLOW_IN_3 * C_IN_3 + FLOW_IN_4 * C_IN_4;$

ENERGY BALANCE

 $FLOW_OUT * T_OUT = FLOW_IN_1 * T_IN_1 + FLOW_IN_2 * T_IN_2 +$
 $FLOW_IN_3 * T_IN_3 + FLOW_IN_4 * T_IN_4;$

MODEL SPLITTER

TYPE

T_IN, T_OUT_1, T_OUT_2 AS TEMPERATURE

FLOW_IN, FLOW_OUT_1, FLOW_OUT_2 AS FLOWRATE

C_IN, C_OUT_1, C_OUT_2 AS CONCENTRATION

STREAM

INPUT T_IN, FLOW_IN, C_IN

OUTPUT 1 T_OUT_1, FLOW_OUT_1, C_OUT_1

OUTPUT 2 T_OUT_2, FLOW_OUT_2, C_OUT_2

EQUATION

 $T_IN = T_OUT_1;$ $T_IN * FLOW_IN = T_OUT_1 * FLOW_OUT_1 + T_OUT_2 * FLOW_OUT_2;$ $C_IN = C_OUT_1;$ $C_IN * FLOW_IN = C_OUT_1 * FLOW_OUT_1 + C_OUT_2 * FLOW_OUT_2;$ $FLOW_IN = FLOW_OUT_1 + FLOW_OUT_2;$

FLOWSHEET

STREAM SP1 INPUT OF SPLIT1 IS FEED 1

STREAM SP2 INPUT OF SPLIT2 IS FEED 2

STREAM SP3 INPUT OF SPLIT3 IS FEED 3

STREAM SP4 INPUT OF SPLIT4 IS FEED 4

STREAM MIXED5 OUTPUT OF MIX5 IS PRODUC

STREAM SPLIT1 OUTPUT 1 OF SPLIT1 IS INPUT OF CS1

STREAM SPLIT2 OUTPUT 2 OF SPLIT1 IS INPUT 1 OF MIX1

STREAM REAC1 OUTPUT OF CS1 IS INPUT 2 OF MIX1

STREAM SPLIT3 OUTPUT 1 OF SPLIT2 IS INPUT OF CS3

STREAM SPLIT4 OUTPUT 2 OF SPLIT2 IS INPUT 1 OF MIX2

STREAM REAC3 OUTPUT OF CS3 IS INPUT 2 OF MIX2

STREAM SPLIT5 OUTPUT 1 OF SPLIT3 IS INPUT OF CS5

STREAM SPLIT6 OUTPUT 2 OF SPLIT3 IS INPUT 1 OF MIX3

STREAM REAC5 OUTPUT OF CS5 IS INPUT 2 OF MIX3

STREAM SPLIT7 OUTPUT 1 OF SPLIT4 IS INPUT OF CS7

STREAM	SPLIT8	OUTPUT 2	OF	SPLIT4	IS	INPUT 1 OF MIX4
STREAM	REAC7	OUTPUT	OF	CS7	IS	INPUT 2 OF MIX4
STREAM	MIXED1	OUTPUT	OF	MIX1	IS	INPUT OF CS2
STREAM	MIXED2	OUTPUT	OF	MIX2	IS	INPUT OF CS4
STREAM	MIXED3	OUTPU	OF	MIX3	IS	INPUT OF CS6
STREAM	MIXED4	OUTPUT	OF	MIX4	IS	INPUT OF CS8
STREAM	REAC2	OUTPUT	OF	CS2	IS	INPUT 1 OF MIX5
STREAM	REAC4	OUTPUT	OF	CS4	IS	INPUT 2 OF MIX5
STREAM	REAC6	OUTPUT	OF	CS6	IS	INPUT 3 OF MIX5
STREAM	REAC8	OUTPUT	OF	CS8	IS	INPUT 4 OF MIX5

UNIT	CS1	IS	A	CSTR		

UNIT	CS2	IS	A	CSTR		

UNIT	CS3	IS	A	CSTR		

UNIT	CS4	IS	A	CSTR		

UNIT	CS5	IS	A	CSTR		

UNIT	CS6	IS	A	CSTR		

UNIT	CS7	IS	A	CSTR		

UNIT	CS8	IS	A	CSTR		

UNIT	MIX1	IS	A	MIXER		

UNIT	MIX2	IS	A	MIXER		

UNIT	MIX3	IS	A	MIXER		

UNIT	MIX4	IS	A	MIXER		

UNIT	MIX5	IS	A	MIXR		

UNIT	SPLIT1	IS	A	SPLITTER		

UNIT	SPLIT2	IS	A	SPLITTER		

UNIT	SPLIT3	IS	A	SPLITTER		

UNIT	SPLIT4	IS	A	SPLITTER		

Chapter 3

Switchability and Operability Assessment in Chemical Processes

1	Introduction	3.1
2	Switchability analysis	3.2
2.1	Process constraints and nonlinear feature.....	3.2
2.2	Model time delays, uncertainties and disturbances.....	3.3
3	Switchability formulation	3.4
4	Solution methods for switchability problems	3.5
4.1	Sequential optimization.....	3.6
4.2	Simultaneous optimization and integration.....	3.8
5	Problem formulation	3.8
5.1	Problem formulation using sequential technique.....	3.11
5.2	Problem formulation using simultaneous technique.....	3.13
5.2.1	Global orthogonal collocation.....	3.14
5.2.2	Orthogonal collocation on finite elements.....	3.17
6	Case studies	3.21
6.1	Case study 1: a single CSTR.....	3.21
6.1.1	Dynamic closed-loop back-off problem.....	3.25
6.1.2	Switchability problem.....	3.29
6.1.3	Testing the feasibility of the solutions.....	3.40
6.2	Case study 2: two CSTRs in series	3.46
6.2.1	Dynamic closed-loop back-off problem.....	3.48

6.2.2	Switchability problem.....	3.49
6.2.3	Testing the feasibility of the solutions.....	3.57
6.2.4	Switching from startup operating conditions.....	3.60
7	Conclusion.....	3.63
8	Nomenclature.....	3.66
9	References.....	3.67
	Appendix 3A.....	3.69

The concept of flexibility and the quantitative analysis of this property in a given system have been reviewed in Chapter 2. Flexibility study is concerned with the ability of a plant to operate within a range of conditions. To ensure a feasible operation under disturbances, a new strategy is introduced to calculate the steady state open loop back-off from nominal optimum. This strategy can be expanded to consider dynamic cases, when the dynamic plant is controlled. Chapter 3 studies the ability of a chemical plant to switch safely and optimally from one operating condition to another. A formulation for simultaneous operability and switchability is proposed, leading to an uncertain dynamic nonlinear programming (NLP) problem. Two different approaches can be used to solve the NLP problem. Due to possible disturbances entering the plant during the transition, closed-loop back-off from nominal trajectories of control variables should also be considered. The effectiveness of the proposed strategy is tested through two case studies. Different optimization problems generated in this chapter are solved using the software packages SPEEDUP and GAMS with MINOS 5.2 optimizer.

1. Introduction

A process system should be designed so that it has the ability to respond to changeovers in downstream demands, product specifications, feed stock and the environment regulations in an optimal and safe manner. During normal operations, the supervisory and regulatory layers of the control system are responsible for the feasible moving between different operating conditions caused by those changeovers. However, conventional controllers do not always satisfy constraints and interactions within a complex plant, neither can they automatically give sufficient control range for an efficient switch. This leads to the switchability problem in a chemical plant. A thorough review of previous works specifically on switchability problems will be presented in section 4.

In order to cope with all likely disturbances throughout a switch, the switchability problem is simultaneously formulated with the flexibility and controllability problems. The integrated strategy reviewed in Chapter 2 for operability analysis has been used as the starting platform, which results in economically desirable steady state conditions at the beginning and the end of the transition. To ensure a safe and feasible changeover, path constraints are efficiently dealt with by placing bounds on

interior points. Minimizing the integral squared deviation of the state and control variables drives them to their new target values in a short period of time.

A framework within the optimization environment is proposed, introducing an uncertain dynamic NLP problem that can be solved by existing techniques. The aims of this chapter are:

- To formulate the simultaneous operability and switchability problem.
- To solve the dynamic NLP problems in two case studies using different techniques and test the numerical results against plant simulations.
- To study the effect of problem formulation on optimal solutions.

Three main features of the operability analysis namely flexibility, controllability and switchability are the attributes of the above problem. Chapter 2 is concerned with the flexibility analysis. The following section presents the relationship between controllability and switchability.

2. Switchability Analysis

As defined in Chapter 1, controllability represents the ability of a plant to move fast and smoothly from one operating condition to another and deal effectively with disturbances. Therefore, switchability is only a part of controllability, which describes how readily a process is able to switch between different operating states. The other part of controllability deals with possible disturbances and uncertainties during the transition. The range of disturbances must be small enough for the linear assumption to hold if the classical control theory is used. Switchability can take into account:

- Process limitations under the form of path constraints.
- Nonlinear response and control constraints.
- Time delays, model uncertainties and deterministic disturbances.

2.1. Process Constraints and Nonlinear Feature

A switching problem normally deals with three types of constraints:

- Inequality constraints representing process and production limitations, safety restrictions and physical property specifications. These constraints are bounded by minimum and maximum values and put under the form of path constraints.
- Equality constraints representing initial and final values of the state variables. They are set in single starting and end time constraints. The final end time constraints are naturally dealt with by extending the changeover period long enough for the system to reach the final steady state.
- Inequality constraints set to avoid abrupt changes that a unit cannot handle. These changes commonly occur in a switching problem. For example, constraints on the first derivative of the inputs are set to monitor how quickly a valve would open or close. They are dealt with by augmenting the states of the system with these inputs and letting their derivatives become new input variables.

Since the switchability problem is also formulated for a closed-loop system, constraints representing the restriction of control actions by physical and safety factors should be considered.

Switchability analysis employs the solution method based on nonlinear models. To maintain this special feature in the problem formulation, although a linear control system is used, simulations are performed using nonlinear dynamic process models instead of linearized models. This would result in larger problems to be solved and consequently longer computational time. However, at this stage the switchability problem is solved off-line and computational time is not a main issue.

2.2. Model Time Delays, Uncertainties and Deterministic Disturbances

Time delays are very common in chemical processes. Process delays generally deteriorate dynamic performances, since controllers cannot react immediately to disturbances. In a switching problem, state delays can be included in model equations as shown later.

The mechanism of disturbance effect on a process is often known in the chemical engineering field (Morari, 1980). The region of variation for deterministic disturbances and uncertainties is defined in Chapter 2 as: $\Gamma = \{\mathbf{d}: \mathbf{d}^L \leq \mathbf{d} \leq \mathbf{d}^U\}$. A step change in time domain is commonly encountered and disturbances to be rejected are

modeled as step changes of magnitude $\Delta d = d^U - d^n$ or $\Delta d = d^n - d^L$. Carvalho (1989) defined the occurrence of a single step change in a process as an event. He classified the problem types into three categories:

- Class I assumes that the possibility for more than two events simultaneously occur is very low. The process can completely reject a disturbance before facing a new one.
- Class II assumes that multiple events can simultaneously occur, and they can be completely rejected before a new event occurs.
- Class III allows a second event to occur θ time units after the first and before the process can completely reject the first event.

To formulate the switchability problem for a closed-loop process, only the first two classes are considered.

Switchability and controllability, however, are difficult to define quantitatively. The analysis is dependent on the specific problem under investigation.

3. Switchability Formulation

Switchability covers all problems involving changeover policies, startup and shutdown operations. These problems belong to an important dynamic optimization group referred to as optimal control problems in which some of the equality constraints are ordinary differential equations (ODEs). The original problem (P0) in Chapter 2 can be written as:

$$\text{Minimize:} \quad F[x(t), u(t), m(t), p, cp, d^n, t, t_f] \quad (S0)$$

Subject to:

$$(dx/dt) = f[x(t), u(t), m(t), p, cp, d^n, t, t_f] \quad x_0 = x(0)$$

$$c_i[x(t), u(t), m(t), p, cp, d^n, t, t_f] = 0 \quad i \in E$$

$$g_j[x(t), u(t), m(t), p, cp, d^n, t, t_f] \leq 0 \quad j \in I$$

$$u^L \leq u(t) \leq u^U$$

The integral quadratic objective function is commonly selected for the switching problem because of its simplicity and effectiveness. Minimizing the integral squared deviation of the state and control variables will drive them to the new target in a short period of time. The objective function becomes:

$$F = \int_0^{t_f} [w_1 (x - x_f)^2 + w_2 (u - u_{sf})^2] dt \quad (3.1)$$

Vector w_i represents the weighting factors. The subscript “sf” denotes the value at the final or second steady state.

S0 is an optimal control problem, which can be solved by some sophisticated mathematical methods. The theory of optimal control has been significantly developed since the 1950s. Different techniques were used to solve chemical engineering problems in reactor design, batch process operation, process startup, changeover policy, etc. It was not an easy task to find the optimal control policy particularly for a nonlinear system. Therefore, instead of solving the dynamic optimization problems directly, many authors have proposed a number of approximate methods. Solution methods with a review of previous works specifically on switchability problems are presented in the following section.

4. Solution Methods for Switchability Problems

One of the first approaches in the 1960s was using properties of the linear quadratic problem to approximate the optimal control of general nonlinear systems. Equation (3.2) was written in the form of equation (3.2a).

$$\frac{dx}{dt} = f(x, u, t) \quad x_0 = x(0) \quad (3.2)$$

$$\frac{dx}{dt} = A(x, t)x + B(x, t)u \quad (3.2a)$$

The linear quadratic problem was solved at different values of x . The method was applied to the control of a gas absorber by Lesser and Lapidus (1966). The effect of bounding the controls from one or both sides was also illustrated, but it required a large computer storage capacity just to solve a linear programming problem. With the development of “minicomputers” in the beginning of 1970s, using a smaller computer, Jarvis and Wright (1972) applied this method to the same liquid-liquid extraction process done by Pang (1970) in a larger digital computer. However, in a CSTR startup example, Hicks and Ray (1971) found that the control variable parameterization methods were better than the approximate control policies. The techniques for parameterization of the state variables were superior in many respects to other techniques. Until the decade of fast development of optimization techniques and software packages, Biegler (1984) proposed a completely different strategy for optimization of a dynamic system. This method will be described later.

Generally, the solution methods can be classified into two categories: sequential optimization approach and simultaneous optimization and integration approach.

4.1. Sequential Optimization

The first category is referred to as sequential optimization and solution strategies, since the ODEs are integrated to completion at each iteration. Because of this fact, most of the computational time is spent on the integration of system equations that provides gradient information. The classical method, Control Vector Iteration (CVI), requires the maximum of the Halmiltonian with respect to the control variable. The control profile is discretized. An initial guess of the control profile is given, the algorithm integrates the state and the adjoint equations, and the control profile is then updated. In another more straightforward method, namely Control Vector Parameterization (CVP), some functional forms in terms of time are used to approximate the control profiles. A set of coefficients is guessed. The algorithm is iterated until the optimal set of coefficients is found. This approach was well illustrated in the startup CSTR problem (Hicks and Ray). Path constraints, however, were not mentioned in this example.

Sargent and Sulivent (1977) described the method of discretizing and approximating the control profile by piecewise continuous basis functions, but it still

required the integration of the adjoint equations. The authors used the optimal control package OPCON (Sargent and Sulivent, 1979) to solve the problem of feed changeover policies for refinery distillation units. The objective function was minimizing a measure of off-specification product. Path constraints in this case were converted to the type of constraints bounded by minimum and maximum values. The optimal switching location was proved to occur when the key component was at the midpoint of the two target specifications.

To handle a large model containing over one hundred equations in some cases, Howell (1984) used the optimal control package SPEEVOP. This package was a combination of the flowsheeting package SPEEDUP and the minimization program VFO2AD. The author attempted to find the optimal control policy directly by using a set of piecewise constant (discrete) values to approximate the control action of a heat exchanger network. The objective index included:

- a term to represent the direct cost of the control action,
- a term to account for the off-specification product, and
- a term to represent the final state error when the switching action is complete.

However, it was shown that the solution found by SPEEVOP did not represent the optimal control policy using continuous controls. Within each control interval, the outlet temperature started at one degree higher than the target, and linearly fell down to one degree below it by the end. This resulted in a saw-tooth path response of the outlet temperature. Howell decided to use SPEEVOP to find the optimal set point response for the closed loop system. The proportional plus integral controllers were tuned using Cohen and Coon method. The control action was determined explicitly by the difference between the actual and target temperatures.

McAuley and MacGregor (1992) considered the addition of a quadratic penalty function to the original objective function. They solved the optimal grade transition problem by approximating the control variable profiles as a series of ramps. The end-points of the ramps were the decision variables chosen by the optimizer MINOS 5.1.

Recently, White et al. (1996) have analyzed the switchability of two different processes: a cryogenic air separation and a binary distillation column. The authors did

not provide much information on solution techniques except that the control action was approximated by a linear profile in each interval of time and was continuous.

4.2. Simultaneous Optimization and Integration

To avoid solving the system of ODEs, the simultaneous optimization and integration approach is introduced. In this technique, state and sometimes control variables are replaced by approximating functions. These functions can be easily differentiated and substituted in the set of differential equations to convert it to a set of algebraic equations. Thus the approximated problem now becomes a NLP problem and can be solved by any optimization technique. Biegler proposed this method first in 1984 to solve a batch reactor problem, quite similar to a switching problem. He applied a very popular approximating technique, the so-called Orthogonal Collocation (OC) approach, to the system of ODEs. Later, Renfro et al. (1987) generalized the method by using Global Spline Collocation. This allows the solution of much stiffer systems of equations and boundary value problems. They solved the CSTR startup problem of Hicks and Ray again and got the same solution in only 5.6 seconds CPU time. As another remedy for problems having stiff and discontinuous solutions, the Orthogonal Collocation on Finite Elements (OCOFE) can be used to replace the OC approach (Biegler, 1991). The following sections present more details on OCOFE.

The simultaneous optimization and integration approach provides a promising research area for the future. However, up to the present not many of its applications have been found in solving switching problems. The main disadvantage is that it cannot be used for large and complicated problems. Whereas the sequential optimization is more practical for engineering applications though it requires much greater computational time. Table 3.1 compares the advantages and disadvantages of the techniques. The use of simultaneous approach for closed loop systems is one of the main aims of this thesis but other solution methods are also discussed.

5. Problem Formulations

The novelty of this chapter is that the switchability concept will be expanded and incorporated with the operability analysis. To formulate these problems simultaneously, the scheme on page 3.10 is pursued.

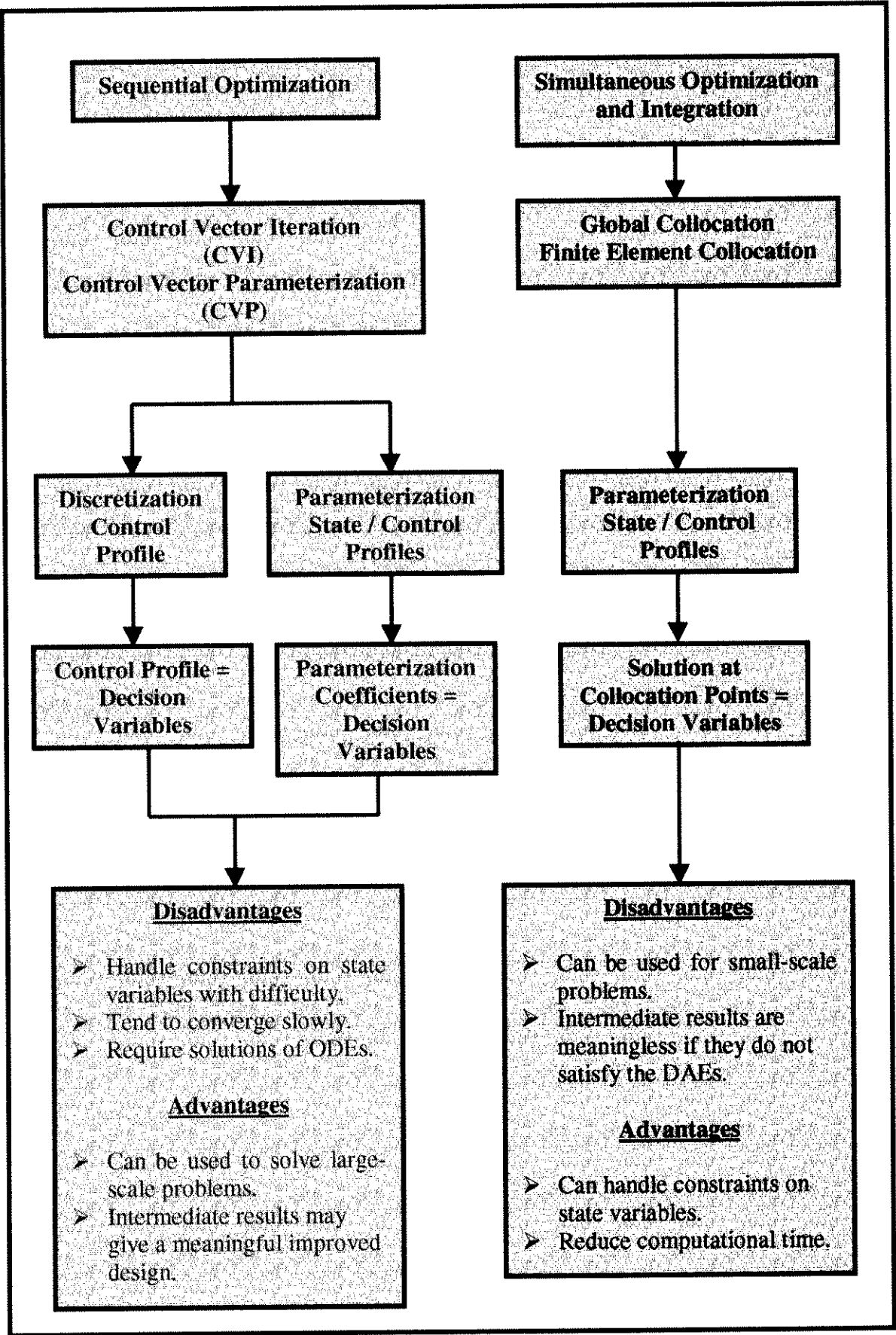


Table 3.1 Two Common Approaches to Solve a Switching Problem

- The first step determines the operating conditions at the beginning and the end of a switch. They are nominal optimal states under specified conditions and are solutions of steady state optimization problems. Due to possible disturbances, uncertainties and imperfect control systems, the plant has to operate at the back-off conditions from nominal states. These solutions are obtained from solving the open loop or dynamic closed-loop back-off problems, if the dynamic plant is controlled (see Chapter 2).
- The second step involves optimal trajectories connecting the states found in the first step. These trajectories are solutions of problem (S0). Following the optimal control profile does not guarantee no path constraint violations, if disturbances enter the process during a transition. The back-off trajectory should be obtained from solving problem (S1), if the disturbance belongs to the single event class or (S2), if the disturbance belongs to the multiple event class. Problems (S1) and (S2) are similar to (S0) but the matrix of uncertain parameter is different. The set $\mathbf{d}^k$ has only one element in problem (S1) but more than one element in problem (S2).

$$\text{Minimize:} \quad F[\mathbf{x}(t), \mathbf{u}(t), \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^k, t, t_f] \quad (\text{S0})$$

Subject to:

$$(\mathbf{dx}/dt) = \mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^k, t, t_f] \quad \mathbf{x}_0 = \mathbf{x}(0)$$

$$\mathbf{c}_i[\mathbf{x}(t), \mathbf{u}(t), \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^k, t, t_f] = 0 \quad i \in E$$

$$\mathbf{g}_j[\mathbf{x}(t), \mathbf{u}(t), \mathbf{m}(t), \mathbf{p}, \mathbf{cp}, \mathbf{d}^k, t, t_f] \leq 0 \quad j \in I$$

$$\mathbf{u}^L \leq \mathbf{u}(t) \leq \mathbf{u}^U$$

In this case the objective function becomes:

$$F = \int_0^{t_f} [w_1(\mathbf{x} - \mathbf{x}_f)^2 + w_2(\mathbf{u} - \mathbf{u}_{sf})^2] dt$$

For problem (S1):

$$\mathbf{d}^k = [\mathbf{d}]$$

For problem (S2):

$$\mathbf{d}^k = [\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_n]$$

- The final step tests the feasibility of solutions found in the second step. The optimal control profiles are applied to the system with possible combinations of

disturbances. If there is any constraint violation, matrix $\mathbf{d}^k$ is updated, and the second step is repeated as shown in Chapter 2.

The types of problems to be solved and solutions generated in the above scheme are shown in Figure 3.1. Similar dynamic optimization problems (P7 or S0) are solved for a dynamic closed-loop back-off condition or an optimal control trajectory. The only difference is in the objective function. For the first case, the object is commonly a cost or a profit index, evaluated at a specific time such as at the beginning or by the end of a dynamic response. This case is referred to as a single objective function problem, but still requires sophisticated mathematical techniques, since the constraints must be satisfied at all time steps. The integral quadratic function is very common for the second case. In order to minimize the deviation of the state and control variables from their final steady state values, the sum of the squared error is evaluated at all time steps. Hence the same mathematical techniques, either sequential optimization or simultaneous integration and optimization can be used for these cases.

5.1. Problem Formulation Using Sequential Optimization Technique

The conceptual solution algorithm includes five steps:

1. Discretizing or parameterizing the control trajectory and providing the initial profile.
2. Solving the set of mixed algebraic and differential equations (ADEs) and evaluating the objective function and the constraints.
3. Calculating the gradient of the objective function and the constraints.
4. Submitting information of objective function, constraints and their gradients to an optimization package.
5. Updating the control profile and going back to step 2 until an optimal solution is found.

Since the sequential technique requires solutions of the ADEs at all iterations, the most time consuming parts of the algorithm are steps 2 and 3. SPEEDUP is selected to do the integration and provide the information required by the optimization package. Figure 3.2 shows the logical flow of information between the integrator and the optimizer.

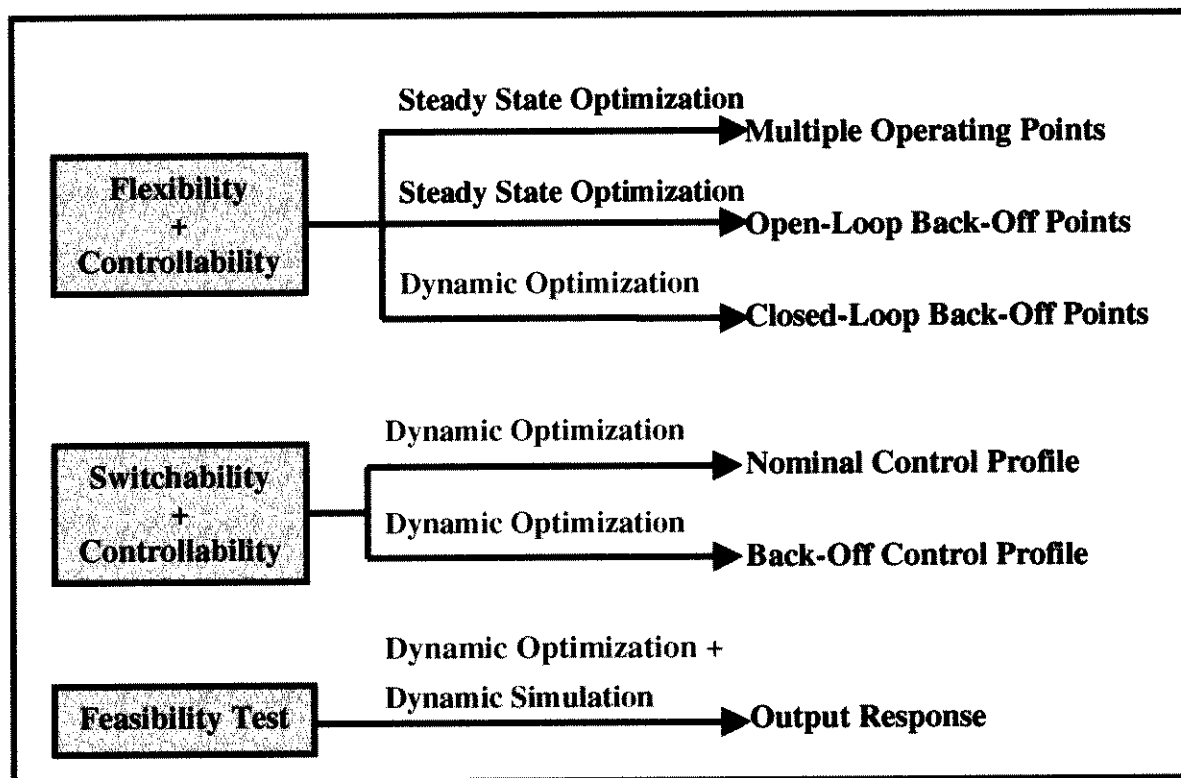


Figure 3.1 Steps to Solve a Switching Problem

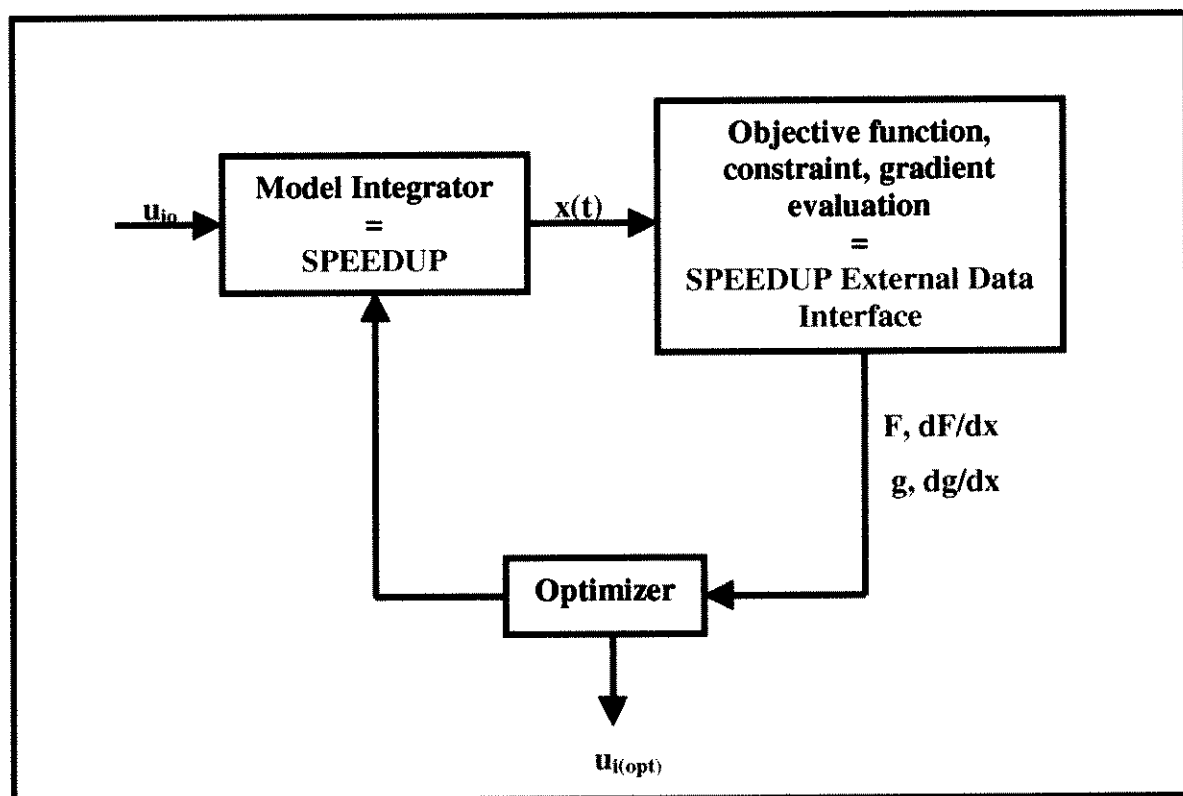


Figure 3.2 Logical Flow of Information Between Integrator and Optimizer

Constraints on control variables, bounded by minimum and maximum values, are set directly within the optimizer. The initial and final steady states and the dynamic simulation are performed in SPEEDUP. Values of other types of path constraints on state variables are also obtained from SPEEDUP dynamic simulations. However, instead of providing values of constraints at all time steps (each value at each time step), only the maximum and minimum values are submitted to the optimizer. Therefore, the number of path constraints is consequently reduced from mn to $2m$ (m is the number of path constraints; n is the number of time steps). When it is impossible to analytically determine the gradients of the objective function and the constraints, SPEEDUP calculates the gradients using finite difference method. The External Data Interface (EDI) mechanism in SPEEDUP passes information between the integrator and the optimizer.

The performance of the control program strongly depends on the selection and interfacing with the optimizer. MINOS is a Fortran-based computer program designed to solve large-scale optimization problems. It solves NLP problems using a reduced-gradient algorithm in conjunction with a quasi-Newton algorithm. OPT is another NLP code that uses the Successive Quadratic Programming algorithm (SQP) described in Biegler and Cuthrell (1985). The SQP routine implements the Powell quadratic programming code. OPT is simpler to use but less efficient than MINOS. For full details of the optimizers, readers should consult Multagh and Saunders (1995) or Biegler and Cuthrell (1985). Modified versions of these two optimizers are used in this chapter.

5.2. Problem Formulation Using Simultaneous Integration and Optimization Technique

One different way to solve a dynamic optimization problem is to convert the ODEs to algebraic equations. A very popular approximating method is the Orthogonal Collocation (OC) or the modified form, Orthogonal Collocation on Finite Elements (OCOFE). The trial function in this approach is taken as a series of orthogonal polynomials, the collocation points are taken as roots to one of those polynomials, and the dependent variables are solution values at the collocation points rather than the coefficients in the expansion. Consequently, the method has several advantages. Namely, the collocation points are picked automatically, thus avoiding the arbitrary

choice by the user, and the error decreases much faster as the number of terms increases (Finlayson, 1980).

5.2.1. Global orthogonal collocation

Instead of writing simple polynomial approximation for the state variables $x(t)$

$$x_n = x_o + t \sum_{i=1}^n a_i P_{i-1}$$

and including the coefficients a_i as decision variables for the optimization problem, the Lagrange interpolation polynomial is applied:

$$x_n(t) = \sum_{i=0}^n x_i \Phi_i(t) \quad (3.3)$$

where:

$$\Phi_i(t) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(t - t_j)}{(t_i - t_j)}$$

The Lagrange polynomial is chosen so that $\Phi_i(t_j)$ has the property of the Kronecker delta (δ_{ij}) of rank two, that is:

$$\begin{aligned} \Phi_i(t_j) &= 1 & \text{if } i = j \\ \Phi_i(t_j) &= 0 & \text{if } i \neq j \end{aligned}$$

The control profiles may also be approximated by:

$$u_n(t) = \sum_{i=1}^n u_i \phi_i(t) \quad \text{where} \quad \phi_i(t) = \prod_{\substack{j=1 \\ j \neq i}}^n \frac{(t - t_j)}{(t_i - t_j)} \quad (3.4)$$

and u_i can be decision variables but it is not limited to this form. The difference in the order of Φ_i and ϕ_i is due to the existence of the initial condition $x_0 = x(0)$.

Here $t_0 = 0$ and t_i ($i = 1, 2, \dots, n$) are the roots of an n^{th} order Legendre polynomial defined from 0 to t_f . Choosing $x_i \equiv x_n(t_i)$ that have physical significance as decision variables instead of a_i , it is much easier to supply meaningful bounds and starting points. The Legendre polynomial of n^{th} order has n roots and the coefficients are determined by requiring the successive polynomials to be orthogonal to all polynomials of order less than n , with some weighting function $w(t) \geq 0$.

$$\int_a^b w(t) P_m(t) P_n(t) dt = 0, \quad m = 0, 1, 2, \dots, n-1 \quad (3.5)$$

The roots of the Legendre polynomials in Table A.1 (see Appendix A) are served as collocation points in the dynamic closed-loop back-off and the switching problems. In equation (3.5) the values of $w(t)$, a and b are respectively selected as 1, 0 and 1.

$$\int_0^1 P_m(t) P_n(t) dt = 0, \quad m = 0, 1, 2, \dots, n-1 \quad (3.6)$$

Equation (3.3) can be differentiated with respect to t to give:

$$\frac{dx_n(t)}{dt} = \sum_{i=0}^n x_i \Psi_i(t) \quad (3.7)$$

where

$$\Psi_i = \frac{\sum_{\substack{k=0 \\ k \neq 1}}^n \prod_{\substack{j=0 \\ j \neq 1 \\ j \neq k}}^n (t - t_j)}{\prod_{\substack{j=0 \\ j \neq 1}}^n (t_i - t_j)}$$

Substitution of equation (3.7) into the state equation yields the residual equation:

$$\mathbf{R}(t) = \sum_{i=0}^n \mathbf{x}_i \Psi_i(t) - \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{p}) \quad (3.8)$$

To obtain the best solution, an adjustable constant or function is chosen so that the weighted residual becomes zero.

$$\int_0^1 \mathbf{R}(t) \mathbf{W}_i(t) dt = 0, \quad i = 1, 2, \dots, n \quad (3.9)$$

This is referred as the method of weighted residuals (MWR). A few common weighted-functions can be found in Finlayson:

➤ The *least square* method uses:

$$\mathbf{W}_i = \frac{\delta \mathbf{R}(t)}{\delta \mathbf{x}_i}$$

or

$$\int_0^1 \mathbf{R}(t) \frac{\delta \mathbf{R}(t)}{\delta \mathbf{x}_i} dt = \frac{1}{2} \int_0^1 [\mathbf{R}(t)]^2 dt$$

so that the mean square residual is minimized over $\mathbf{x}_i$.

➤ The *Galekin* method uses:

$$\mathbf{W}_i = \frac{\delta \mathbf{x}_{n+1}(t)}{\delta \mathbf{x}_i}$$

$$\int_0^1 \mathbf{R}(t) \Phi_i(t) dt = 0$$

- The *collocation* method uses the dirac delta function $W_i = \delta(t - t_i)$, which has the following property:

$$\int_0^1 W_i R(t) dt = R(t_s) = 0$$

The last method is the easiest to apply since the residual is evaluated only at n specified collocation points t_s . As n increases, the residual becomes zero at more and more points and presumably approaches zero everywhere. The approximated problem now becomes a NLP and can be solved by employing a NLP solver code.

For functions that vary sharply, an accurate approximation using global orthogonal collocation would require a very high n^{th} order polynomial. The method of OCOFE is introduced to avoid this requirement. The major advantage of this method is that it defines the trial functions only over a part of the region, and then pieces the adjacent functions together to provide an approximation over the whole domain. Thus small regions can be utilized near the steep gradients and the approximation is improved (see Finlayson). Using this approach, larger and more difficult system models can be successfully optimized.

5.2.2. Orthogonal collocation on finite elements

In this method, the domain is divided into NFE elements. Each finite element (FE) has NCOL internal collocation points and is bounded by two knots α_i and α_{i+1} . The FE length is given by:

$$\begin{aligned} \Delta\alpha_i &= \alpha_{i+1} - \alpha_i, & i &= 1, 2, \dots, \text{NFE} \\ \alpha_1 &= t_o, \alpha_{\text{NFE}+1} &= t_f \end{aligned} \quad (3.10)$$

In each element the OC method is applied as before. Since the relative locations of the points in the element are the same, the variable $\tau \in [0, 1]$ is mapped as:

$$t = \alpha_i + \tau \Delta\alpha_i \quad (3.11)$$

In order to use the model written in GAMS, it is convenient to use double subscripts "ij", where "i" refers the i^{th} FE and "j" refers to the collocation points, as shown in Figure 3.3. Thus equation (3.12) relates the collocation points in each element with the global points.

$$t_{ij} = \alpha_i + \tau_j \Delta \alpha_i \quad (3.12)$$

$$\begin{array}{lll} \text{where:} & \tau_j = 0 & \text{if } j = 0 \\ & \tau_j = 1 & \text{if } j = \text{NCOL} + 1 \\ & \tau_j = \text{collocation points} & \text{if } j = 1, 2, \dots, \text{NCOL} \end{array}$$

For $t \in [\alpha_i, \alpha_{i+1}]$, equations (3.3), (3.4) and (3.7), in section 5.2.1 can be written as:

$$x(t) = \sum_{j=0}^{\text{NCOL}} x_{ij} \Phi_{ij}(t) \quad (3.13)$$

where

$$\Phi_{ij}(t) = \prod_{\substack{n=0 \\ n \neq j}}^{\text{NCOL}} \frac{(t - t_{in})}{(t_{ij} - t_{in})} = \prod_{\substack{n=0 \\ n \neq j}}^{\text{NCOL}} \frac{(\tau - \tau_{in})}{(\tau_{ij} - \tau_{in})} = \Phi_j(\tau)$$

$$\begin{array}{ll} \text{and} & \Phi_{ij}(t_{in}) = \Phi_j(\tau_n) = 1 \quad \text{if } j = n \\ & \Phi_{ij}(t_{in}) = \Phi_j(\tau_n) = 0 \quad \text{if } j \neq n \end{array}$$

The approximation for the control profile becomes:

$$u(t) = \sum_{j=1}^{\text{NCOL}} u_{ij} \phi_{ij}(t) \quad \phi_{ij}(t) = \phi_j(\tau) = \prod_{\substack{n=1 \\ n \neq j}}^{\text{NCOL}} \frac{(\tau - \tau_n)}{(\tau_j - \tau_n)} \quad (3.14)$$

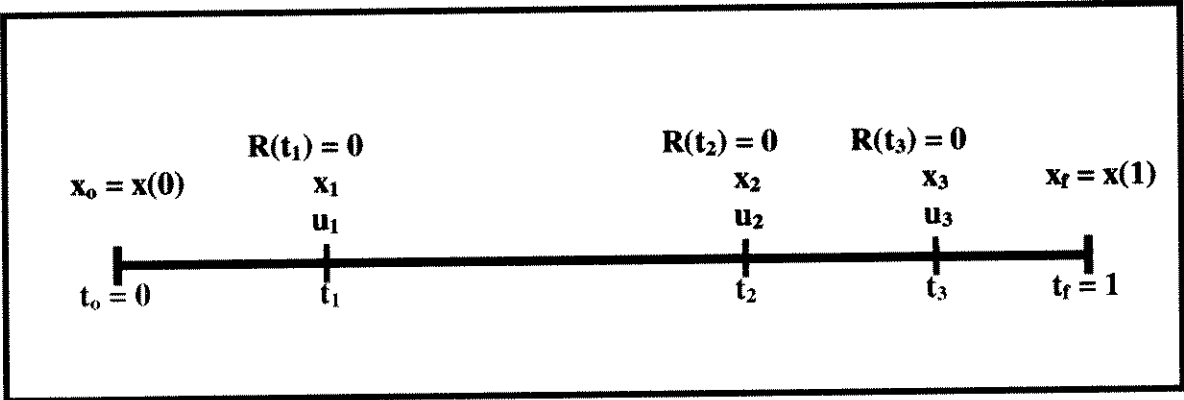


Figure 3.3.a Global Collocation (NCOL = 3)

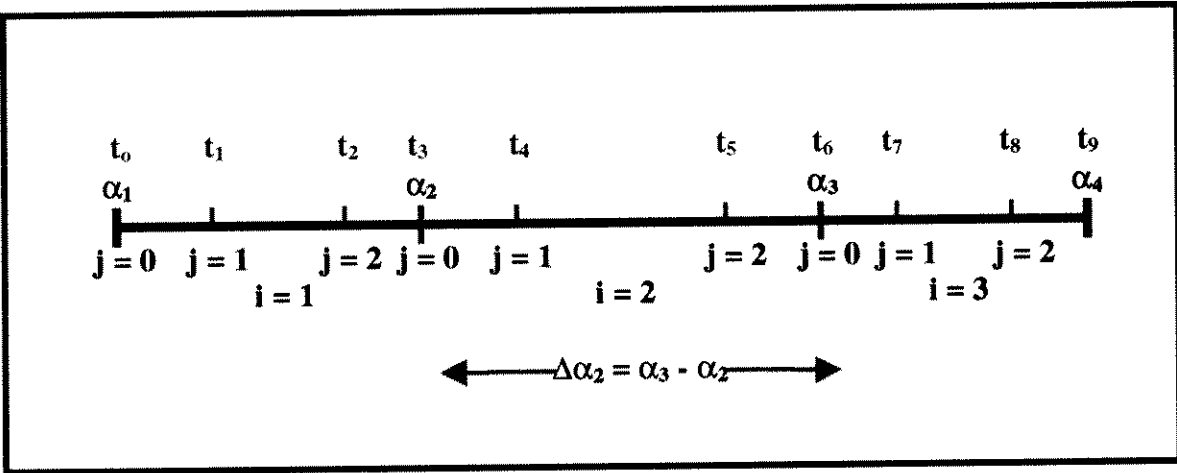


Figure 3.3.b Finite Element Collocation (NCOL = 2, NFE = 3)

The differential equation changes to:

$$\frac{dx(t)}{dt} = \sum_{j=0}^{NCOL} x_{ij} \Psi_{ij}(t) = \sum_{j=0}^{NCOL} x_{ij} \frac{\Psi_j(\tau)}{\Delta\alpha_i} \quad (3.15)$$

where:

$$\Delta\alpha_i \Psi_{ij}(t) = \Psi_j(\tau) = \frac{\sum_{\substack{k=0 \\ k \neq j}}^{NCOL} \prod_{\substack{n=0 \\ n \neq j \\ n \neq k}}^{NCOL} (\tau - \tau_n)}{\prod_{\substack{n=0 \\ n \neq j}}^{NCOL} (\tau_j - \tau_n)}$$

The residual equation evaluated at the collocation points is:

$$R(t_{is}) = \frac{1}{\Delta\alpha_i} \sum_{j=0}^{NCOL} x_{ij} \Psi_j(\tau_s) - f(x_{is}, u_{is}, p) = 0$$

$$x_o = x(0); \quad s = 1, 2, \dots, NCOL; \quad i = 1, 2, \dots, NFE \quad (3.16)$$

The initial condition $x_o = x(0)$ is used for the first element. An additional set of (NFE - 1) equations is required to make the polynomials continuous at the interior knot $\alpha_i, i = 1, 2, \dots, NFE$.

$$x_{io} = \sum_{j=0}^{NCOL} x_{i-1,j} \Phi_j(\tau=1) \quad i = 1, 2, \dots, NFE \quad (3.17)$$

The final condition could be:

$$\sum_1^{NFE} \Delta\alpha_i = t_f \quad (3.18)$$

$\Delta\alpha_i$ can also be chosen as decision variables by controlling the accuracy of the approximation at the end of each FE.

$$-\varepsilon \leq \sum_{j=0}^{N_{COL}} x_{ij} \Phi_{ij}(\tau=1) - f[x(\alpha_{i+1}), u(\alpha_{i+1}), p] \leq +\varepsilon \quad (3.19)$$

Table 3.2 summarizes the switchability problem formulation in discrete form.

6. Case Studies

The examples in Chapter 2 will be used again as the case studies to clarify the different steps of the switchability procedure. The algorithm to calculate the dynamic closed-loop back-off condition has been introduced before. Since it requires the same sophisticated mathematical techniques to solve either a dynamic back-off or a switchability problem, the case studies will demonstrate:

1. The potential recovery that a control system can provide through the dynamic flexibility and controllability analysis.
2. The ability of a process to switch between operating states through the switchability and controllability analysis.

6.1. Case Study 1: A Single CSTR

The first case study is the problem of a single continuous-stirred tank reactor (CSTR). The flowsheet is similar to that on page 2.17 but this plant has two control loops. Details of the flowsheet are shown in Figure 3.4. The main problems to be solved include:

1. Operating conditions at nominal feed concentration ($C_{in} = 20 \text{ mol.l}^{-1}$) and 75% of the nominal concentration ($C_{in} = 15 \text{ mol.l}^{-1}$).
2. Feed policies to switch between the above operating states.

Objective function

Minimize

$$F = w_1 \sum_{i=1}^{NFE} \sum_{j=0}^{NCOL} (x_{ij} - x_{sf})^2 - w_2 \sum_{i=1}^{NFE} \sum_{j=1}^{NCOL} (u_{ij} - u_{sf})^2$$

subject to

Residual equation

$$r(t_{is}) = \sum_{j=0}^{NCOL} x_{ij} \psi_j(\tau_s) - f(x_{is}, u_{is}, p) \Delta \alpha_i = 0$$

$$s = 1, 2, \dots, NCOL \quad i = 1, 2, \dots, NFE$$

Continuity equation

$$x_{i0} = \sum_{j=0}^{NCOL} x_{i-1,j} \phi_j(\tau=1) \quad i = 2, 3, \dots, NFE$$

where

$$\phi_j(\tau) = \phi_{ij}(t) = \prod_{\substack{n=0 \\ n \neq j}}^{NCOL} \frac{(t - t_{in})}{(t_j - t_{in})} = \prod_{\substack{n=0 \\ n \neq j}}^{NCOL} \frac{(\tau - \tau_{in})}{(\tau_j - \tau_{in})}$$

$$\Delta \alpha_i \psi_{ij}(t) = \psi_j(\tau) = \frac{\sum_{\substack{k=0 \\ k \neq j}}^{NCOL} \prod_{\substack{n=0 \\ n \neq j \\ n \neq k}}^{NCOL} (\tau - \tau_n)}{\prod_{\substack{n=0 \\ n \neq j}}^{NCOL} (\tau_j - \tau_n)}$$

$$\text{Initial condition} \quad x_0 = x(0)$$

$$\begin{aligned} \text{Inequality constraint} \quad & g(x_{is}, u_{is}, p) \leq 0 \\ & \Delta \alpha_i \geq 0 \end{aligned}$$

$$\text{Equality constraint} \quad c(x_{is}, u_{is}, p) = 0$$

Final condition

$$\sum_{i=1}^{NFE} \Delta \alpha_i = t_f$$

Table 3.2 Switchability Problem Formulation in Discrete Form

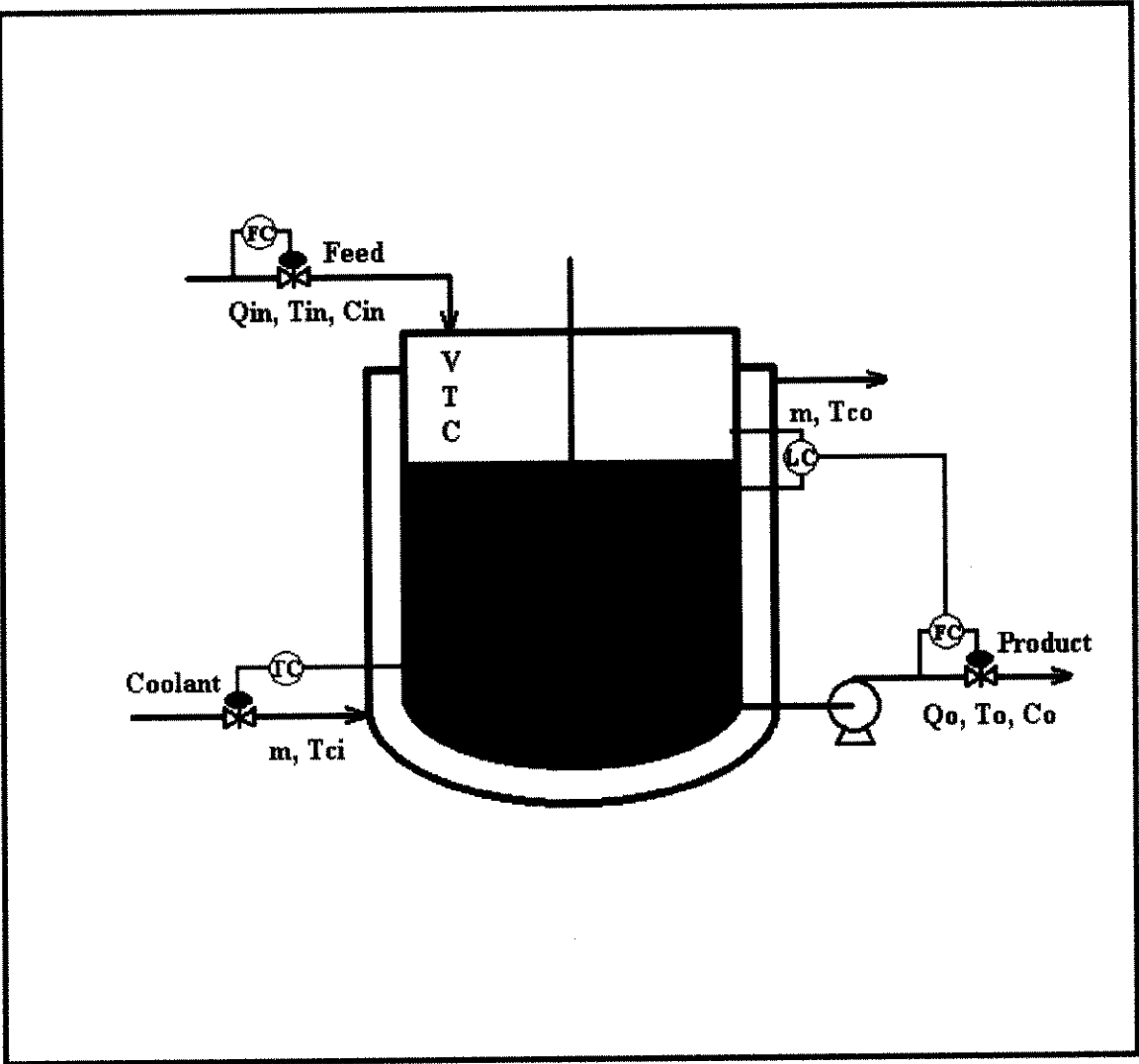


Figure 3.4 Single CSTR with Temperature and Level Controllers

The equality constraints describing the model of the system are similar to those on page 2.16 (2.5 to 2.10) with additional equations related to the controllers (3.21 to 3.25).

$$\text{Rate of consuming A:} \quad \text{Rate} = -k_0 e^{(-E/RaT)} VC \quad (2.5)$$

$$\text{Mass balance for A} \quad \{d(VC)/dt\} = \text{Rate} + Q_{in}C_{in} - Q_oC_o \quad (2.6)$$

$$\text{Rate of heat removal} \quad \text{Cool} = Ua(T - T_{co}) = m(T_{ci} - T_{co}) \quad (2.7)$$

$$\text{Energy balance} \quad \{d(VT)/dt\} = DH * \text{Rate} + Q_{in}T_{in} - Q_oT_o - \text{Cool} \quad (2.8)$$

$$\text{where} \quad DH = -\{\Delta H_r/(\rho_r C_p)\} \quad (2.9)$$

$$\text{Perfect mixing} \quad C = C_o; T = T_o \quad (2.10)$$

$$\text{Overall mass balance} \quad V_{max}(dH/dt) = Q_{in} - Q_o \quad (3.20)$$

$$V = V_{max}H \quad (3.21)$$

$$\text{Temperature control} \quad m = \text{Gain}_t[\text{Stp}_t - T + (Int_t/Rst_t)] + m_{ss} \quad (3.22)$$

$$\{d(Int_t)/dt\} = \text{Stp}_t - T \quad (3.23)$$

$$\text{Level control} \quad Q_o = Q_{max}\text{Gain}_h[\text{Stp}_h - H + (Int_h/Rst_h)] + Q_{ss} \quad (3.24)$$

$$\{d(Int_h)/dt\} = \text{Stp}_h - H \quad (3.25)$$

The differential terms (dC/dt) , (dT/dt) in equations (2.6), (2.8) are not equal to zero if dynamic simulations are performed. Equation (2.11) in Chapter 2 is replaced by equation (3.20) to take into account the dynamics of the inventory.

If the temperature in the tank is controlled, the coolant flowrate is not fixed but it varies within the lower and upper values. More constraints are posed on the limits of level, outlet and coolant flowrates. All these constraints can be active at any time step.

Safety restriction	$T \leq 350 \text{ K}$	Constraint 1
	$0.5 \leq H \leq 0.9$	Constraint 2
Process limitation	$\text{Cool} \leq 20 \text{ l.K.s}^{-1}$	Constraint 3
	$0.1 \leq m \leq 8.0 \text{ l.s}^{-1}$	Constraint 4
Maximum, minimum throughput	$0.05 \leq Q_{\text{in}}, Q_o \leq 0.8 \text{ l.s}^{-1}$	Constraint 5
	$C_o \leq 0.3 \text{ mol.l}^{-1}$	Constraint 6

The same set of disturbances on page 2.16 is used but the feed temperature (T_{in}) and the coolant inlet temperature (T_{ci}) are considered as fast disturbances. The occurrence of a step change in T_{in} or T_{ci} is an event (Carvallo, 1989). Meanwhile the heat transfer coefficient (Ua) is treated as a slow disturbance or an uncertain parameter. Therefore, in the dynamic optimization problems Ua is a constant ($Ua = 0.33, 0.35$ or 0.37), while T_{in} and T_{ci} are modeled as step changes of magnitude $\Delta T = (\text{upper bound} - \text{nominal value})$ or $\Delta T = (\text{nominal value} - \text{lower bound})$.

	Lower Bound	Nominal Value	Upper Bound
$T_{\text{in}}(\text{K})$	295	300	305
$T_{\text{ci}}(\text{K})$	280	283	286
$Ua(\text{l/s})$	0.33	0.35	0.37

6.1.1. Dynamic closed-loop back-off problem

As presented in Chapter 2, the six-step procedure for open loop and closed-loop back-off calculations is applied. The open loop back-off operating conditions are obtained after three iterations. The matrix of disturbances and uncertain parameters in the last iteration becomes:

$$d^n = \begin{bmatrix} T_{in} & Ua & T_{ci} \\ 300 & 0.35 & 283 \\ 305 & 0.33 & 286 \\ 295 & 0.37 & 280 \end{bmatrix}$$

Because of the disturbances on the feed temperature (T_{in}), the coolant inlet temperature (T_{ci}) and the uncertain heat transfer coefficient (Ua), the plant has to operate at the open loop back-off condition: $Q_{in} = 0.296 \text{ l.s}^{-1}$; $V = 349 \text{ l}$ (see Table 3.3a). The profit loss due to backing off from the nominal state is about 20%. A temperature control loop is introduced to recover this loss. Adjusting the coolant flowrate controls the temperature in the reactor. Controller gains and reset times are also included in the optimization problem as decision variables with initial guesses given by Ziegler-Nichols method. Two equations: (3.24) and (3.25), and also constraint 2 are removed from the problem. The term (dH/dt) in equation (3.20) is equal to zero. The net profit evaluated at time zero is selected as the objective function:

$$\text{Profit}(t=0) = \text{product value}(t=0) - \text{raw material cost}(t=0) - \text{cost of cooling}(t=0)$$

$$\text{Obj} (\$/\text{time}) = pv * Q_{in}(t=0) * (C_{in} - C_o(t=0)) - mc * Q_{in}(t=0) * C_{in} - cc * \text{Cool}(t=0) \quad (3.26)$$

The dynamic optimization problem is solved for three decision variables: feed flowrate (Q_{in}), inventory (V) and temperature set point (Stp_r). The latter variable was not seen before in the case study because the problem had two degrees of freedom. The addition of a temperature control loop increases the number of degrees of freedom in this case. Since these decision variables define the operating conditions at steady state, they are evaluated at a single time step ($t=0$). However, it has to be solved as a dynamic optimization problem because path constraints must be satisfied at all time steps.

As discussed in Chapter 2, the recovery strongly depends on the control strategy. A proportional (P) controller can bring the recovery up to 100% but it produces an offset. Consequently the temperature response cannot reach the desired set point. A PI

controller is used to avoid this problem. A sensitivity analysis with different values of temperature controller gain and reset time shows the following trends:

- The recovery increases with gain. On the contrary, the final time (t_f) for the system to reach steady state, maximum values of coolant flowrate ($m_{\max}$) and cooling ($\text{cool}_{\max}$) required decrease with a higher gain value.
- A higher reset time value would decrease $\text{Cool}_{\max}$ and $m_{\max}$ but increase t_f .
- The recovery has an upper limit. Even extremely large values of gain or reset time can not significantly improve the recovery beyond this limit.

As there is no unit interaction, highest values of gain and reset time may generally be used for the PI controller. Additional constraints are required to control t_f , if reset time is included as a decision variable in the optimization.

$$-\epsilon < T(t_f > \theta) - \text{Stp}_t < +\epsilon$$

Constraint 7

The differential equations in the above problem are converted to algebraic equations using OCOFE method. GAMS with MINOS 5.2 optimizer is used to solve the NLP problem. Two cases are considered separately to prepare for the coming switching problem in section 6.1.2. Class I assumes a single step change in T_{in} only. Class II assumes a multiple step change in T_{in} and T_{ci} . The matrices of disturbances and uncertain parameters in the second iteration respectively for Class I and Class II are:

$$d_I^1 = \begin{bmatrix} T_{\text{in}} & U_a \\ 300 & 0.35 \\ 305 & 0.33 \end{bmatrix} \quad d_{II}^1 = \begin{bmatrix} T_{\text{in}} & U_a & T_{\text{ci}} \\ 300 & 0.35 & 283 \\ 305 & 0.33 & 286 \end{bmatrix}$$

Permanent feasible solutions are obtained after two iterations. The closed-loop back-off conditions are compared with the open loop and nominal cases in Table 3.3a. The difference between Class I and Class II is that the maximum amount of cooling required for the latter case is higher. Since this amount of cooling does not hit the upper limit, the recoveries are almost the same in both cases. The maximum percentage of recovery is 78 %.

Case	Feed Conditions	Objective Index (F \$.hr ⁻¹)	Inlet Flowrate (Q _{in} m.s ⁻¹)	Inventory (V l)	Set Point Temperature (Stp _t K)
<i>Nominal</i>	T _{in} = 300 T _{ci} = 283 U _a = 0.35	71.0	0.362	245	350.0
<i>Open Loop Back-Off</i>	295 < T _{in} < 305 280 < T _{ci} < 286 0.33 < U _a < 0.37	58.4	0.296	349	344.5
<i>Dynamic Back-Off (Class I)</i>	T _{in} → 305 T _{ci} = 283 U _a = 0.33	67.9	0.346	235	349.9
<i>Dynamic Back-Off (Class II)</i>	T _{in} → 305 T _{ci} → 286 U _a = 0.33	67.8	0.345	235	349.9

Table 3.3a Optimal Operating Conditions (C_{in} = 20)

In this example, possible highest values of gain (K_c) and reset time (τ) are assumed to be 40 and 100, respectively. The temperature controller can provide maximum recovery with $K_c = 10$, $\tau = 25$. Similar calculations are done for the case where the feed concentration drops by 25% ($C_{in} = 15$). Feasible solutions are shown in Table 3.3b. Highest values of gain and reset time ($K_c = 40$, $\tau = 100$) are used. To control the ending time in Class II, the optimization problem must include the reset time as a decision variable. Constraint 7 becomes:

$$-10^{-3} < T(t_f \geq 100) - \text{Stp}_t < +10^{-3}$$

The optimal value of reset time is $\tau = 90$.

Case	Feed Conditions	Objective Index ($F \$ \cdot \text{hr}^{-1}$)	Inlet Flowrate ($Q_{\text{in}} \text{ m} \cdot \text{s}^{-1}$)	Inventory (V l)	Set Point Temperature ($\text{Stp}_t \text{ K}$)
<i>Nominal</i>	$T_{\text{in}} = 300$ $T_{\text{ci}} = 283$ $U_a = 0.35$	109.5	0.746	377	350.0
<i>Open Loop Back-Off</i>	$295 < T_{\text{in}} < 305$ $280 < T_{\text{ci}} < 286$ $0.33 < U_a < 0.37$	81.0	0.550	482	344.6
<i>Dynamic Back-Off (Class I)</i>	$T_{\text{in}} \rightarrow 305$ $T_{\text{ci}} = 283$ $U_a = 0.33$	98.8	0.674	359	349.0
<i>Dynamic Back-Off (Class II)</i>	$T_{\text{in}} \rightarrow 305$ $T_{\text{ci}} \rightarrow 286$ $U_a = 0.33$	96.4	0.657	358	348.5

Table 3.3b Optimal Operating Conditions ($C_{\text{in}} = 15$)

As shown in Tables 3.3a and 3.3b, if the feed concentration (C_{in}) drops by 25%, the operating conditions completely change. The next step attempts to find the best trajectories to connect these operating conditions.

6.1.2. Switchability problem

To perform a switch on feed flowrate and inventory, a level control loop is introduced to avoid overflowing or dry running of the tank. Using proportional plus integral (PI) controllers, manipulating the outflow from the tank will control the level. The problem includes all equality constraints on page 3.24, (2.5) to (2.10) and (3.20) to (3.25). The inlet and outlet flowrates are related to each other by equation (3.20). The integral squared deviation of the state and control variables evaluated at all time steps is selected as the objective function.

$$F = \int_{t_0}^{t_f} [w_p (Q_{in} - Q_{sf})^2 + w_c (C - C_{sf})^2 + w_t (T - T_{sf})^2 + w_h (H - H_{sf})^2] dt \quad (3.27)$$

The dynamic optimization problem is solved for the best trajectory of the inlet flowrate (Q_{in}), when the feed concentration drops by 25% ($C_{in} = 20 \rightarrow 15$). The same mathematical techniques in section (6.1.1) are used, since decision variables are evaluated and path constraints must be satisfied at all time steps. Two special cases are considered:

- Switching Inventory (SI): These problems are a mixture of regulator and servo problems, since feed changes are accompanied by set point changes. Liquid levels in reactors represent inventories. To avoid abrupt changes in the levels that may upset outflow and downstream operations, the level set points must follow some trajectories. The best trajectory is obtained from solving the problem that includes an additional deviation term in the objective function.

$$F = \int_{t_0}^{t_f} [w_p (Q_{in} - Q_{sf})^2 + w_c (C - C_{sf})^2 + w_t (T - T_{sf})^2 + w_h (H - H_{sf})^2 + w_{hsp} (Sp_h - Sp_{hsf})^2] dt \quad (3.28)$$

- Fixed Inventory (FI): These problems are regulator problems. Another way to avoid enormous changes in levels is allowing them to have a constant set point value during the switch. In this case, the dynamic closed-loop back-off problem in section (6.1.1) should be:

1. The optimal operating conditions at the second or final steady state ($C_{in} = 15 \text{ mol.l}^{-1}$) are solved first for three decision variables: feed flowrate (Q_{in}), inventory (V) and temperature set point (Stp_t). Results were shown in Table 3.3b.
2. The optimal operating conditions at the first or beginning steady state ($C_{in} = 20 \text{ mol.l}^{-1}$) are solved next for two decision variables: feed flowrate (Q_{in}) and temperature set point (Stp_t). The inventory is a parameter having the same

optimal value found above ($V1 = V2 = 360$ l). Results will be different from those presented in Table 3.3a.

Table 3.4 shows different cases considered for the switching policies. In all graphs blue-broken lines show the constraints and magenta-broken lines show the targets to reach. The following cases have been considered:

❖ Nominal condition

This case finds the switching policy between nominal operating conditions. Disturbances and uncertain parameters haven't been introduced yet, but the plant should have the level controller for safe feed and inventory changeovers. There is no feasible solution. Constraint 6 ($C_o < 0.3$) is violated. Figure 3.5 shows concentration, temperature and outflow responses. These profiles are from an infeasible solution but can be used to compare the trend of fixed and switching inventories. Green curves are for (FI) and red ones for (SI) cases. The red curves in Figure 3.5a show that in order to increase the liquid volume in the tank, at the beginning of the switch the outlet valve has to be closed and the inlet valve widely open. That results in a greater amount of constraint violation in (SI) than in (FI) (see Figure 3.5b, Concentration and Temperature Responses), but as a trade-off the temperature in the first case responds more rapidly.

An additional set of constraints is now included to take into account the response of the inlet valve. For instant, at the beginning of a switch the derivative of the inflow with respect to time has lower and upper bounds.

$$-10^{-2} \leq \frac{dQ_{in}}{dt}(t \leq 20) \leq +10^{-2}$$

Constraint 8

❖ Open loop back-off condition

This case finds the switching policy between open loop back-off operating conditions. Multi event disturbances and an uncertain parameter affect the system. The plant has the level controller ($K_c = 40$, $\tau = 100$) but the temperature has not been controlled yet.

Cases	First Steady State ($C_{in} = 20$)	Second Steady State ($C_{in} = 15$)	Results
Nominal Condition <i>Fixed Inventory (FI)</i> <i>Switching Inventory (SI)</i>	$T_{in} = 300$ $T_{ci} = 283$ $Ua = 0.35$ $Q_{ss} = 0.357$ $V = 378$ $Q_{ss} = 0.361$ $V = 246$ $Stp_h = 0.492$	$T_{in} = 300$ $T_{ci} = 283$ $Ua = 0.35$ $Q_{ss} = 0.746$ $V = 378$ $Q_{ss} = 0.746$ $V = 378$ $Stp_h = 0.756$	Figure 3.5 a, b
Open-Loop Back-Off <i>Fixed Inventory (FI)</i> <i>Switching Inventory (SI)</i>	$Ua = 0.33$ $T_{in} = 300$ $T_{ci} = 283$ $Q_{ss} = 0.285$ $V = 500$ $Q_{ss} = 0.286$ $V = 374$ $Stp_h = 0.598$	$Ua = 0.33$ $T_{in} \rightarrow 305$ $T_{ci} \rightarrow 288$ $Q_{ss} = 0.532$ $V = 500$ $Q_{ss} = 0.532$ $V = 500$ $Stp_h = 0.800$	Figure 3.6 a, b, c, d
Closed-Loop Back-Off Class I <i>Fixed Inventory (FI)</i> <i>Switching Inventory (SI)</i>	$Ua = 0.33$ $T_{in} = 300$ $T_{ci} = 283$ $Q_{ss} = 0.342$ $V = 360$ $Q_{ss} = 0.346$ $V = 243$ $Stp_h = 0.54$	$Ua = 0.33$ $T_{in} \rightarrow 305$ $T_{ci} = 283$ $Q_{ss} = 0.674$ $V = 360$ $Q_{ss} = 0.674$ $V = 360$ $Stp_h = 0.800$	Figure 3.7
Closed-Loop Back-Off Class II <i>Fixed Inventory (FI)</i> <i>Switching Inventory (SI)</i>	$Ua = 0.33$ $T_{in} = 300$ $T_{ci} = 283$ $Q_{ss} = 0.342$ $V = 360$ $Q_{ss} = 0.286$ $V = 243$ $Stp_h = 0.54$	$Ua = 0.33$ $T_{in} \rightarrow 305$ $T_{ci} \rightarrow 286$ $Q_{ss} = 0.657$ $V = 360$ $Q_{ss} = 0.657$ $V = 360$ $Stp_h = 0.800$	Figure 3.8

Table 3.4 Different Switching Cases

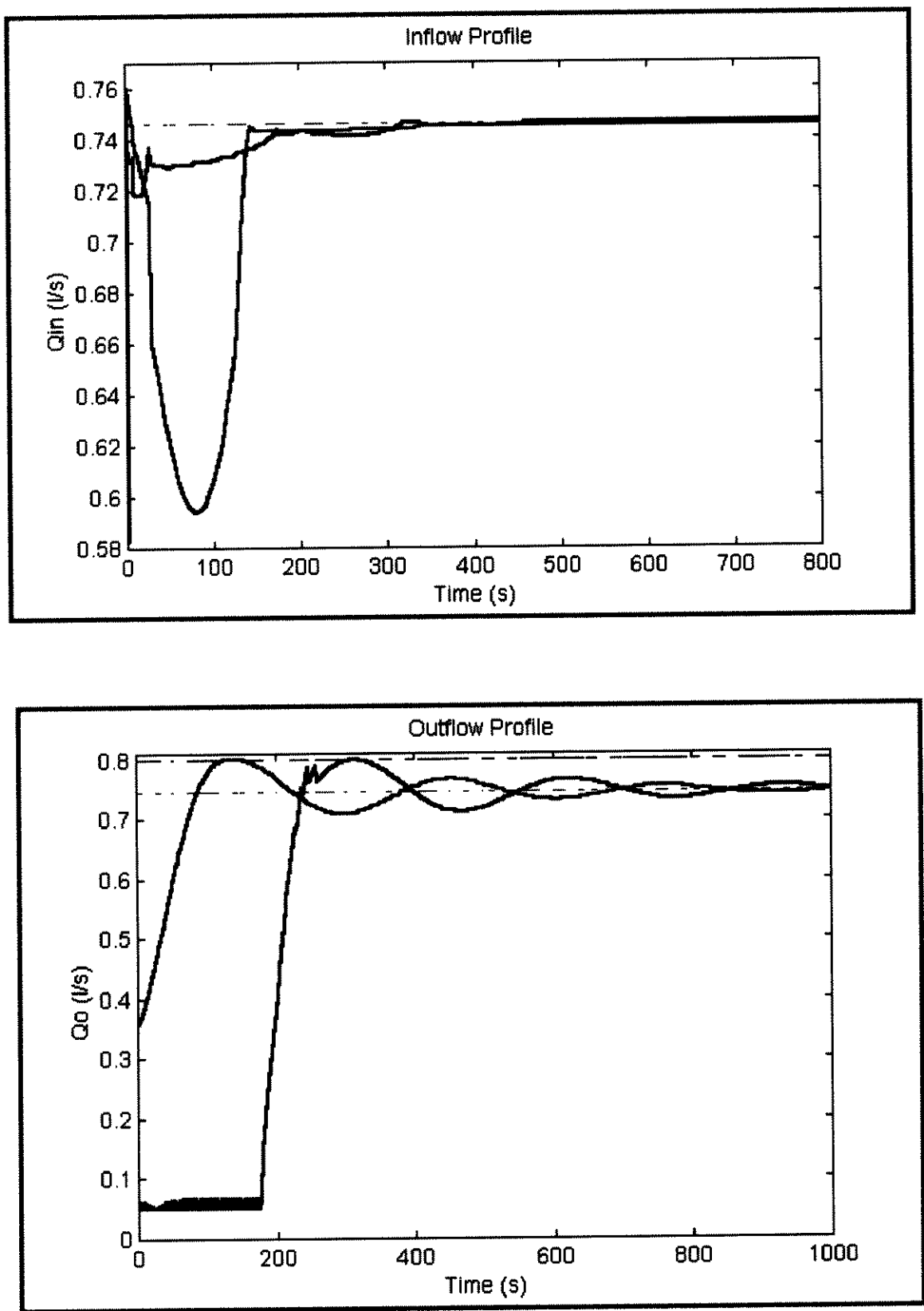


Figure 3.5a Inflow and Outflow Responses (Nominal Case)
(Green curve: Fixed Inventory)
(Red curve: Switching Inventory)
(Broken line: Constraint or target to reach)

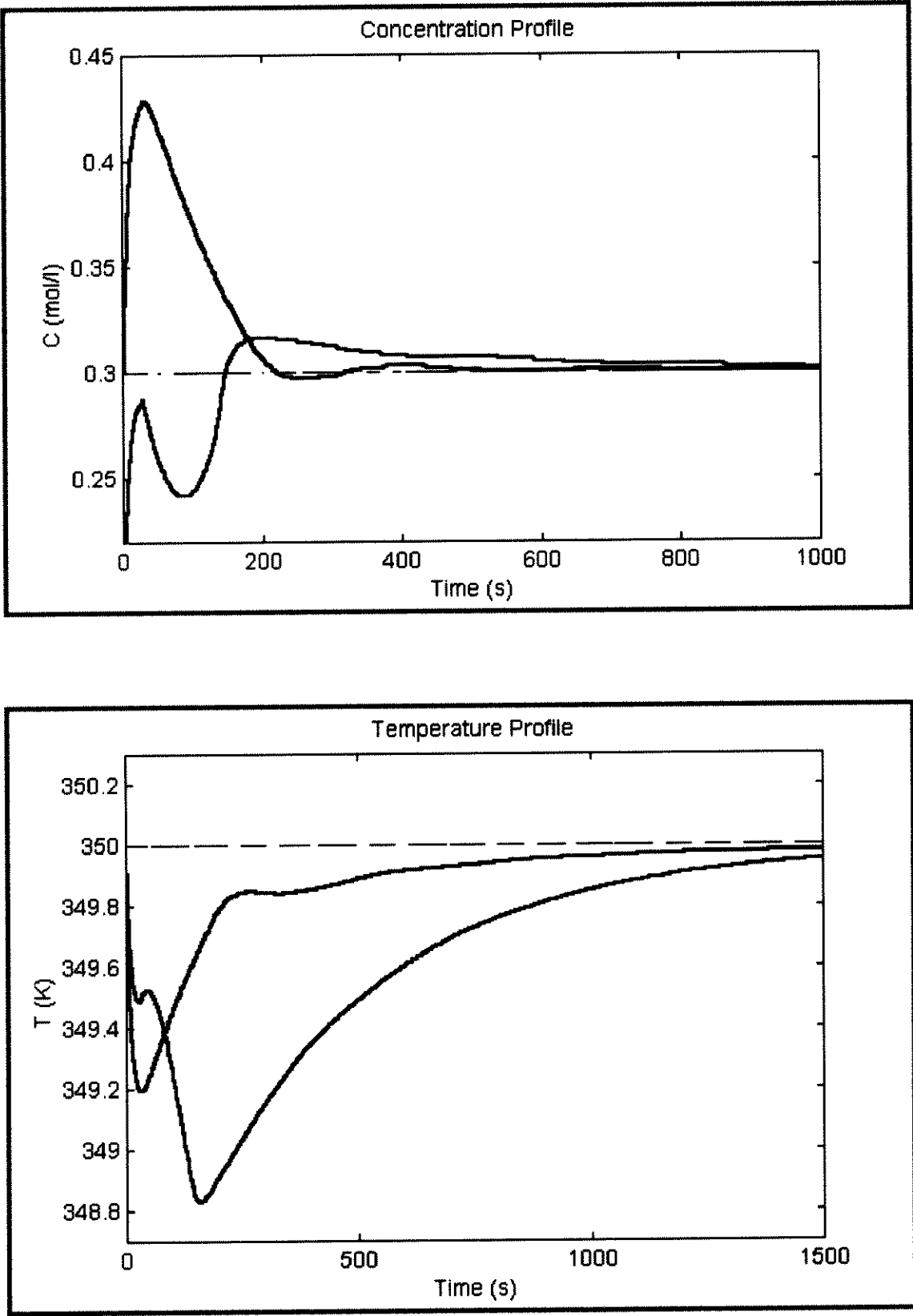


Figure 3.5b Concentration and Temperature Responses (Nominal Case)

(Green curve: Fixed Inventory)

(Red curve: Switching Inventory)

A step change profile in feed flowrate is also a feasible solution because no path constraints are violated. Such a step profile is, however, not the optimal trajectory because it takes much more time for the temperature to reach steady state. Consequently, the process might not be able to completely reject multiple disturbances before facing a new one and Class II assumption is not held. Figures 3.6a and b show the effect of weighting factor on system responses. Since there is no temperature controller, the temperature deviation term included in equation (3.27) acts like a PI controller with the weighting factor as a controller gain. As the temperature weighting factor is increased, the temperature response is faster. Responses represented by green curves have a weighting factor ($w_t = 0.001$) ten times less than red curves ($w_t = 0.01$). Figure 3.6 also shows the effect of constraints posed on response time of the inlet valve.

$$-10^{-2} \leq \frac{dQ_{in}}{dt}(t \leq \theta) \leq +10^{-2}$$

Yellow curves and red curves have the same temperature weighting factor. However, θ takes the value of 110 seconds in the first and 60 seconds in the latter case. These constraints are always active. Therefore, the response curves are shifted forward as under the effect of time delays.

As discussed in the nominal case, (FI) is generally more favorable than (SI). Temperature and concentration responses of FI are slower than those of SI cases. On the contrary, the outflow and level response of the first are much better than the latter. Temperature, level, inflow and outflow responses of these cases are plotted in Figures 3.6c and d.

❖ Dynamic closed-loop back-off condition

This case finds the switching policy between dynamic closed-loop back-off operating conditions. A single disturbance (Class I) and an uncertain parameter are dealt with first, then multiple disturbances (Class II) are considered.

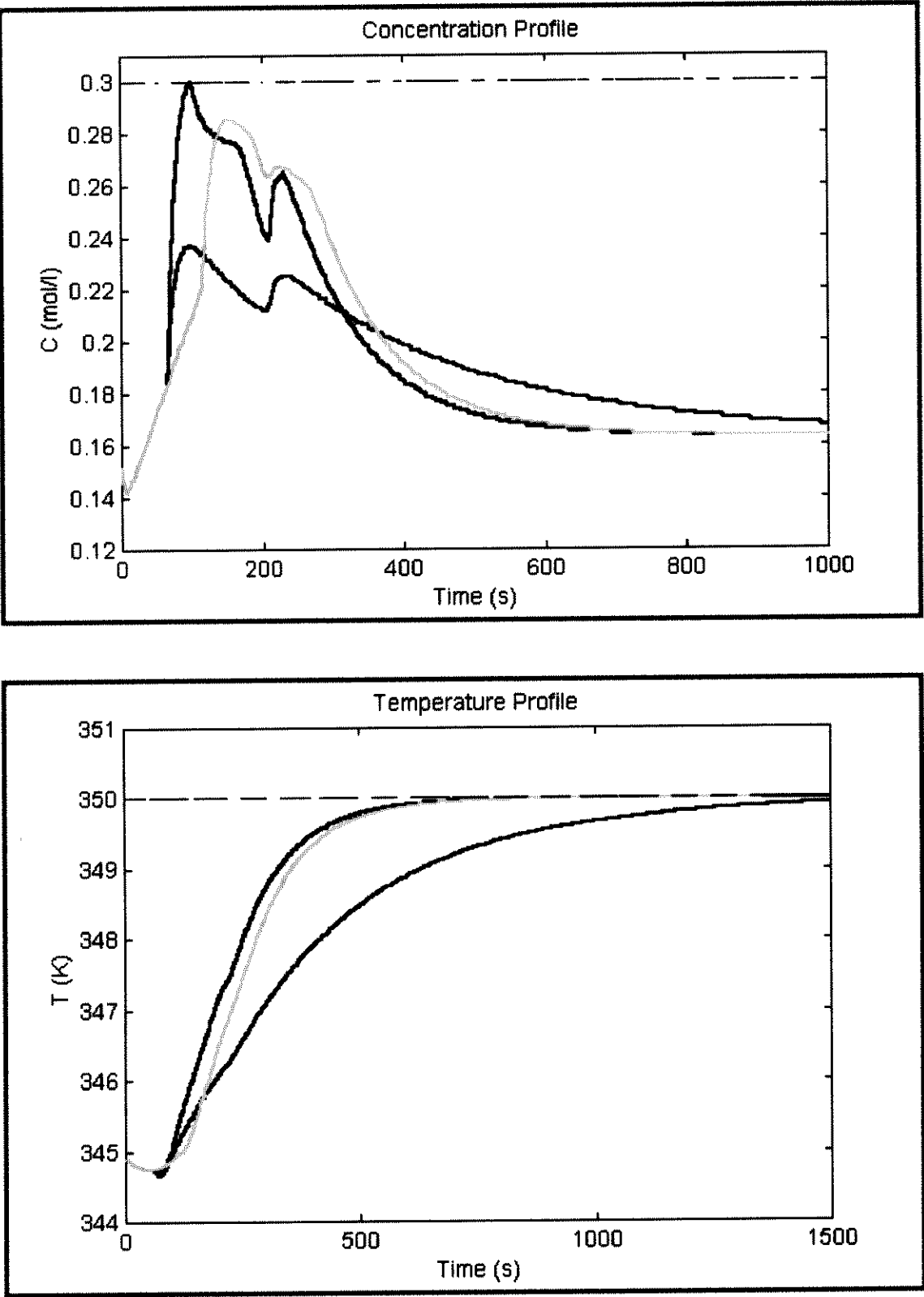


Figure 3.6a Concentration and Temperature Responses (Open Loop Back-Off Case)
(Green curve: weighting factor $w_t = 0.001$, constraints on inlet valve for $t < 60$ s)
(Red curve: weighting factor $w_t = 0.01$, constraints on inlet valve for $t < 60$ s)
(Yellow curve: weighting factor $w_t = 0.01$, constraints on inlet valve for $t < 110$ s)

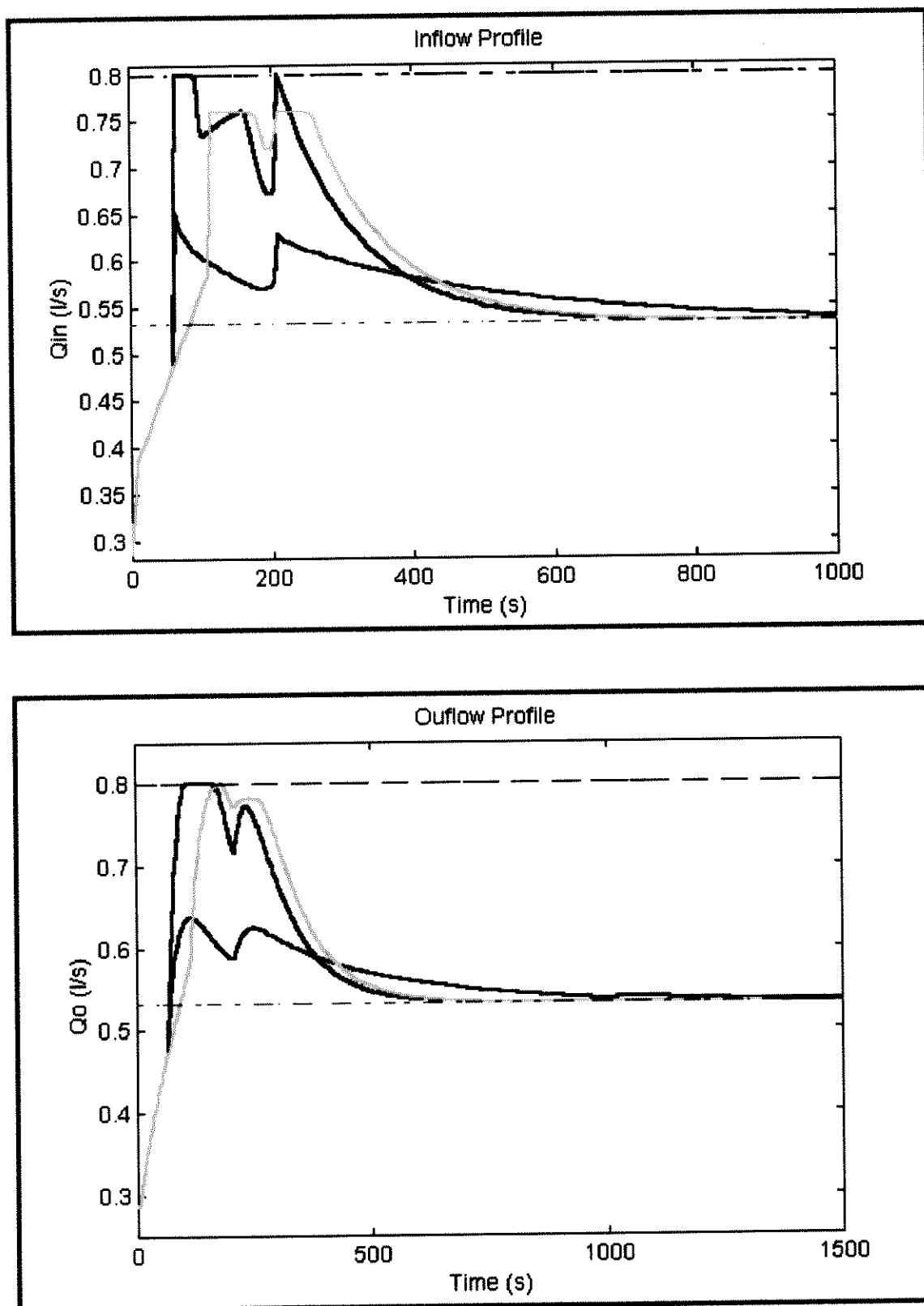


Figure 3.6b Inflow and Outflow Responses (Open Loop Back-Off Case)

(Green curve: weighting factor $w_t = 0.001$, constraints on inlet valve for $t < 60$ s)

(Red curve: weighting factor $w_t = 0.01$, constraints on inlet valve for $t < 60$ s)

(Yellow curve: weighting factor $w_t = 0.01$, constraints on inlet valve for $t < 110$ s)

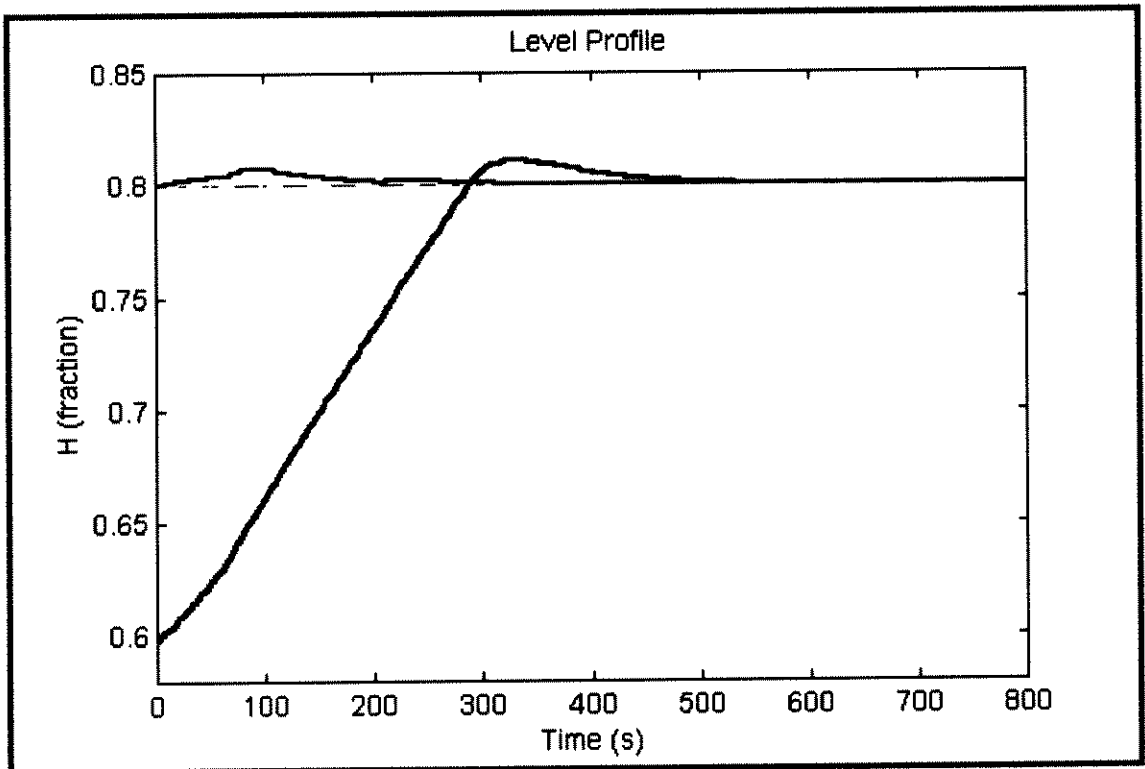
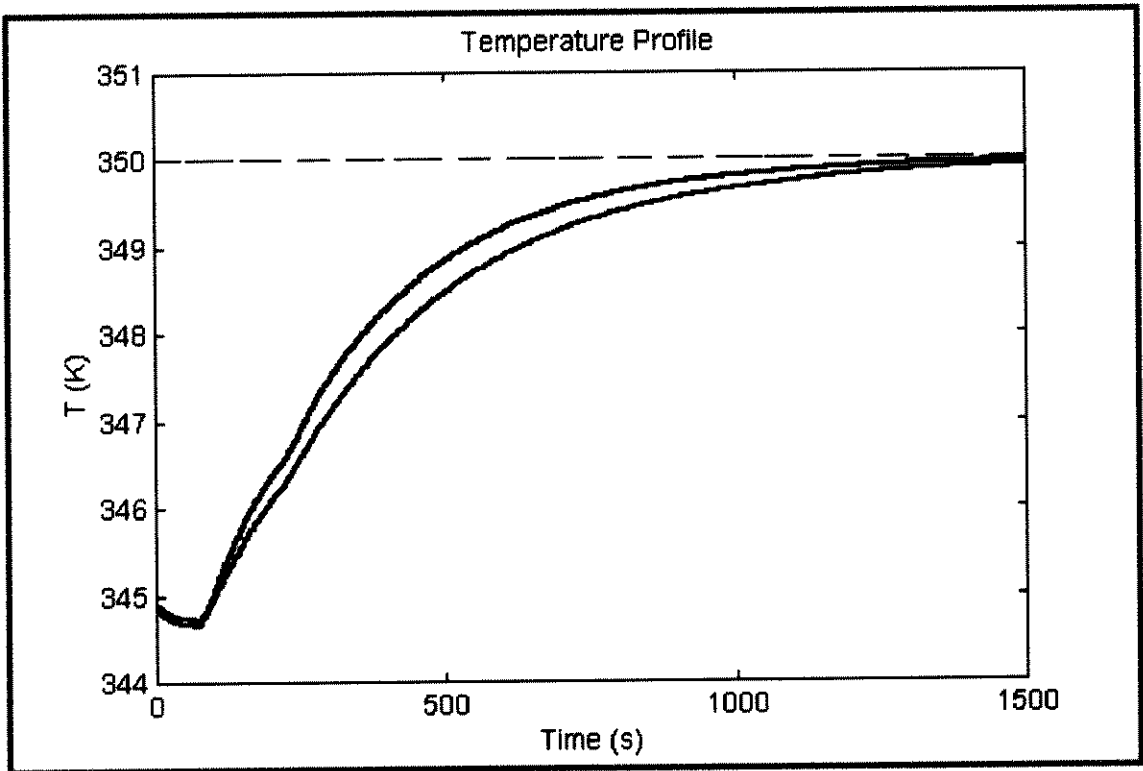


Figure 3.6c Temperature and Level Responses (Open Loop Back-Off Case)

(Green curve: Fixed Inventory)

(Red curve: Switching Inventory)

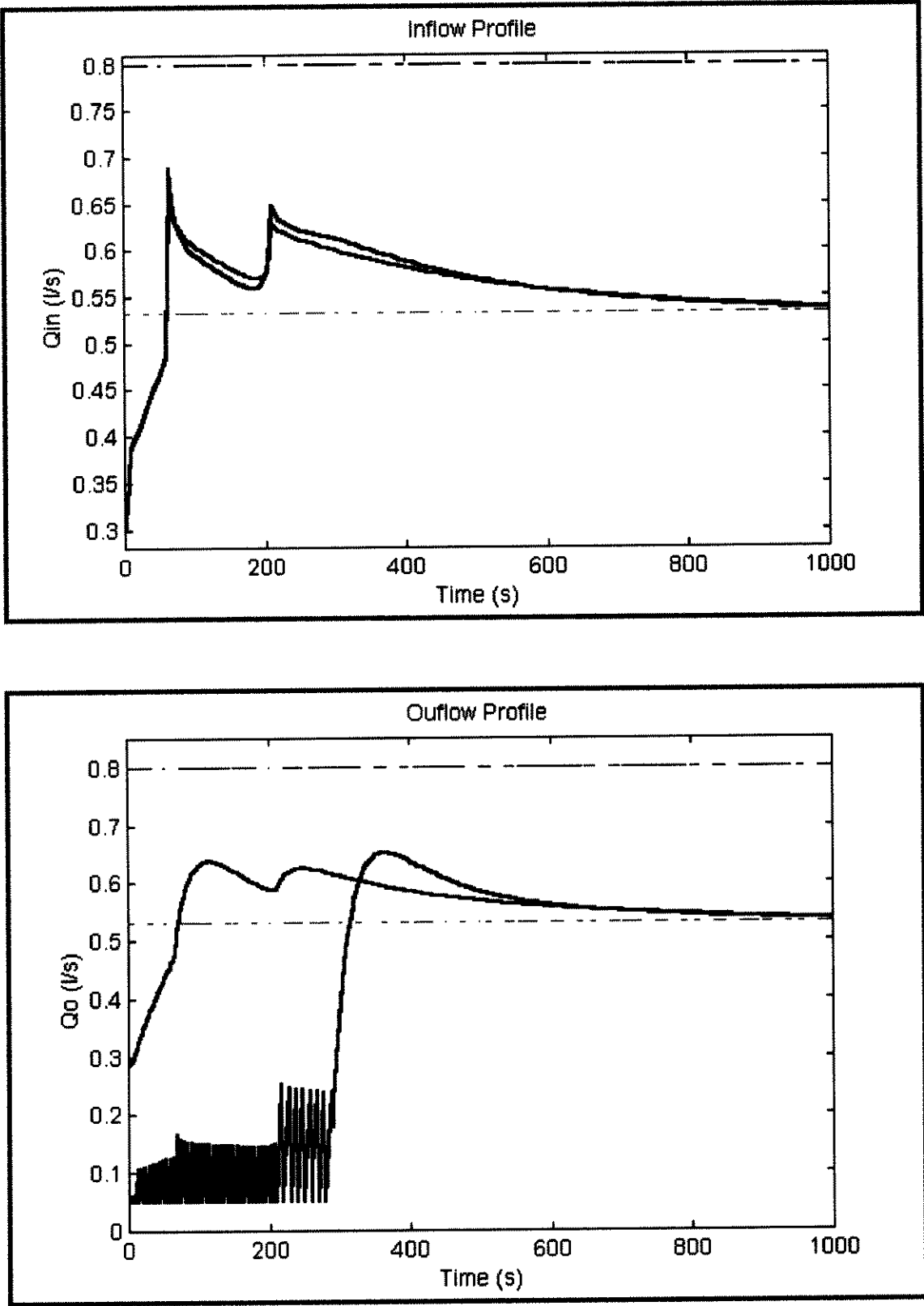


Figure 3.6d Inflow and Outflow Responses (Open Loop Back-Off Case)
(Green curve: Fixed Inventory)
(Red curve: Switching Inventory)

The plant has both level and temperature control loops. The level controller has highest values of gain and reset time ($K_{ch} = 40$, $\tau_h = 100$). The gain and reset time of the temperature controller depend on the temperature set point policy. This policy can be a step change profile or an optimal trajectory obtained from solving the objective function similar to equation (3.28):

$$F = \int_{t_0}^{t_f} [w_p (Q_m - Q_{sf})^2 + w_c (C - C_{sf})^2 + w_t (T - T_{sf})^2 + w_e (H - H_{sf})^2 + w_{sp} (Sp_t - Sp_{sf})^2] dt$$

Figure 3.7 compares two temperature set point policies. The red curves are for the step change set point policy and the green curves for the optimal set point trajectory (or temperature set point tracking). It takes only 260 iterations to solve the step change set point problem. Meanwhile more than 400 iterations are required to solve the temperature set point tracking problem, although the temperature gain used is eight times greater than in the first case. The inflow profiles of these cases are quite similar, as the temperature difference between two ends of the switch is less than two degrees. Despite lengthy iteration, the temperature set-point tracking is more favorable for switching problems with great temperature differences, as it will be shown in the second case study.

The response curves for multiple disturbances are similar to a single disturbance except that longer trajectories and a greater number of iteration are required. Figure 3.8 compares inflow and temperature responses of single-disturbance and multiple-disturbance cases.

6.1.3. Testing the feasibility of the solutions

The optimal trajectories of the inlet flowrate (Q_m) found in the above cases are tested with different combinations of disturbances. If there is any constraint violation the switchability problem must be solved again with the updated matrix of disturbances.

$$d^k = d^n \cap d^{n+1} \cap d^{n+2} \cap \dots$$

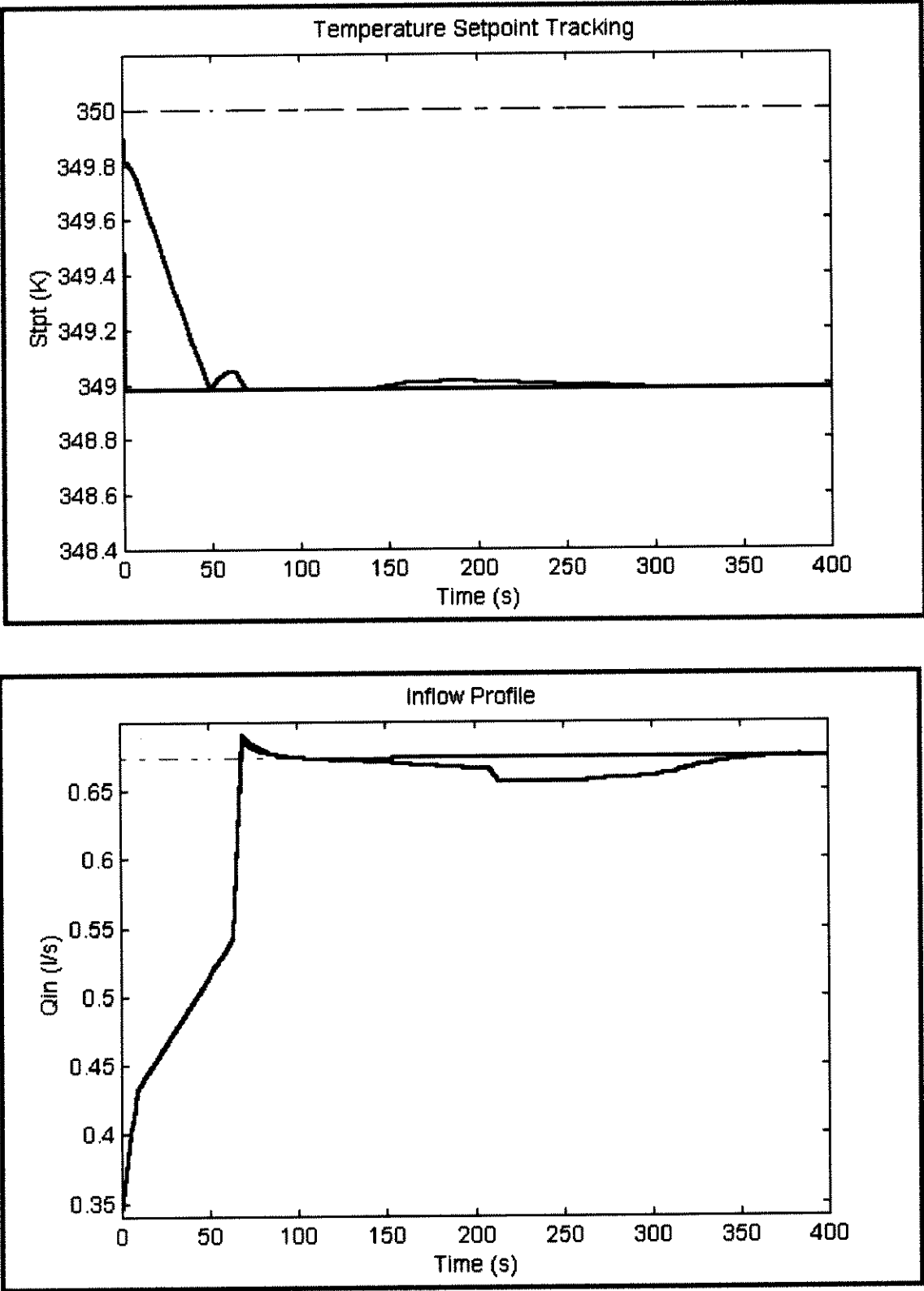


Figure 3.7 Temperature Set Point Policies and Corresponding Inflow Profiles
(Dynamic Closed-Loop Back-Off Case – Class I)
(Green curve: Temperature set point tracking case)
(Red curve: Step change set point policy)

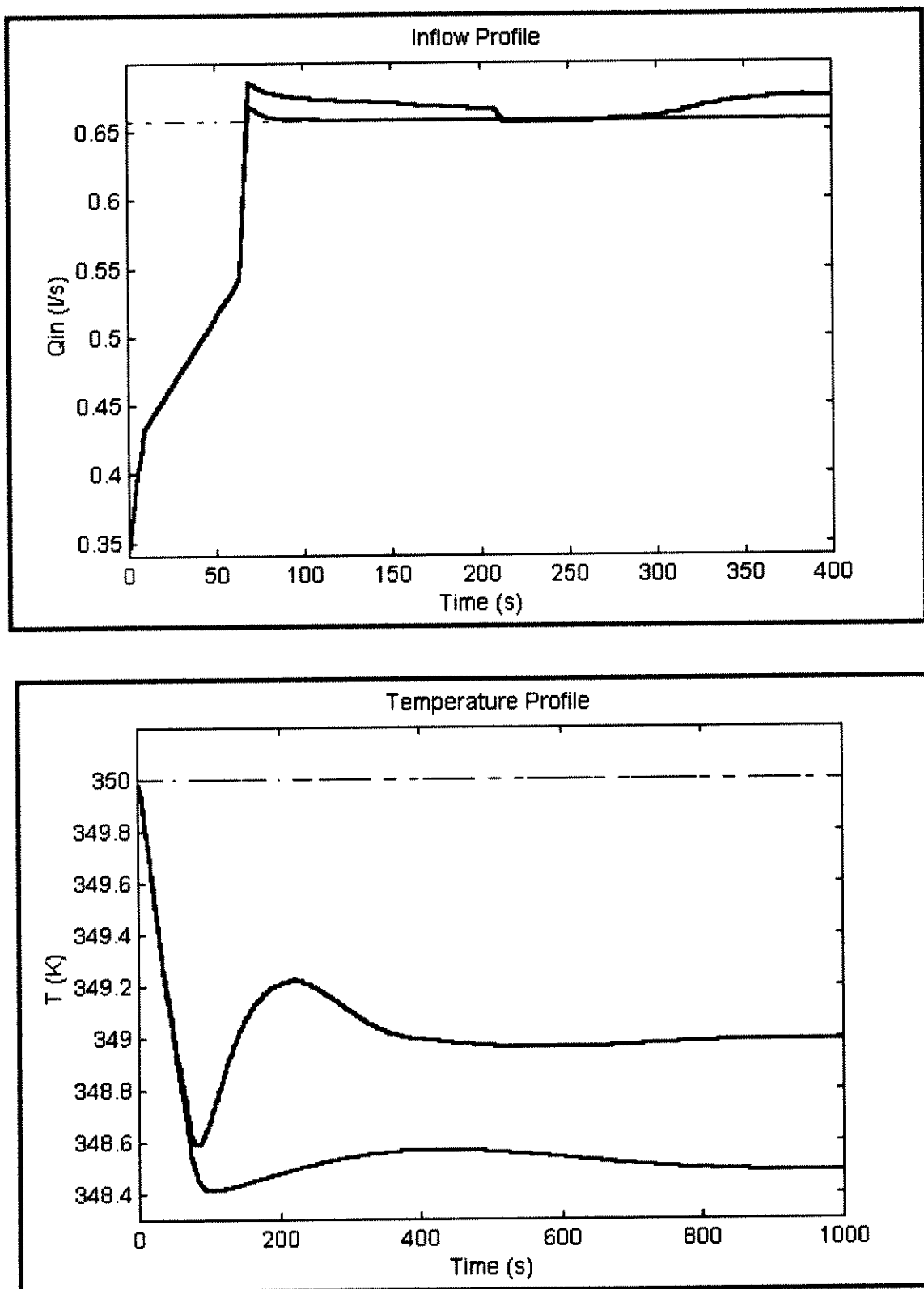


Figure 3.8 Inflow Profiles and Corresponding Temperature Responses

(Dynamic Closed-Loop Back-Off Case)

(Red curve: Class I disturbance)

(Green curve: Class II disturbance)

The inflow profile shown by the green curve in Figure 3.8 is used as an example for testing the feasibility of the solutions. The data points constructing this profile are solutions of the switchability problem at the collocation points (see Figure 3.3). The points provided by GAMS with MINOS optimizer are used again in SPEEDUP to set the values of the feed flowrate that change with time in the dynamic simulation. The External Data Interface (EDI) can be used to transmit numerical values from GAMS to SPEEDUP. This feature will be discussed in the next chapter. A different option is to fit the data points in one or some polynomials of order n^{th} , then use the mathematical expression to define the value of the feed flowrate at any time. For example, the data points constructing the green inflow profile in Figure 3.8, are represented by two straight lines:

$$\text{For } 1 \leq t \leq 9 \quad Q_{\text{in}} = 0.01t + 0.342$$

$$\text{For } 9 \leq t \leq 64 \quad Q_{\text{in}} = 0.002t + 0.414$$

The inflow profile is then approximated by a series of steps. Each step has the value set by the data point. Figure 3.9 shows how well the data points are fitted in the curve. The red curve is the approximating inflow profile, while the green curve plots the data points.

With the feed flowrate known at each time step, SPEEDUP performs dynamic simulations. If the constraints are satisfied with all combinations of disturbances, the solution is feasible. Figure 3.10 plots coolant profiles from SPEEDUP dynamic simulations. The figure presents the trajectories of constraint 4 ($m \leq 8$) and the corresponding temperature profiles, since adjusting the coolant flowrate controls the temperature in the reactor. Constraint 4 is one of the active constraints. During the transition, using a high gain for the temperature controller, the manipulated variable hits the upper bound and remains at this bound for some period of time (red curve). A low gain for the temperature controller results in a less aggressive manipulated variable but the temperature response is more sluggish (green curve). The yellow curve represents a compromising control strategy: a high temperature controller gain with temperature set point tracking. The manipulated variable behaves aggressively for about one minute but the temperature quickly reaches the set point.

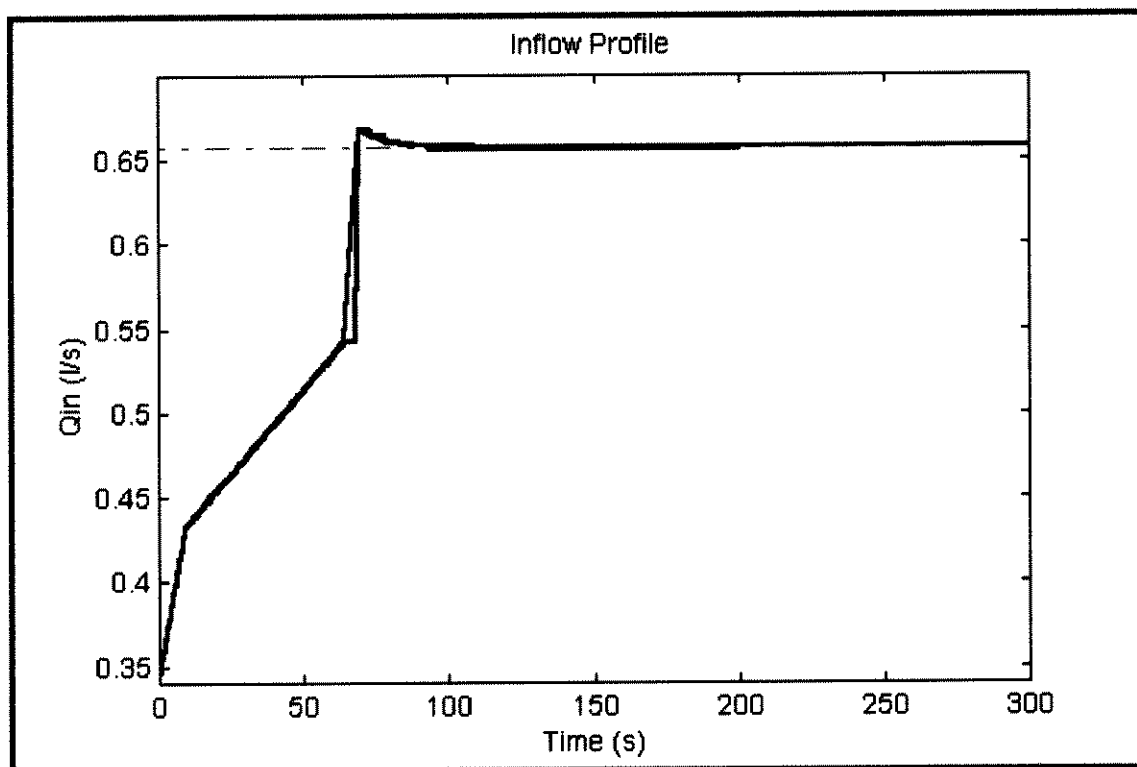


Figure 3.9 Feed Flowrate Curve Fitting (Dynamic Closed-Loop Back-Off Case)

(Green curve: Inflow profile generated by data points)

(Red curve: Approximating inflow profile)

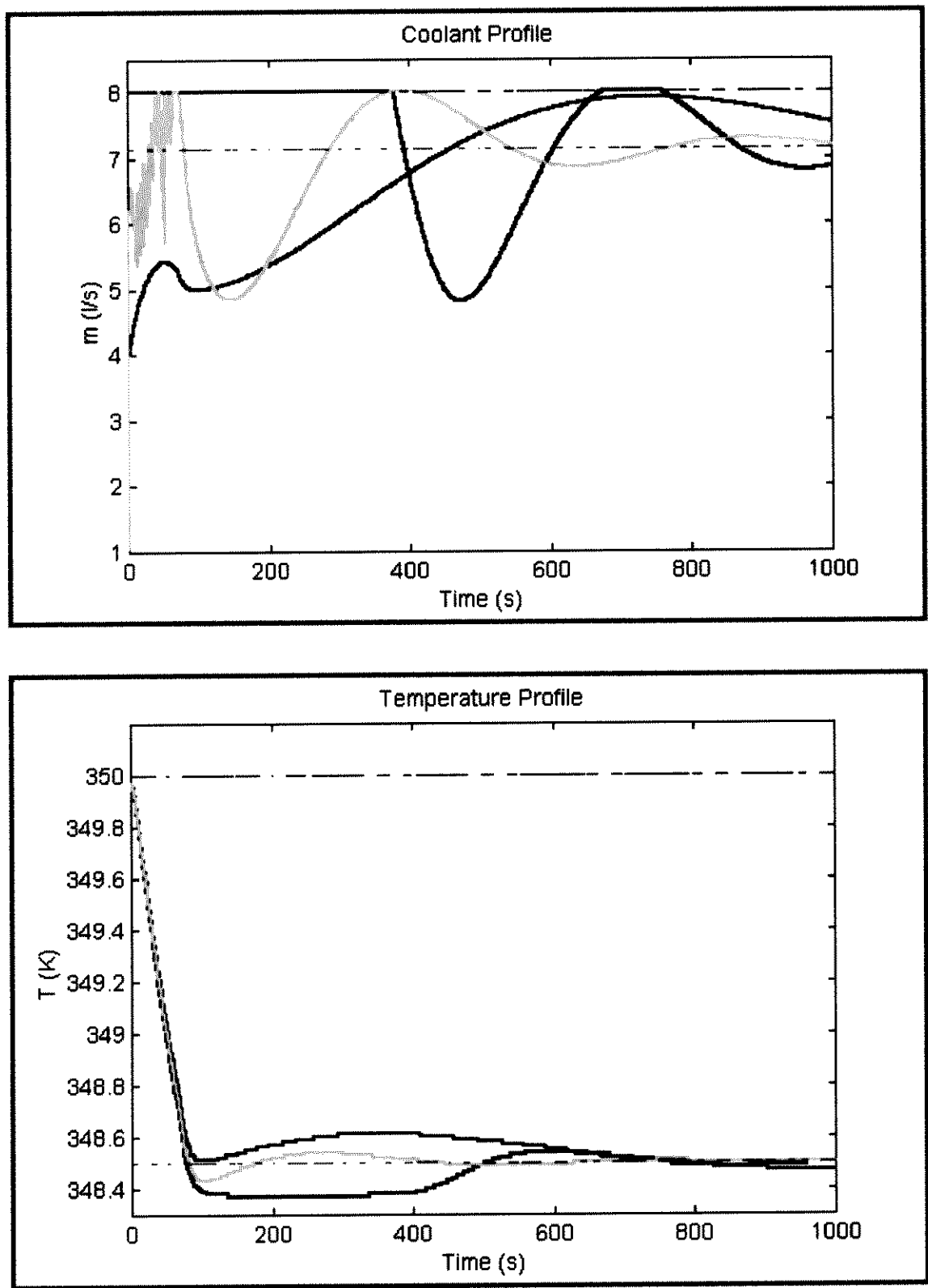


Figure 3.10 Manipulated and Controlled Variable Profiles (From SPEEDUP)

(Green curve: Low temperature controller gain)

(Red curve: High temperature controller gain)

(Yellow curve: High gain and temperature set point tracking)

Some factors that might affect the potential recovery of a dynamic closed-loop back-off problem, the feasibility and optimal solution of a switchability problem are presented through the first case study. In the forward problem the plant moves from high to lower feed concentrations while satisfying all process constraints. In the backward problem the plant has to satisfy the same constraints while switching back from low to higher feed concentrations. These switching problems will be demonstrated in the second case study.

6.2. Case Study 2: Two CSTRs in series

The second case study is the problem of two continuous-stirred tank reactors in series with four control loops, as shown in Figure 3.11. The same set of equality constraints in the first case study is applied for two reactors. Equations (2.12), (2.13) and (2.14) on page 2.21 describe the intermediate mixer. The inequality constraints and the set of uncertain parameters in Chapter 2 are rewritten as:

<i>Safety restriction</i>	$T_1, T_2 \leq 350 \text{ K}$	Constraint 3.1
	$0.3 \leq H_1, H_2 \leq 0.8$	Constraint 3.2
<i>Process limitation</i>	$\text{Cool}_1 \leq 20 \text{ l.K.s}^{-1}$	Constraint 3.3
	$\text{Cool}_2 \leq 15 \text{ l.K.s}^{-1}$	Constraint 3.4
	$0.1 \leq m_1, m_2 \leq 5.0 \text{ l.s}^{-1}$	Constraint 3.5
<i>Maximum, minimum</i>	$0.1 \leq Q_f \leq 0.8 \text{ l.s}^{-1}$	Constraint 3.6
<i>Throughput</i>	$0.05 \leq Q^1_{in}, Q^1_o, Q^2_o \leq 0.8 \text{ l.s}^{-1}$	Constraint 3.7
	$C^2_o \leq 0.3 \text{ mol.l}^{-1}$	Constraint 3.8

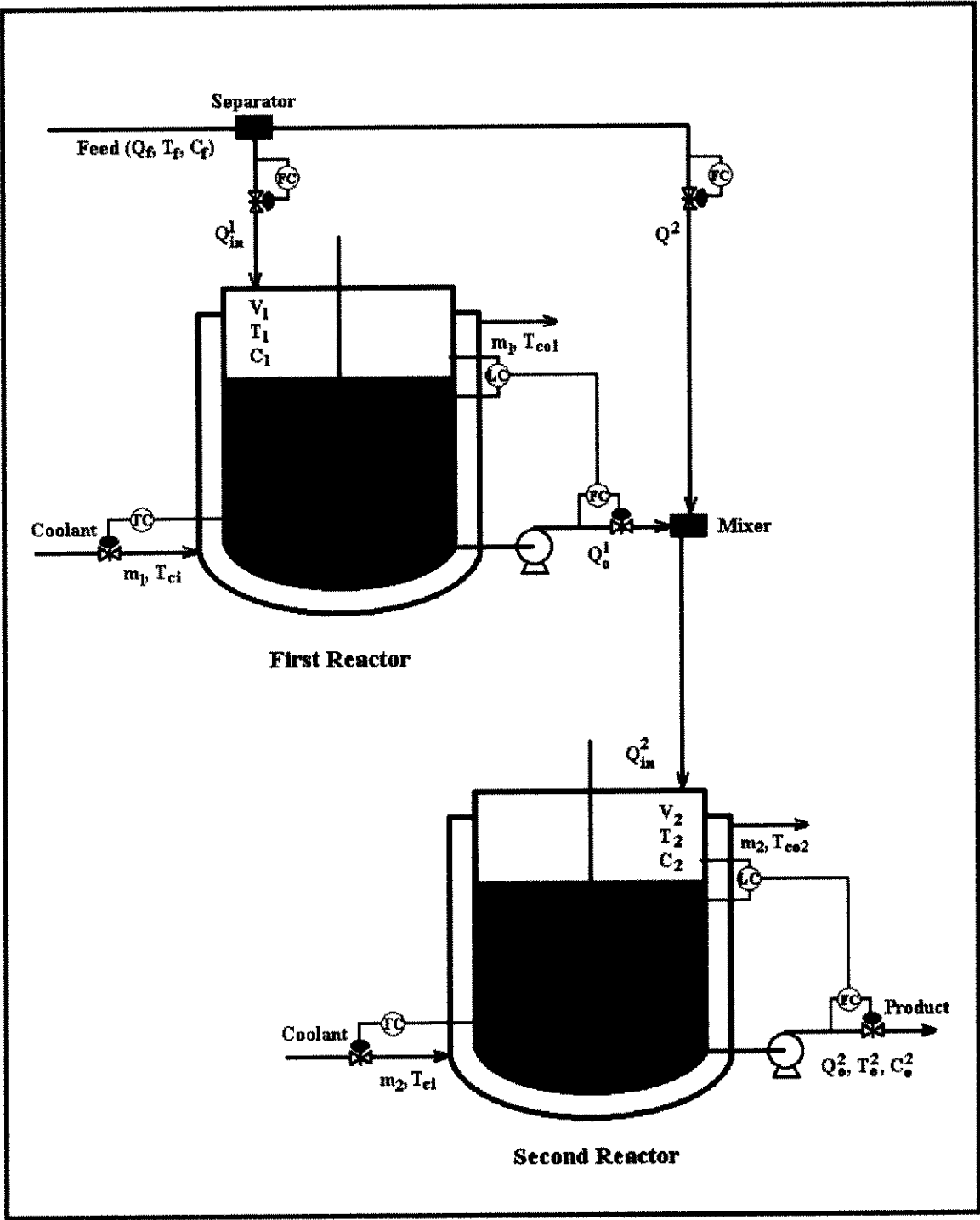


Figure 3.11 Two CSTRs in Series with Temperature and Level Controllers

	Lower Bound	Nominal Value	Upper Bound
$T_{in}(K)$	298	300	305
$T_{ci}(K)$	280	283	286

6.2.1. Dynamic closed-loop back-off problem

The open-loop back-off problem has already been solved in Chapter 2. The back-off operating conditions, which were obtained after four iterations, will be shown again in Table 3.5. The matrix of disturbances and uncertain parameters in the last iteration were:

$$d^n = \begin{bmatrix} T_{in} & T_{ci} \\ 300 & 283 \\ 305 & 286 \\ 305 & 280 \\ 298 & 280 \end{bmatrix}$$

In this chapter, the dynamic closed-loop back-off problem is solved for five decision variables: inventory (V), temperature set point in each reactor (Stpt₁ and Stpt₂), flowrates of two streams from the splitter to the first tank (Q¹_{in}) and to the mixer (Q²). Equation (3.29) defines the objective function.

$$\begin{aligned} \text{Obj } \$/\text{time}) = & pv * Q_R(t=0) * (C_f - C_o^2(t=0)) - mc * Q_R(t=0) * C_f - cc_1 * \text{Cool}^1(t=0) - \\ & cc_2 * \text{Cool}^2(t=0) \end{aligned} \quad (3.29)$$

Since any small change in the first reactor may have a great effect on the second reactor, a sensitivity analysis is carried out first, in order to determine the feasible region of temperature controller gain and reset time. The feasible ranges in this case study are small because of unit interactions. The values of gains and reset times, which give the highest objective index, are selected within the feasible ranges. The configurations of the temperature controllers used in the dynamic back-off problem are $K_{c1} = 0.019$, $\tau_1 = 0.5$, $K_{c2} = 0.14$, $\tau_2 = 10$. Permanent feasible solutions are obtained after two iterations. The open loop back-off and the dynamic closed-loop cases are compared in Table 3.5. The matrix of disturbances in the second iteration is:

$$d_{II}^1 = \begin{bmatrix} T_{in} & T_{ci} \\ 300 & 283 \\ 305 & 286 \end{bmatrix}$$

Case	Objective Index (F \$.hr ⁻¹)	Inventory (V l)	Inflow to CSTR1 (Q ¹ _{in} l.s ⁻¹)	Inflow to Mixer (Q ² l.s ⁻¹)	Set Point T ₁ (Stpt ₁ K)	Set Point T ₂ (Stpt ₂ K)
<i>Nominal</i> T _{in} = 300 T _{ci} = 283	141.4	274	0.551	0.244	350	340.3
<i>Open Loop Back-Off</i> 298 < T _{in} < 305 280 < T _{ci} < 286	116.1	354	0.439	0.220	345.5	335.8
<i>Dynamic Back-Off (Class II)</i> T _{in} → 305 T _{ci} → 286	120.8	201	0.548	0.137	349.5	335.9

Table 3.5 Optimal Operating Conditions (C_{in} = 20)

There is not much difference between the open loop back-off and the dynamic closed-loop back-off cases. In other words, the temperature control loop cannot recover the profit loss caused by disturbances and uncertainties. However, the temperature controllers are still required to keep the operating temperature in the reactors at the set point regardless of possible disturbances.

6.2.2. Switchability problem (to prepare for the shutdown operation)

The switchability problem in this case is moving to the operating state, which is ready for the shutdown operation. When the feed concentration drops by 25%, the total feed goes mostly to the first reactor (Q¹_{in} = 0.75). The stream from the splitter to the mixer reduces to the lower limit (Q² = 0.05). The inventory is also reduced. The problem is solved for the best trajectories of Q¹_{in} and Q². Equation (3.30) is used for the objective function. As the number of variables in this case enormously increases, to

avoid lengthy calculation, the plant is scaled down so that the residence time is ten times smaller. The cases considered to prepare for the shutdown operation are shown in Table 3.6.

$$F = \int_{t_0}^{t_f} \left\{ \sum_{i=1}^2 w_{pi} (Q^i - Q_{sf}^i)^2 + \sum_{i=1}^2 w_{ci} (C^i - C_{sf}^i)^2 + \sum_{i=1}^2 w_{ti} (T^i - T_{sf}^i)^2 + \sum_{i=1}^2 w_{hi} (H^i - H_{sf}^i)^2 \right\} dt \quad (3.30)$$

Cases	First Steady State ($C_{in} = 20$)	Second Steady State ($C_{in} = 15$)	Results
Nominal Condition <i>Fixed Inventory (FI)</i>	$T_{in} = 300$ $T_{ci} = 283$ $Q_{in}^1 = 0.550$ $Q^2 = 0.244$ $V = 274$	$T_{in} = 300$ $T_{ci} = 283$ $Q_{in}^1 = 0.750$ $Q^2 = 0.050$ $V = 274$	Figure 3.12 a,b
Open Loop Back-Off <i>Fixed Inventory (FI)</i> <i>Switching Inventory (SI)</i>	$T_{in} = 300$ $T_{ci} = 283$ $Q_{in}^1 = 0.439$ $Q^2 = 0.220$ $V = 354$ $Q_{in}^1 = 0.439$ $Q^2 = 0.220$ $Stp_h = 0.708$	$T_{in} \rightarrow 305$ $T_{ci} \rightarrow 286$ $Q_{in}^1 = 0.750$ $Q^2 = 0.050$ $V = 354$ $Q_{in}^1 = 0.750$ $Q^2 = 0.05$ $Stp_h = 0.360$	Figure 3.13 Figure 3.14 a, b, c
Closed-Loop Back-Off Class II <i>Step-Change Temperature Set Point</i>	$T_{in} = 300$ $T_{ci} = 283$ $Q_{in}^1 = 0.524$ $Q^2 = 0.126$ $Stpt_1 = 348.8$ $Stpt_2 = 334.6$ $V = 240$	$T_{in} \rightarrow 305$ $T_{ci} \rightarrow 286$ $Q_{in}^1 = 0.750$ $Q^2 = 0.05$ $Stpt_1 = 339.3$ $Stpt_1 = 328.1$ $V = 240$	Figure 3.15 Figure 3.16 Figure 3.17

Table 3.6 Different Shutdown Cases

❖ Nominal condition

This case solves for the trajectories connecting the nominal conditions. It is assumed that there is no disturbance on the process and the plant is operating at nominal conditions. The effects of level controller gain and reset time on optimal solutions are plotted in Figure 3.12. The integral squared deviation objective function reduces with a higher gain and reset time up to a certain limit. Using high values of gain beyond that limit, the problem fails to converge. Without a temperature control loop, the plant has to operate at the open loop back-off condition during a normal operation. Therefore, switching operations under back-off conditions are studied with more emphasis.

❖ Open loop back-off condition

This case solves for the trajectories connecting the open-loop back-off operating conditions presented in Table 3.6. Figure 3.13 shows the effect of constraints posed on response time of the inlet valve. Due to these constraints the flow from the splitter to the mixer reduces by half then remains constant for a period of time before completely being off. The feed trajectory to the reactor is shifted forward (red curves). To prepare for the shutdown operation, the valve connecting the splitter and the mixer is closed and the flow of this stream tends to the lowest limit. Meanwhile, the valve connecting the splitter and the reactor is fully opened so all the flow from the splitter goes to the first reactor. Figure 3.14 compares FI (green curves) and SI (red curves). The plots indicate FI switching has shorter flow trajectories, lower temperature drops and smoother outflow. The SI case is harder to achieve because it is a mixture of regulator and servo problems. However, it truly prepares for a shutdown operation in which the feed concentration drops, the by-pass stream is off, operating temperatures and the inventories reduce optimally.

❖ Dynamic closed-loop back-off condition

This case finds the switching policy between dynamic closed-loop back-off operating conditions when all level and temperature control loops are closed. Multiple disturbances (Class II) are considered to compare with the previous condition. The switchability problem in this case is very expensive to solve because of its large size.

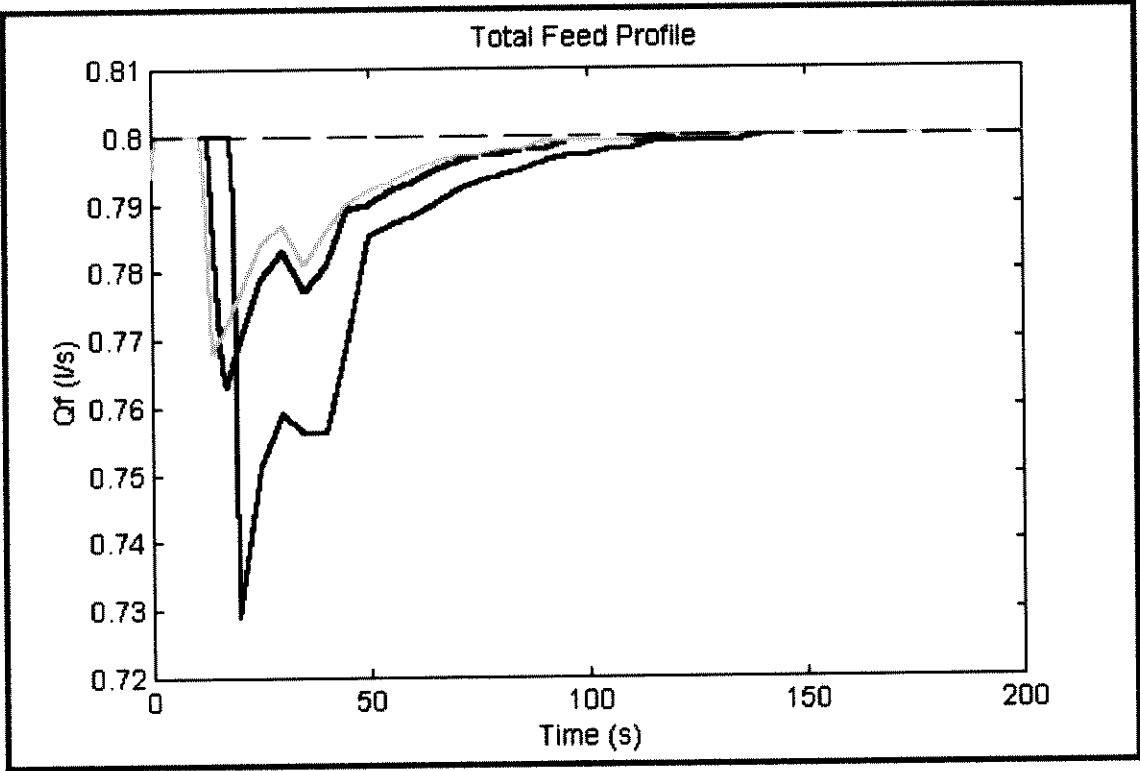


Figure 3.12a Effect of Level Controller Gain (Nominal Case)
(Green: Gain = 4, Red: Gain = 8, Yellow: Gain = 11)

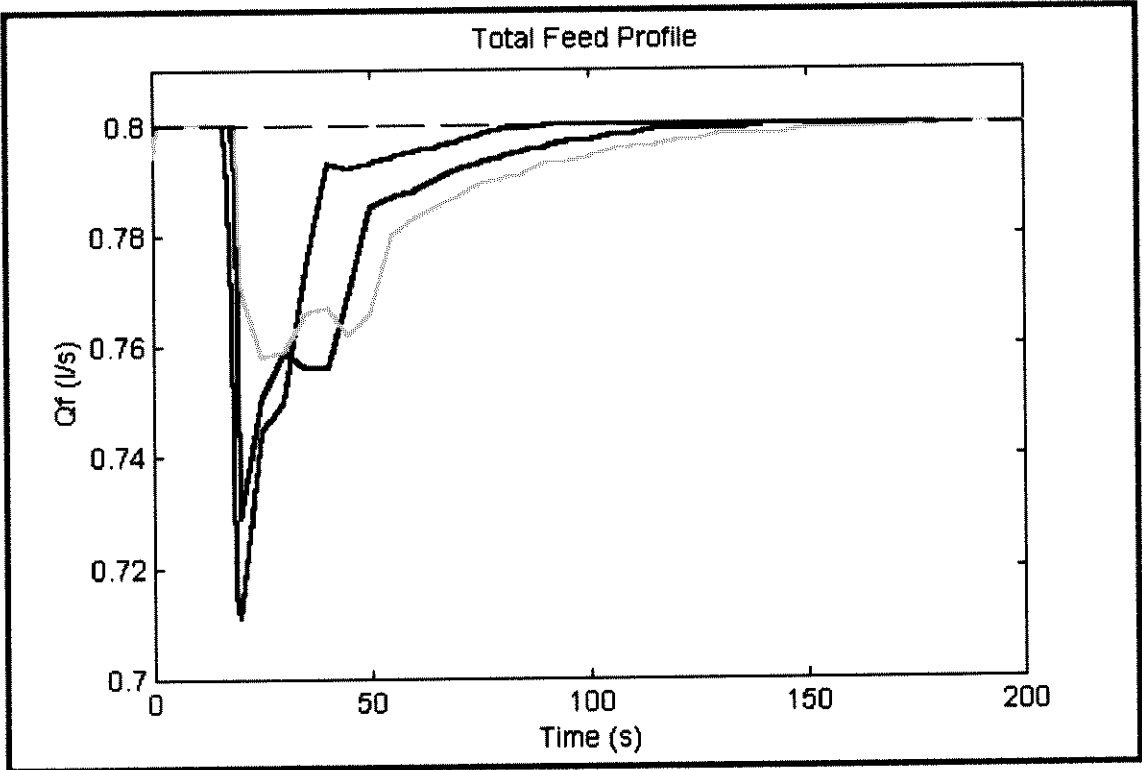


Figure 3.12b Effect of Level Controller Reset Time (Nominal Case)
(Green: Reset Time = 10, Red: Reset Time = 20, Yellow: Reset Time = 30)

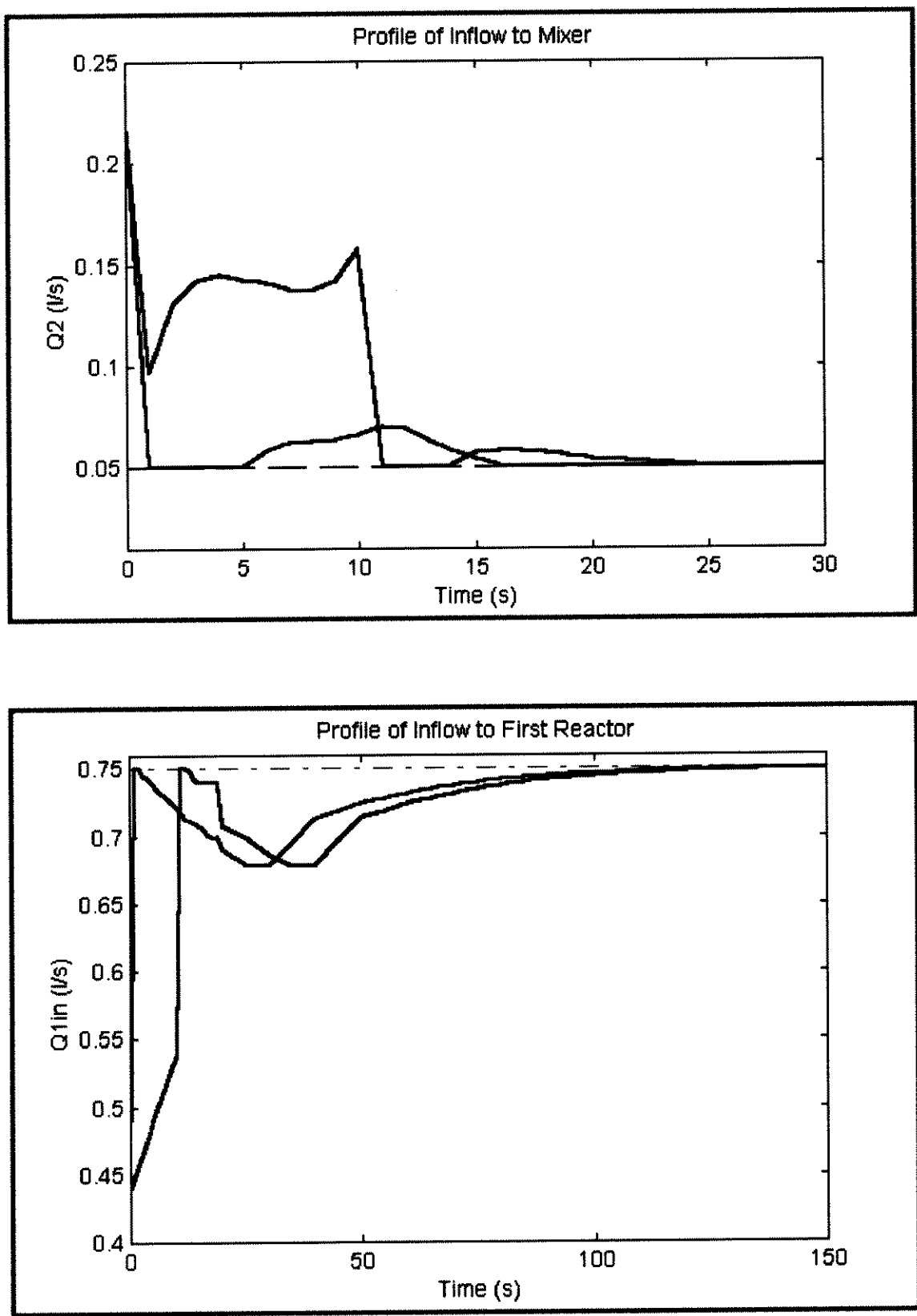


Figure 3.13 Effect of Constraint on Inlet Valve (Open Loop Back-Off Case)

(Green curve: No constraints on inlet valve)

(Red curve: Constraints on inlet valve)

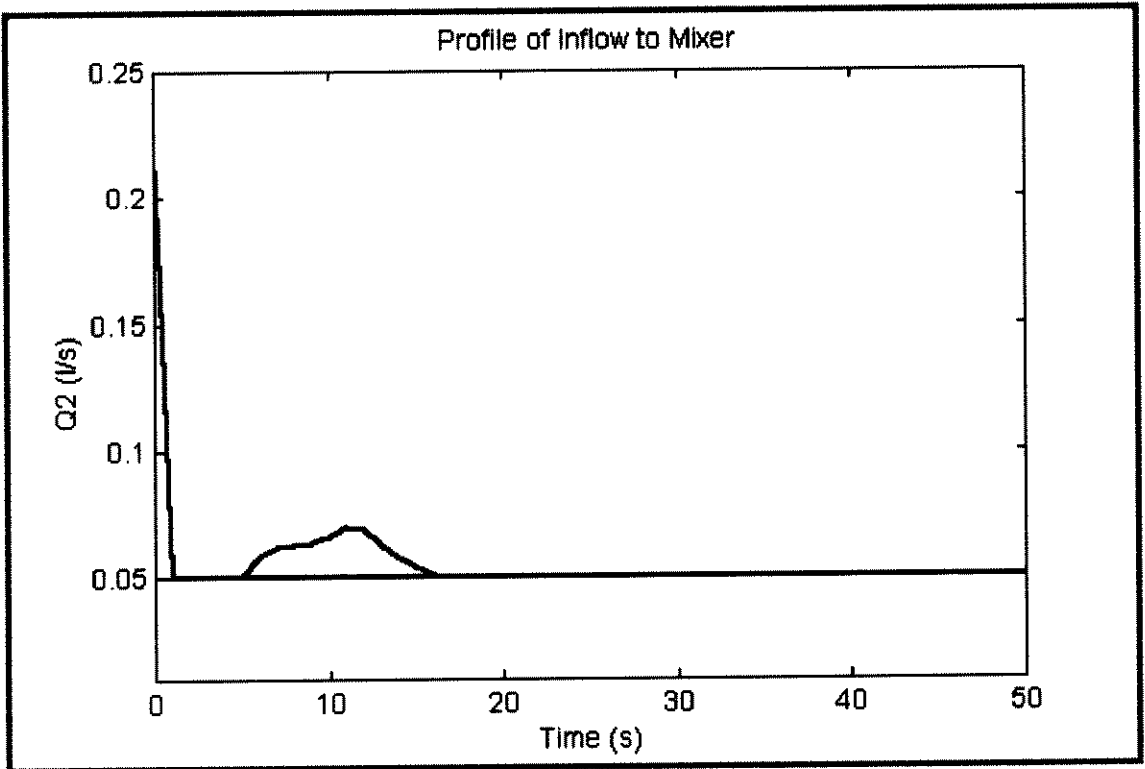
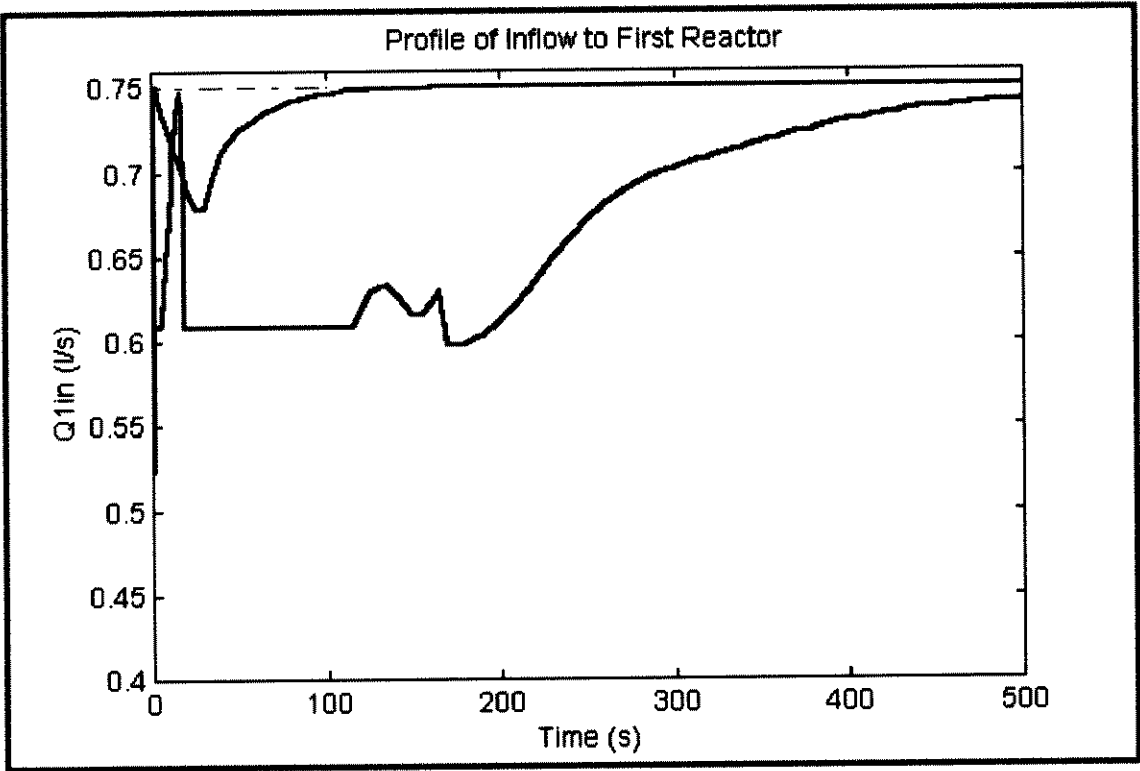


Figure 3.14a Inflow Profiles (Open Loop Back-Off Case)

(Green curve: Fixed Inventory (FI) case)

(Red curve: Switching Inventory (SI) case)

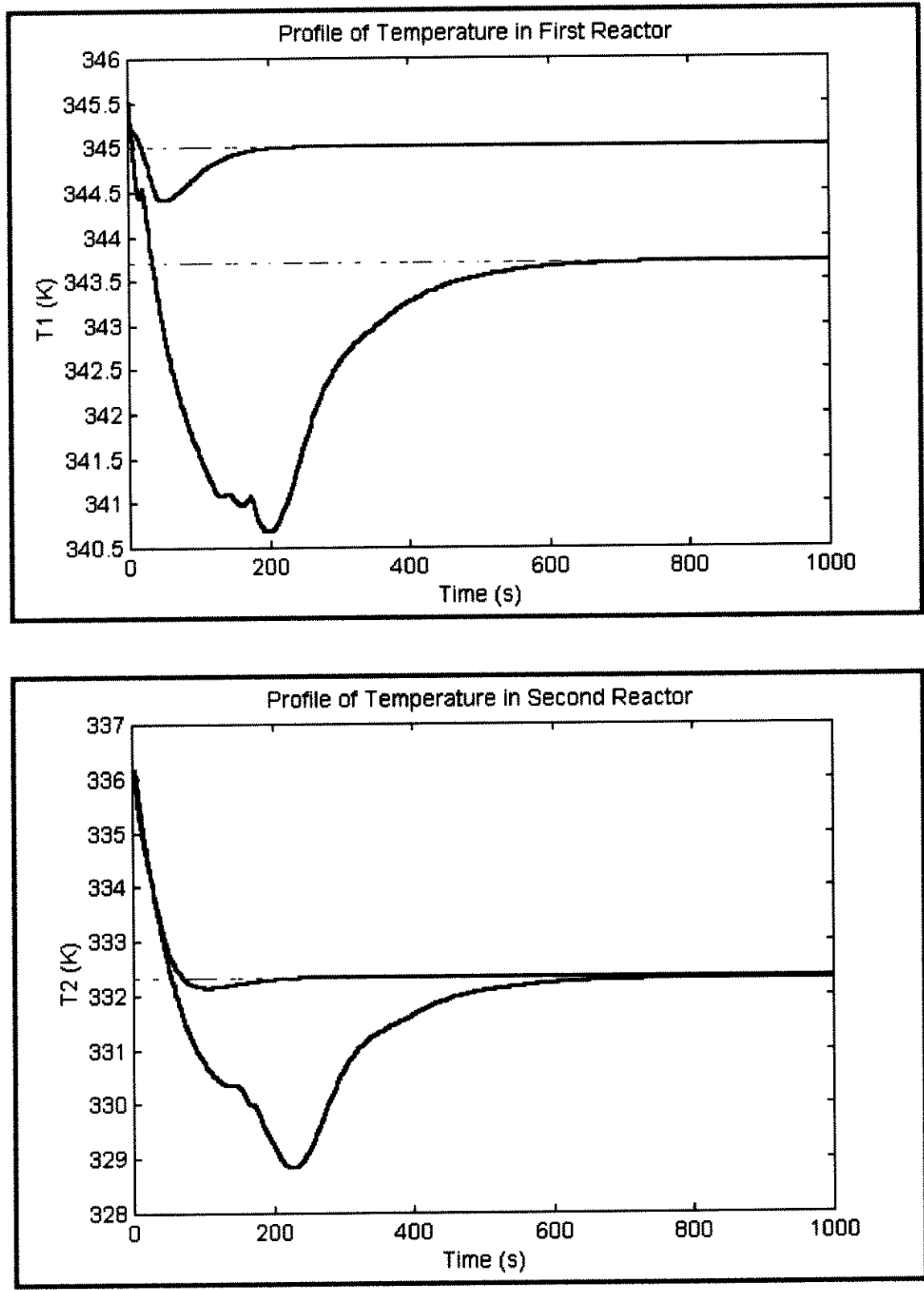


Figure 3.14b Temperature Profiles (Open Loop Back-Off Case)
(Green curve: Fixed Inventory (FI) case)
(Red curve: Switching Inventory (SI) case)

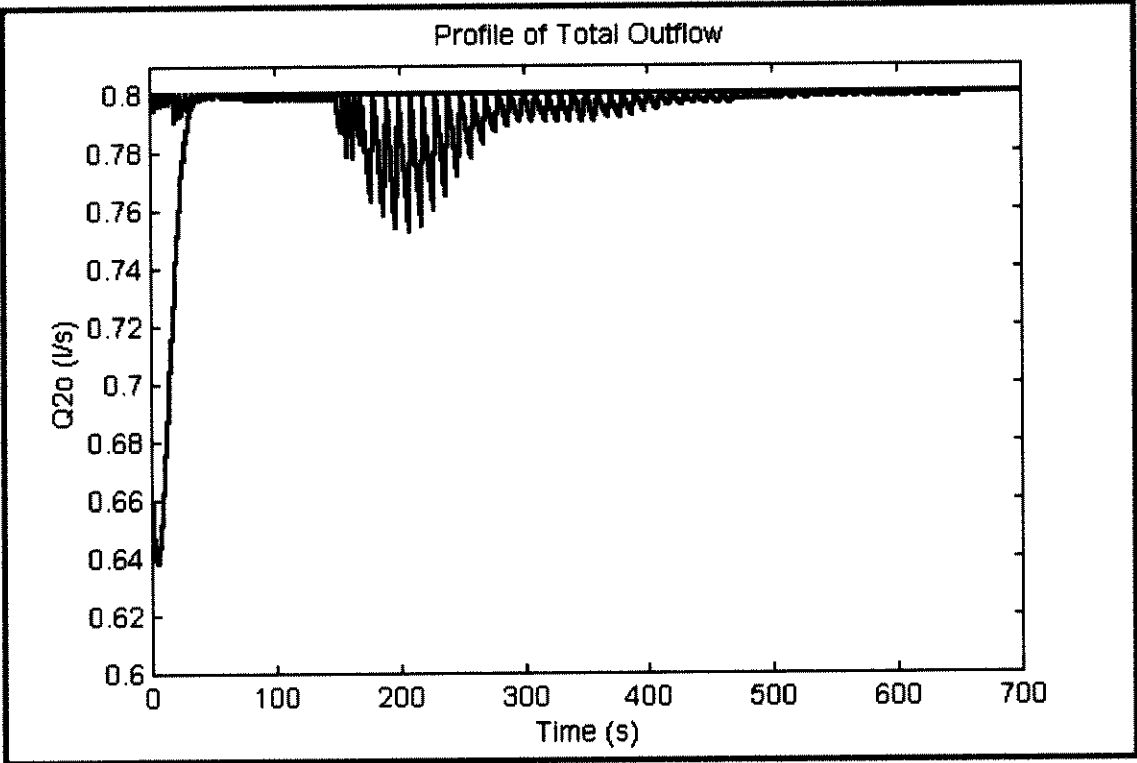


Figure 3.14c Total Outflow Profiles (Open Loop Back-Off Case)
(Green curve: Fixed Inventory (FI) case)
(Red curve: Switching Inventory (SI) case)

Table 3.7 lists sizes of open loop and closed-loop back-off problems, and limits in the solver (MINOS) for comparison.

	Open Loop Back-Off	Closed-Loop Back-Off	MINOS
<i>Number of single equations</i>	7937	14047	32767
<i>Number of single variables</i>	8415	15137	32767
<i>Work space required to solve</i>	7 MB	12.7 MB	

Table 3.7 Sizes of Back-Off Problems and Limits in The Solver

Figure 3.15 compares inflow profiles of open and closed-loop conditions. These profiles will be fed back later, as inputs in the dynamic simulations, with different combinations of disturbances to test the feasibility of the solutions. As mentioned before, the temperature control loop cannot recover the profit loss caused by disturbances and uncertainties, but it is essential to maintain the operating temperature in the reactors at the set point. This feature will be shown in the following section.

6.2.3. Testing the feasibility of the solutions

The optimal trajectories of the inlet flowrates (Q_{in}^1) and (Q^2) found in the above cases are tested with different combinations of disturbances:

$$298K \leq T_{in} \leq 305K$$

$$280K \leq T_{ci} \leq 286K$$

For the open loop back-off condition all constraints listed on page 3.46 are satisfied with T_{in} and T_{ci} varying within the lower and upper bounds. For the dynamic closed-loop back-off condition, constraint 3.4 ($Cool_2 \leq 15$) is violated, when T_{in} changes from its nominal value to the upper bound and T_{ci} changes from its nominal value to the lower bound.

$$T_{in} = 300K \rightarrow 305K$$

$$T_{ci} = 283K \rightarrow 280K$$

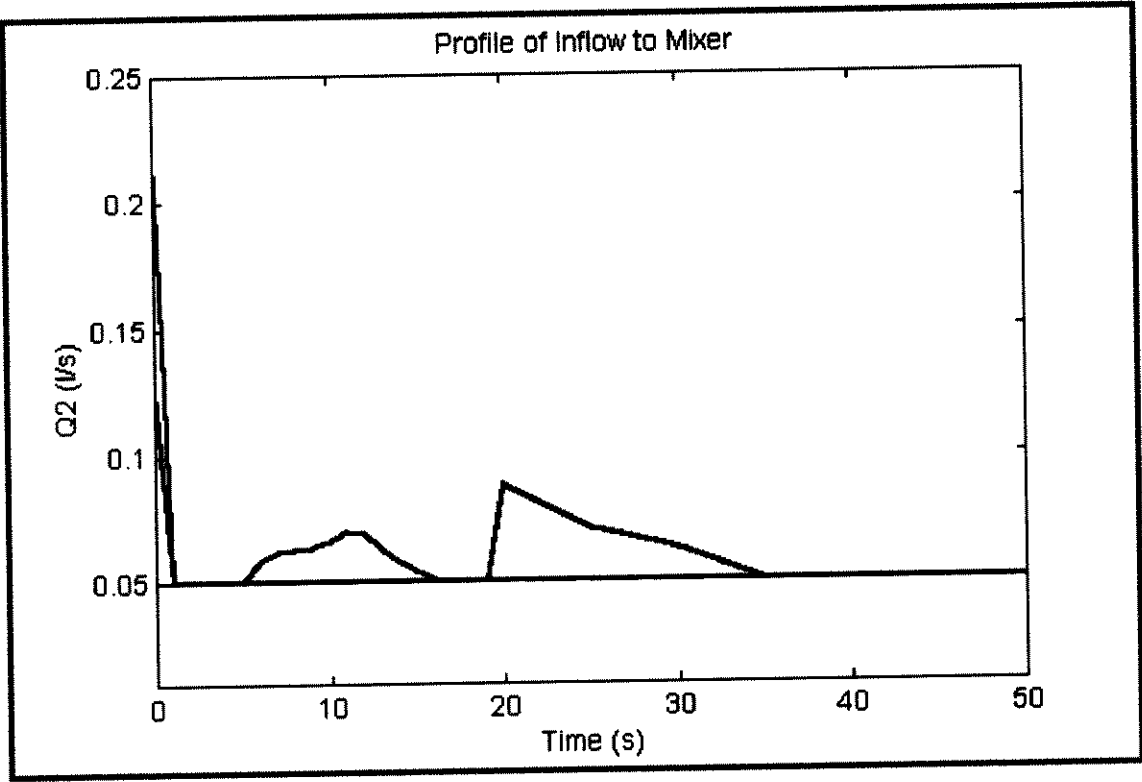
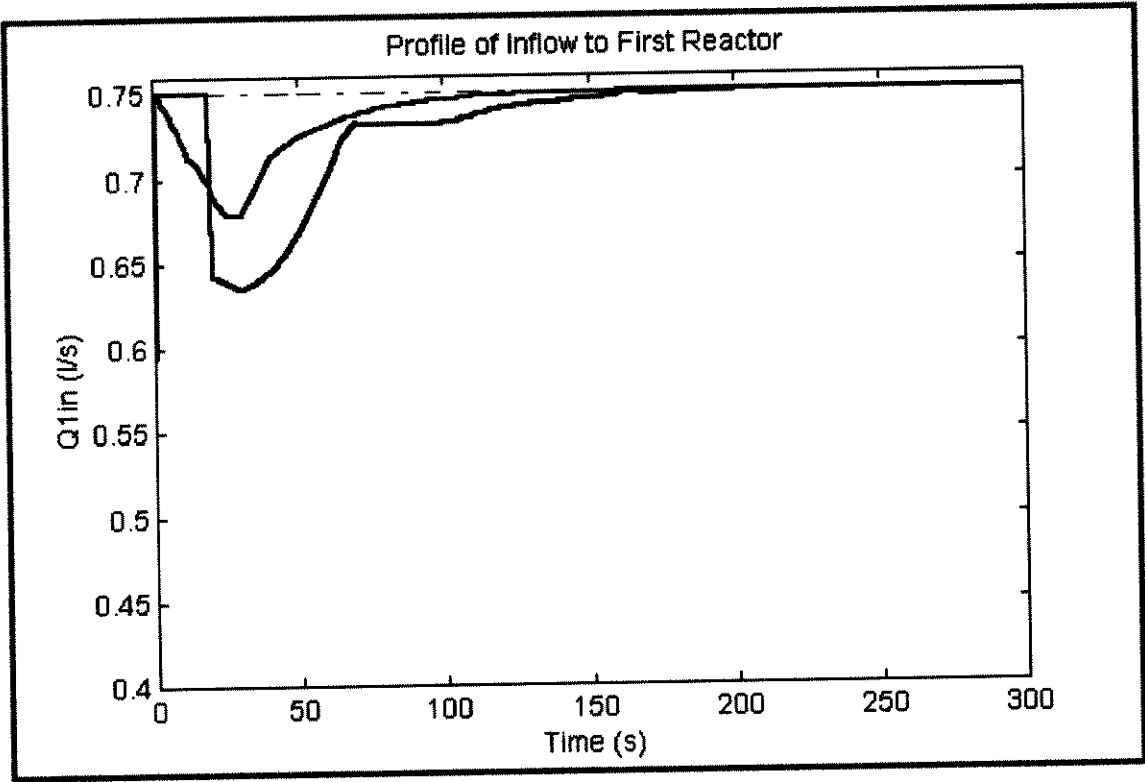


Figure 3.15 Inflow Profiles (Closed-Loop Back-Off Case)
(Green curve: Open loop back-off)
(Red curve: Closed-loop back-off)

The switchability problem must be solved again with the updated matrix of disturbances. A similar procedure has been presented in Chapter 2, but in this case the problems must be solved for two systems of two CSTRs in series, using dynamic optimization techniques. Each system is subject to a different set of disturbances given in the following matrix:

$$d^n = \begin{bmatrix} T_{in} & T_{ci} \\ 305 & 286 \\ 305 & 280 \end{bmatrix}$$

The size of the problem is enormously increased with four CSTRs and eight controllers. The simultaneous optimization and integration technique is not able to handle this case because of the size limitation of the software and the solver. The sequential optimization technique should be used instead but computational time is the main issue. Further discussions on solution methods will be presented in Chapter 5. For this special case study, a simpler remedy can be used. As the path constraint is violated at the very beginning of the trajectory, the switchability problem can be solved again with a small time delay on the temperature set point of the second reactor. The value of this time delay is so small that it does not have any effect on the optimal inlet flowrate trajectories found before, but it changes the cooling profile effectively.

Figure 3.16 plots the profiles of the cooling in the second reactor with different values of disturbances. The corresponding temperature profiles are found in the same figure. These results are obtained from SPEEDUP dynamic simulations.

- Green curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 286K$.
- Red curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 280K$, the cooling exceeds the constraint (blue line).
- Yellow curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 280K$, with a small time delay on temperature set point of the second reactor. The cooling just meets the constraint.

More constraints must be satisfied when introducing the temperature control loop to the plant. These constraints might be limitations of the coolant, the amount of cooling and the controller itself. Since the number of dynamic terms in the switchability problem is increased with the number of controllers in the plant, it is not

easy to solve the fully controlled problem. However, as a trade off, the temperature in the reactor, if controlled, always converges to the set point despite the variations in feed or coolant temperatures. Meanwhile if the temperature is not controlled, then it will vary with any change in feed and coolant temperatures.

As an example, Figure 3.17 plots profiles of temperatures in the first reactor, both controlled and uncontrolled.

- Green curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 286K$
- Red curve: $T_{in} = 300K \rightarrow 298K$ and $T_{ci} = 283K \rightarrow 280K$

In the first graph of Figure 3.17, the reactor temperature might be any point in the area bounded by the red and green curves, when feed and coolant temperatures vary within their lower and upper bounds. The second graph shows the convergence of the controlled temperature and its set point (magenta line).

Up to this stage, only the forward problem, moving from high to lower feed concentrations, has been studied. The last section of this case study is reserved for the backward problem, in which the plant switches back from low to higher feed concentrations while satisfying the same path constraints and under the same effect of disturbances.

6.2.4. Switching from Startup Operating Conditions

The switchability problem under consideration is the reverse case of the FI open loop back-off problem, as shown in Table 3.8. The operating condition of the second steady state in Table 3.6 now becomes condition of the first steady state and vice versa. However, the problem is still subject to the worst case:

$$T_{in} = 300K \rightarrow 305K$$

$$T_{ci} = 283K \rightarrow 286K$$

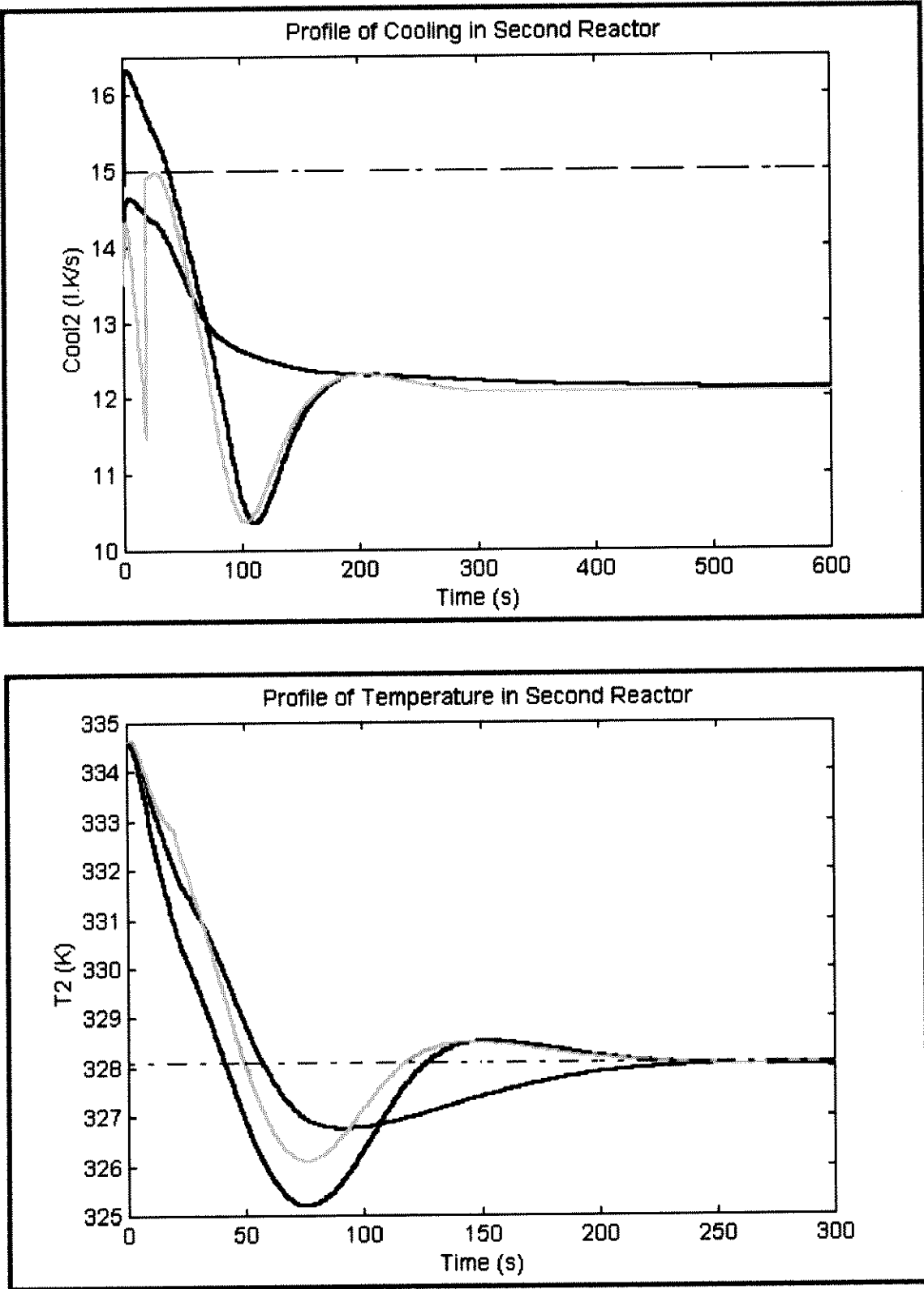


Figure 3.16 Cooling and Corresponding Temperature Profiles (From SPEEDUP)

(Green curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 286K$)

(Red curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 280K$)

(Yellow curve: $T_{in} = 300K \rightarrow 305K$ and $T_{ci} = 283K \rightarrow 280K$, Delay in the set point)

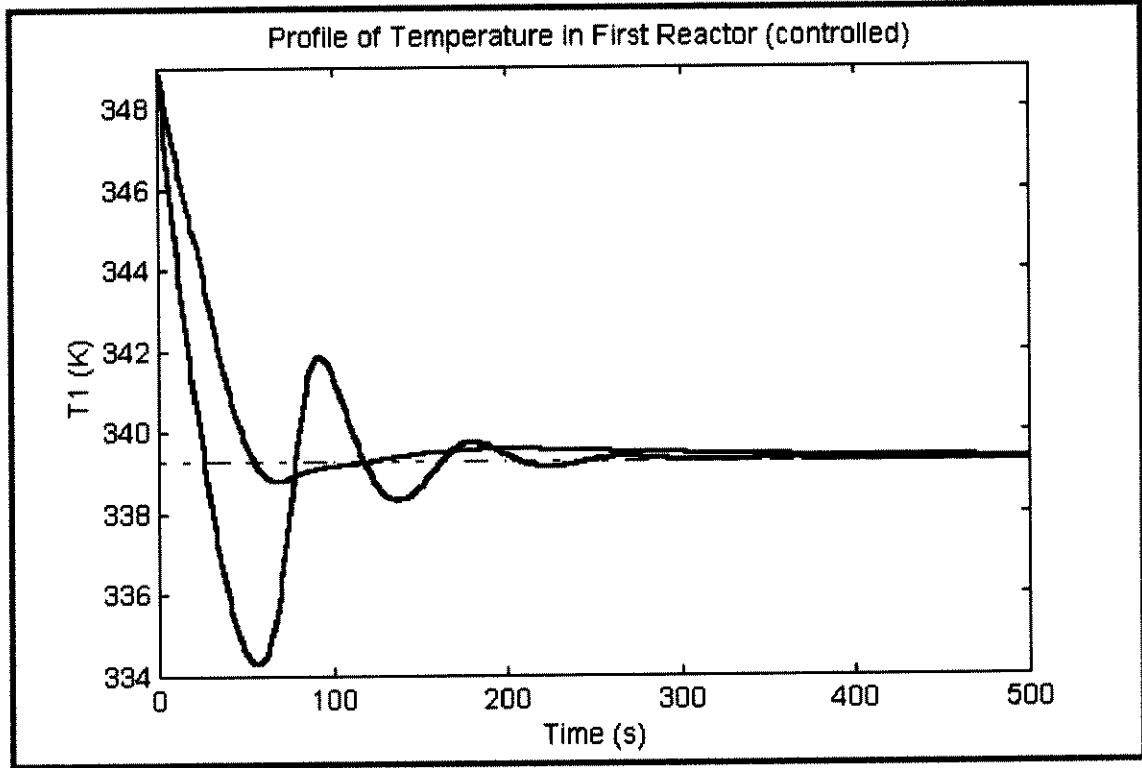
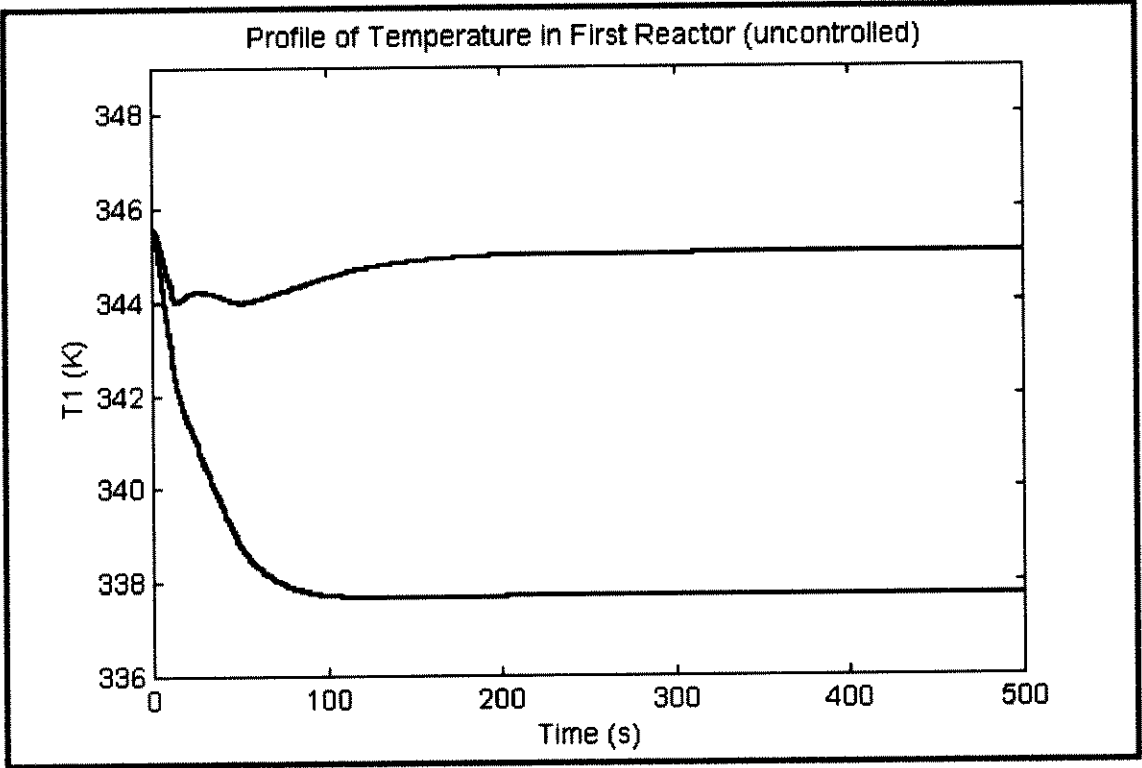


Figure 3.17 Profiles of Temperature in First Reactor (From SPEEDUP)

(Green curve: $T_{in} = 300\text{K} \rightarrow 305\text{K}$ and $T_{ci} = 283\text{K} \rightarrow 286\text{K}$)

(Red curve: $T_{in} = 300\text{K} \rightarrow 298\text{K}$ and $T_{ci} = 283\text{K} \rightarrow 280\text{K}$)

Cases	First Steady State ($C_{in} = 15$)	Second Steady State ($C_{in} = 20$)	Results
Open Loop Back-Off <i>Fixed Inventory (FI)</i>	$T_{in} = 300$ $T_{ci} = 283$ $Q^1_{in} = 0.750$ $Q^2 = 0.050$ $V = 354$	$T_{in} \rightarrow 305$ $T_{ci} \rightarrow 286$ $Q^1_{in} = 0.439$ $Q^2 = 0.220$ $V = 354$	Figure 3.18 a, b

Table 3.8 Switching Case from Startup Operating Conditions

The optimal profiles are limited by constraint 3.1 ($T_1 \leq 350$ K) and constraint 3.8 ($C_2 \leq 0.3$). Inflow, concentration and temperature profiles are plotted in Figure 3.18. As in the first case study, when there is no temperature controller, the temperature deviation term acts like a PI controller with the weighting factor as a controller gain. Responses represented by green curves have a weighting factor ($w_t = 0.01$) ten times greater than red curves ($w_t = 0.001$). Since the temperature weighting factor is increased, the temperature response is faster. However, that extends the period, which the concentration hits the constraint (Figure 3.18b).

7. Conclusion

Chapter 3 considers the changeover policies, startup and shutdown operations of a chemical plant. The switchability problem is simultaneously formulated with the flexibility and controllability problem. The integrated strategy reviewed in Chapter 2 for flexibility is used first to find economically desirable steady state conditions at the beginning and the end of a transition. Minimizing the integral squared deviation of the variables is the next search for optimal trajectories connecting two ends of a switch. The dynamic optimization problems generated in these steps are solved using two different techniques. The simultaneous optimization and integration approach can handle the path constraints and reduce computational time but cannot be used for large and complicated problems. The sequential optimization approach converges slowly but is more practical for engineering applications. Further comparison of solution methods will be discussed in Chapter 5.

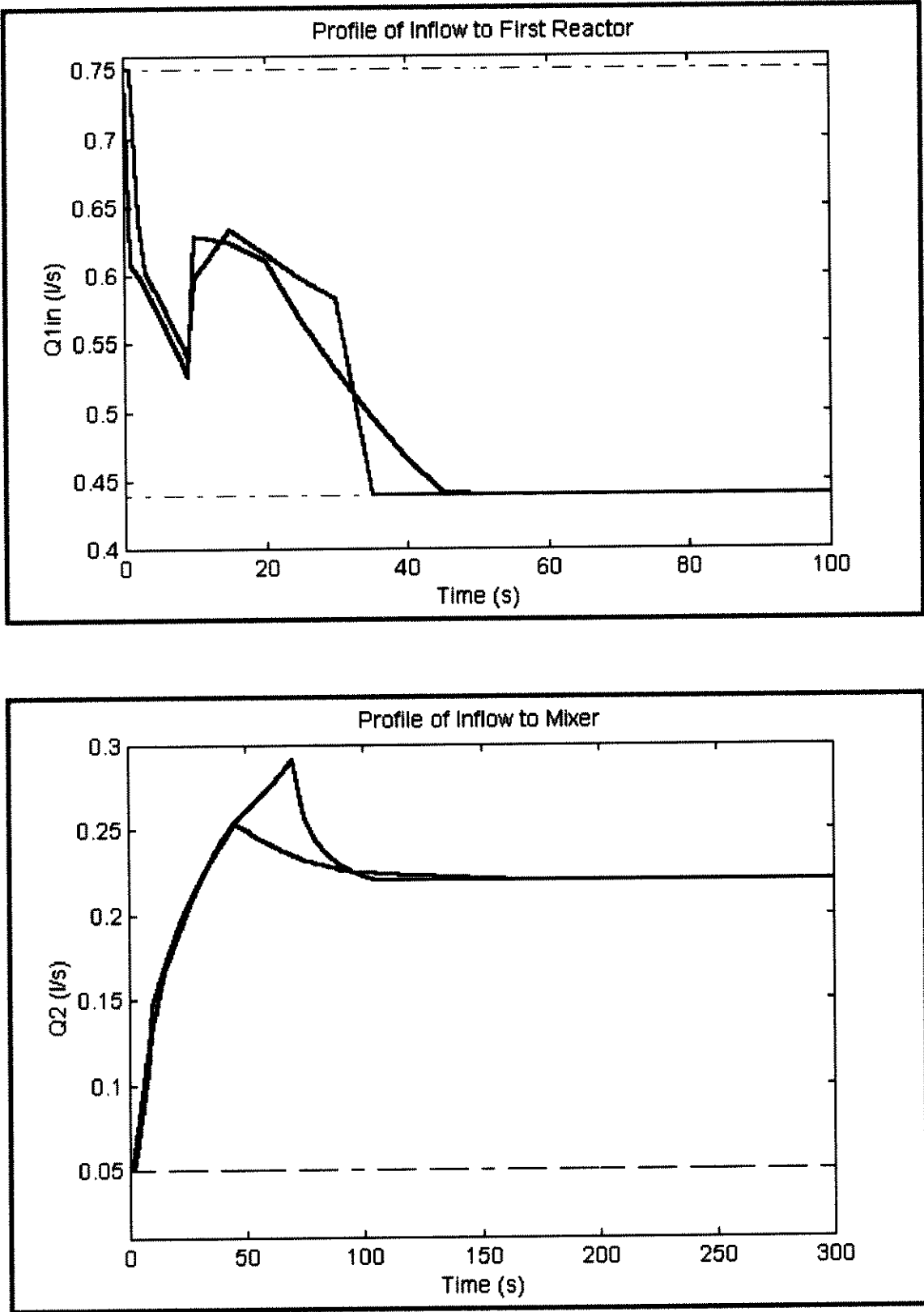


Figure 3.18a Inflow Profiles (Open-Loop Back-Off Case / Startup Problem)

(Green curve: Temperature-weighting factor $w_t = 0.01$)

(Red curve: Temperature-weighting factor $w_t = 0.001$)

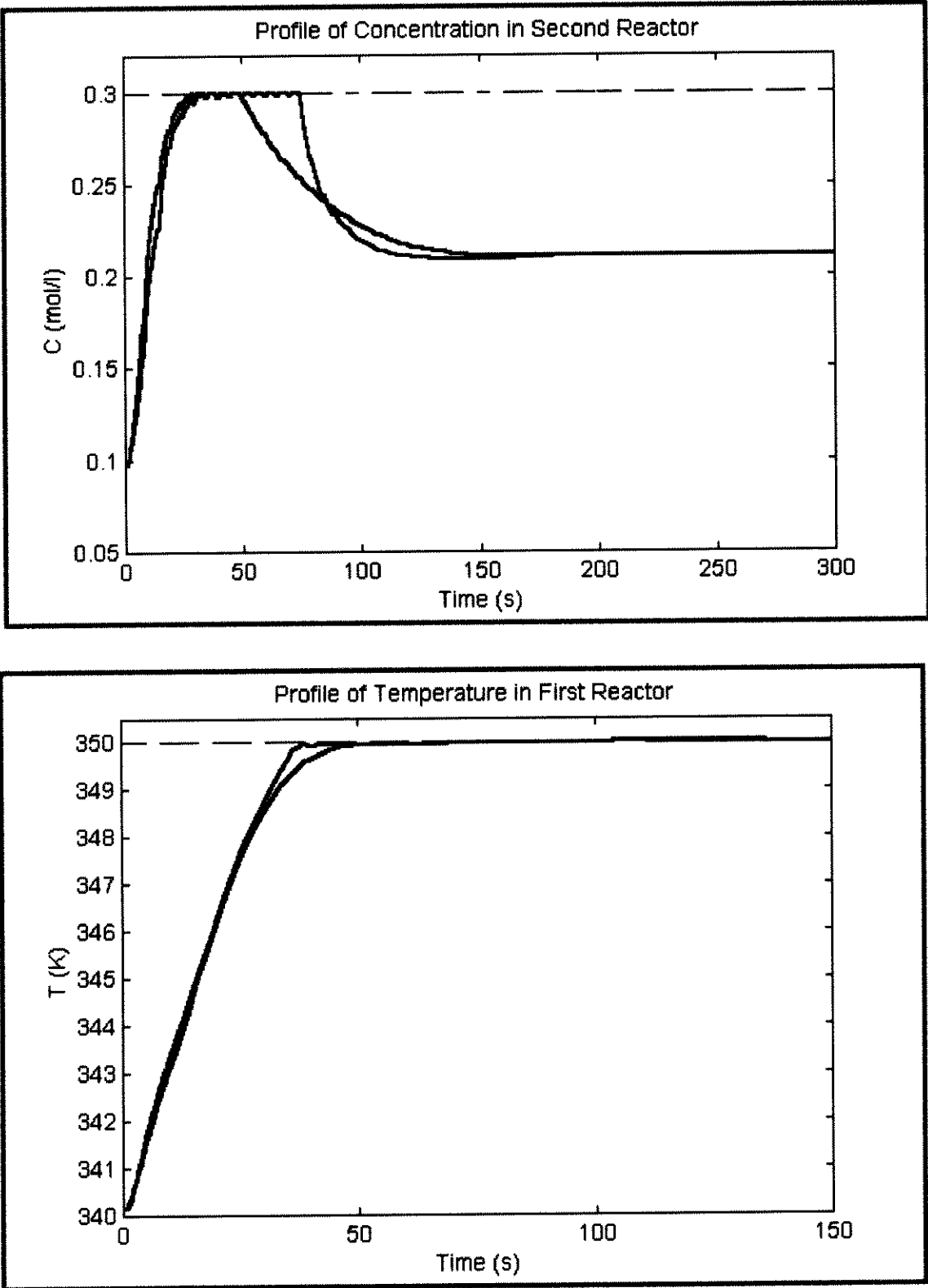


Figure 3.18b Concentration and Temperature Profiles

(Open-Loop Back-Off Case / Startup Problem)

(Green curve: Temperature-weighting factor $w_t = 0.01$)

(Red curve: Temperature-weighting factor $w_t = 0.001$)

Through the case studies, it is shown that:

- The potential recovery of the profit loss caused by disturbances and uncertainties strongly depends on the control strategy. Controller gain, reset time and even set point might be included in the optimization problem as decision variables.
- Some factors affecting the feasibility and optimal solutions of a switchability problem include number of degree of freedom, weighting factor and control strategy.
- The switching problem involving feed changes accompanied by set point changes is lengthy to solve, since it is a mixture of regulator and servo problem. However, it can avoid abrupt changes in manipulated variables as well as path constraint violations.
- The optimal trajectories from solving the switchability problem subject to the worst condition might not be a feasible solution subject to other combinations of disturbances. Although it is tedious and time consuming, feasibility tests should always be carried out to guarantee a safe transition.

Chapter 2 and Chapter 3 have shown the important contribution of controllability in flexibility and switchability analysis. Whether it is a dynamic back-off problem or a switchability problem, both are solved off-line and the optimal solutions mainly depend on the control strategies. The next chapter concentrates on the control scheme that can improve the economic performance of the plant.

8. Nomenclature

c_i	: Set of equality constraints
cc	: Cost of cooling, $\$.(l.K)^{-1}$
C	: Concentration, $mol.l^{-1}$
$cool$	: Removal heat from the reactor to the cooling jacket, $l.K.s^{-1}$
cp	: Vector of controller parameters
C_{pc}	: Coolant heat capacity, $kJ.(kg.K)^{-1}$
d	: Vector of disturbances or uncertain parameters
E	: Activation energy, $l.atm.mol^{-1}$
F	: Objective function or flexibility index
g_j	: Set of inequality constraints
H	: Fraction of liquid over tank volume
ko	: Arrhenius constant, s^{-1}
m	: Coolant flowrate = $(m_c C_{pc} / \rho_r C_{pr})$, $l.s^{-1}$
m_c	: Coolant flowrate, $kg.s^{-1}$
mc	: Material cost, $\$.mol^{-1}$

p	: Vector of process constants
p_v	: Product price, \$.mol ⁻¹
P	: Polynomial
Q	: Flowrate, l.s ⁻¹
R	: Residual function
R_a	: Universal gas constant, l.atm.(K.mol) ⁻¹
Rate	: Rate of reaction, mol.s ⁻¹
t	: Integration variable
T	: Temperature, K
u	: Vector of control (independent) variables
U_a	: Overall heat transfer coefficient/($\rho_r C_{pr}$), l.s ⁻¹
V	: Volume, l
x	: Vector of state (dependent) variables
w	: Weighting function

Greek Letters

$\Delta\alpha_i$	: Length of finite element
Γ	: Disturbance region
ΔH_r	: Heat of reaction, kJ.mol ⁻¹
ρ_r	: Density, kg.l ⁻¹
Φ_i, ϕ_i	: Lagrange polynomial
Ψ_i, ψ_i	: Derivative of Φ_i and ϕ_i with respect to t

Superscripts and subscripts

1	: First CSTR
2	: Second CSTR
c	: Coolant
i, o	: Initial
L	: Lower bound
n	: Nominal value
s	: Steady state
f	: Final or feed
U	: Upper bound

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Appendix 3A

Legendre Polynomials	Roots (t _i)	
P ₀ = 1		
P ₁ = 1 - 2t	0.500000000	
P ₂ = 1 - 6t + 6t ²	0.2113248654	0.7886751346
P ₃ = 1 - 12t + 30t ² - 20t ³	0.1127016654	0.5000000000
	0.8872983346	
P ₄ = 1 - 20t + 90t ² - 140t ³ + 70t ⁴	0.0694318442	0.3300094783
	0.6699905218	0.9305681558
P ₅ = 1 - 30t + 210t ² - 560t ³ + 630t ⁴ - 252t ⁵	0.0469100771	0.2307653450
	0.5000000000	0.7692346551
	0.9530899230	
P ₆ = 1 - 42t + 420t ² - 1680t ³ + 3150t ⁴ - 2772t ⁵ + 924t ⁶	0.0337652429	0.1693953068
	0.3806904070	0.6193095931
	0.8306046933	0.9662347571

Table A.1: Roots of Polynomials Defined by Equation (3.5)
(a = 0, b = 0 and w = 1)

Chapter 4

Switchability and Controllability Analysis – Predictive Control Approach

1	Introduction.....	4.1
2	Model predictive control (MPC).....	4.2
2.1	Dynamic matrix control (DMC).....	4.2
2.2	Nonlinear predictive control (NLPC).....	4.5
3	Case studies.....	4.6
3.1	Case study 1: a single CSTR.....	4.7
3.1.1	Dynamic closed-loop back-off problem with DMC...	4.8
3.1.2	Switchability problem with DMC.....	4.18
3.2	Case study 2: two CSTRs in series	4.26
3.2.1	Dynamic closed-loop back-off problem with DMC...	4.30
3.2.2	Switchability problem with DMC.....	4.32
4	Conclusion.....	4.44
5	Nomenclature.....	4.49
6	References.....	4.49
	Appendix 4A.....	4.50
	Appendix 4B.....	4.53

The essential role of controllability in flexibility and switchability analysis has been shown in the last two chapters. An appropriate control scheme may recover the profit loss due to the effect of disturbances and uncertainties on the process. It also leads to the feasibility and the optimal switching policy of the plant. The simultaneous switching and control problems, either regulator or a mixture of regulator and servo problems are achieved with traditional proportional plus integral (PI) controllers. The controller parameters are initially tuned by conventional Ziegler-Nichols method, but they can be included as decision variables in the optimization problems, which are solved off-line. Chapter 4 will consider the predictive control approaches: linear and nonlinear model predictive control (LMPC and NLPC) techniques. Dynamic matrix control (DMC) based on a linear convolution model is the most cited LMPC. DMC can successfully handle process constraints by using on-line measurements to adjust controller settings. Nonlinear predictive control is a direct extension of the LMPC method, which uses nonlinear dynamic process models. NLPC problems have a general mathematical formulation very similar to that of switchability problems. These two techniques are compared with the traditional PI controller in both back-off and switching aspects through the case studies. Different dynamic optimization problems generated in this chapter are solved using the software packages MATLAB and GAMS with MINOS 5.2 optimizer.

1. Introduction

Inexpensive, well-understood linear system analysis and design tools have traditionally controlled chemical processes for the following reasons:

- ❖ There is an analytical solution that can prove rigorous stability and performance in linear systems.
- ❖ Computational time for linear system simulation as well as implementation is small compared to nonlinear system simulation.

Linear system techniques are limited, if the process is highly nonlinear, under the effect of interactions between manipulated and controlled variables or subject to path constraints on manipulated and state variables. During the past two decades progress in nonlinear control theory, combined with computer software and hardware advances have allowed advanced nonlinear control strategies to be successfully

implemented on chemical processes. However, nonlinear control cannot completely replace the “good-old” linear strategies. The proportional-integral-derivative (PID) controllers still remain in most flow and cascade control loops. Bequette (1991) presented a comprehensive review on techniques using an explicit, nonlinear model of the process for control system design or implementation. Among these categories, the model predictive (MP) method will be considered for the aims of the thesis because its formulation is very similar to the switchability formulation. DMC was the first MP structure successfully applied to chemical processes. The use of DMC is adequate for mildly nonlinear processes, which are subject to small range disturbances; otherwise NLPC is required to improve robustness and to handle constraints, unusual dynamics and time delays. The application of MPC to replace PI controllers will be discussed thoroughly in terms of back off from the nominal condition and switching between operating states.

2. Model Predictive Control (MPC)

Since the early 1970s LMPC, specifically DMC, has been increasingly used and improved in a large number of industrial processes. Cutler and Ramaker (1980) originally presented the basic concepts of DMC. Since DMC can only artificially handle constraints through weighting factors, Garcia and Morshedi (1986) developed quadratic dynamic control (QDMC) to explicitly incorporate process constraints, on both manipulated and controlled variables. To cope with highly nonlinear situations, researchers have successfully extended LMPC to NLPC, using nonlinear dynamic process models rather than linear convolution models. Readers are referred to Bequette (1991) for a thorough literature review on MPC. The following sections briefly present the algorithms for DMC and NLPC, with much focus on the variations of these algorithms in the formulation of control and switching problems.

2.1. Dynamic Matrix Control (DMC)

The DMC algorithm requires a discrete impulse response (convolution) model. This model can be obtained directly from the experimental step response without assuming a model structure or from the solution of the dynamic nonlinear model equations. This flexibility is helpful in modeling unusual process behavior. An illustration of developing a convolution model is shown in Appendix 4A (Marchetti et

al. (1983)). It is proved that the dynamic matrix controller (or gain matrix) K_{DMC} , obtained from minimizing the integral squared deviation between predicted and desired outputs, over a prediction horizon V is:

$$K_{DMC} = (A^T [WW] A + [QQ])^{-1} A^T [WW] \quad (4.1)$$

where:

- [WW] : Diagonal weighting matrix = $ww * I_V$
 [QQ] : Diagonal weighting matrix = $qq * I_U$
 I_V, I_U : Identity matrix of size V and U , respectively
 ww : Adjustable parameter (≥ 0), weighting the controlled variable deviation from set point
 qq : Adjustable parameter (≥ 0), weighting the adjustments of the manipulated variable (move suppression factor)

The weighting matrix [WW] and [QQ] are assumed to be diagonal. This assumption is valid when the behavior of one controlled variable does not depend on the behavior of the other controlled variables; otherwise a penalty should be introduced in the appropriate off-diagonal elements in [WW] for the deviations of both variables.

The control action is calculated from the gain matrix:

$$\Delta u = K_{DMC} E' \quad (4.2)$$

The vector containing the future values of the manipulated variables has V rows but only the value in the first row is implemented. The corrected prediction of controlled variables is obtained from:

$$y_{k+j}^c = y_{k+j-1}^c + \sum_{i=1}^N h_i \Delta u_{k+j-i} \quad (4.3)$$

Definitions of the dynamic coefficient matrix A , the matrix of open loop predicted error E' and coefficients of impulse response h_i can be found in Appendix 4A. Model uncertainties and process disturbances are handled by calculating an additive disturbance as the difference between the process measurement and the model prediction at the current time step. The vector of predicted errors is updated and equation (4.2) is applied again to solve for the next control action.

$$d_k = y_k^m - y_k$$

$$y_{k+i}^{pr} = y_{k+i} + d_k \quad (4.4)$$

The predictive control is really an open-loop optimal control strategy with feed back provided by the disturbance estimate (Bequette). The predictive horizon approach is a natural distinguishing characteristic of MPC that allows the incorporation of future set point changes in the control algorithm.

The algorithm shown in the last paragraph is developed for the single-variable case (SISO). However, it can be extended for the multivariable case (MIMO). The equation calculating K_{DMC} still has the same format as equation (4.1) but the matrices now are composed of individual blocks. The development of these blocks is illustrated in Appendix 4B.

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad [WW] = \begin{bmatrix} [WW]_1 & 0 \\ 0 & [WW]_2 \end{bmatrix} \quad [QQ] = \begin{bmatrix} [QQ]_1 & 0 \\ 0 & [QQ]_2 \end{bmatrix} \quad (4.5)$$

The DMC has a large number of adjustable parameters, all of which influence the control performance (Marlin, 1995). In general, the sample period (Δt) should be a small fraction of the closed-loop dynamics. The prediction horizon (V) should be long enough for the closed-loop system to approach its steady state. The control horizon (U) must be shorter than the prediction horizon. A smaller value of U leads to a robust controller that is relatively insensitive to model errors (Seborg, 1989). The weighting for each controlled variable (ww) represents the relative importance of each deviation

from its set point. Increasing this number reduces the deviation of the corresponding controlled variable. The weighting for each manipulated variable (qq) represents the relative importance of the adjustments to each manipulated variable. Increasing this number will slow down the feedback adjustment and reduce the variability of the manipulated variable, which may be required in some circumstances to improve the robustness of the closed-loop system. This feature will be shown in the case studies. As a result, (qq) is referred to as the move suppression factor.

2.2. Nonlinear Predictive Control (NLPC)

Instead of using a linear convolution model to estimate the control action, the NLPC method uses a nonlinear dynamic process model. The aim is to select a set of future control moves (control horizon), in order to minimize a function based on a desired output trajectory over a prediction horizon. The objective function in this case, very similar to that of the switchability problem, is the integral squared deviation of the model predicted outputs from the set point values over the prediction horizon V . The formulation is:

$$\text{Minimize:} \quad F[y(t), u(t), m(t), cp, d^n] \quad (4.6)$$

Subject to:

$$(dy/dt) = f[y(t), u(t), m(t), p, d^n] \quad x_0 = x(0)$$

$$c_i[y(t), u(t), m(t), p, d^n] = 0 \quad i \in E$$

$$g_j[y(t), u(t), m(t), p, d^n] \leq 0 \quad j \in I$$

$$u^L \leq u(t) \leq u^U$$

where:

$$F = \sum_{i=k+1}^{k+V} (y(i) - y(i)_{sp})^2 \quad (4.7)$$

As in the DMC, although the optimization is based on a control horizon, only the first control action is implemented. Plant output is measured, compensation of plant and model mismatch is performed and the optimization problem (4.6) is solved again. For the open-loop systems, which are stable, the initial conditions of state variables can

be obtained from the solution of the dynamic model equations over the previous time step. The predicted output is given by equation (4.4).

LMPC compared to NLPC uses only the step response coefficients, which are assumed to remain constant, as modeling information to calculate the projected effect of past control moves and the effect of future manipulated variable moves on the predicted output (Sistu et al. (1992)). This assumption no longer holds for a nonlinear system. Although NLPC can explicitly handle path constraints on manipulated and controlled variables, the technique also faces some problems. The major disadvantages are in solving the optimization problem. There is no guarantee of convergence and robustness with respect to stability and performance at all time steps. Computational time is an issue as well with complex models that have relatively fast dynamics. In that situation the QDMC might be a better option. A primary modification of the DMC is required for nonlinear processes. Instead of using the convolution model to predict the output over the prediction horizon V , the projection is made by integrating the nonlinear ODEs from the current state over V , keeping the manipulated variable constant. An important assumption has been made that the dynamic matrix A is constant for the calculation of future control moves. That allows using the constant gain matrix K_{DMC} in computing the control action without solving the optimization problem.

The above theory of LMPC and NLPC has been developed for a control problem. The methodology of implementing these control techniques in a simultaneous control and switching problem will be discussed next through the case studies.

3. Case Studies

A review of two case studies in Chapter 3 shows that the plants need temperature control loops to recover profit losses, due to effects of disturbances and uncertainties. To perform a switch on flowrate and inventory, a level controller is essential to avoid overflowing or dry running of the tank. So far the simultaneous switching and control problems, either regulator or a mixture of regulator and servo problems have been achieved with traditional PI controllers. An attempt has been made to improve these linear control techniques. Although a linear control system is used, the verification is performed via simulations using a nonlinear dynamic process model. Furthermore the tuning parameters are included as decision variables in the optimization

problems, and the set-point optimal trajectory is searched as well for the regulator and servo problem. However, all these cases are solved off-line under the worst situation, since there is no means to incorporate set point and load changes in the control algorithm. Because of discontinuity and interactions between manipulated and controlled variables, there is no guarantee of global optimal values of tuning parameters within a large range of searching. Including set point tracking in an optimization problem sometimes results in increasing the size of the problem so much that the solver cannot handle it. MPC techniques are considered to replace PI controllers hopefully to overcome the disadvantage of the linear control technique. At this stage, on-line measurements are not available but some of the problems are designed for on-line implementation. A few assumptions have been made.

1. The nonlinear dynamic process model is perfect. The effects of the manipulated variable on the real plant and the model are identical. Then the feedback signal is equal to the effect of the disturbance on the controlled variable. Instead of using equation (4.4), the predicted output is the solution of the nonlinear dynamic process model.
2. Since there is no information on current disturbances, the simulations are performed under the worst situation and feasibility tests should be carried out to cover all cases that might occur.

A single CSTR represents the SISO case, and two CSTRs in series is an example of the MIMO case. A full-scale plant is used in the following examples to compare the settling time of the process with different control strategies to reach 99% completion.

3.1. Case study 1: A Single CSTR

The first case study is the problem of a single CSTR shown in Chapter 3. This problem is solved again with the following set of disturbances:

	Lower Bound	Nominal Value	Upper Bound
$T_{in}(K)$	298	300	305
$T_{ci}(K)$	280	283	286
$Ua(l/s)$	0.33	0.33	0.33

The equality constraints describing the model and the inequality constraints are found on pages 3.24-3.25.

3.1.1. Dynamic closed-loop back-off problem with DMC

The results shown in Table 4.1 are solutions of the dynamic closed-loop back-off problem with the PI temperature controller. The tuning parameters are: gain, $K_c = 40$ and reset time, $\tau = 100$.

Feed Condition	Inlet Flowrate ($Q_{in} \text{ ms}^{-1}$)	Set Point Temp. ($Stp_t \text{ K}$)	Inventory (V l)
$T_{in} = 300 \rightarrow 305$ $T_{ci} = 283 \rightarrow 286$ $C_{in} = 20$	0.342	349.97	360
$T_{in} = 300 \rightarrow 305$ $T_{ci} = 283 \rightarrow 286$ $C_{in} = 15$	0.657	348.53	360

Table 4.1 Dynamic Closed-Loop Back-Off Operating Conditions (A Single CSTR)

The operating conditions in Table 4.1 are also used in the switching problem as the first and final steady-state conditions. Some following figures plot outputs of the closed-loop plant, operating at the dynamic back-off conditions. The DMC is introduced to compare with the PI controller. Equations (3.22) and (3.23), related to the temperature PI controller, are replaced by the following equations to calculate the vector of control actions over the prediction horizon. The terms in the bracket indicate matrices or vectors.

$$[dMV] = [K_{DMC}][E'] \quad (4.8)$$

The gain matrix K_{DMC} is given by equation (4.1). The dynamic coefficient matrix A is constructed on the response curve to a unit step change in coolant flowrate. That graph plots temperature difference against time. Further discussion on the matrix A will be presented later. The matrix of open loop predicted error E' in this case becomes:

$$[E'] = [Stp_t] - [T^{pr}] \quad (4.9)$$

where:

$$\begin{aligned} d_k &= T_k - T_{meas} \\ T_{k+i}^{pr} &= T_{k+i} - d_k \quad i = 1, 2, \dots, V \end{aligned} \quad (4.10)$$

Here the subscripts “meas” and “k” denote on-line measured values and values at the current time step, respectively. Vector T is the set of temperatures obtained from solving the dynamic process model equations (equations 2.5 – 2.10).

[dmv] has V rows but only the value in the first row is implemented. After each sample time, the matrix [dmv] will be updated to include the first row of [dmv] and all elements of [dmv] can be summed up to obtain the value of the manipulated variable used in the next step.

$$m = \sum [dmv] + m_{ss} \quad (4.11)$$

If the DMC replaces the PI temperature controller, equation (4.11) is used instead of equation (3.22) to calculate the coolant flowrate.

The effects of DMC tuning parameters on responses are also discussed. For this simple plant, the DMC does not offer any significant advantage over a well-tuned PI. As shown in Figure 4.1, DMC and PI controllers give very similar temperature responses. The green curve is the response of the PI controller, red and yellow curves are of the DMC. The configuration used for the DMC includes $\Delta t = 5$; $V = 40$; $U = 1$; $ww = 1$; $qq = 0$ (red curve) or 10 (yellow curve). Both figures plot temperature responses of the plant, operating at (a) the first condition ($C_{in} = 20$) and (b) the final condition ($C_{in} = 15$) for step changes in feed and coolant temperatures ($T_{in} = 300 \rightarrow 305$; $T_{ci} = 283 \rightarrow 286$). In case (b), $qq=15$ (yellow curve) is used instead of $qq = 10$ as in case (a) because the flowrate at the final state is higher than at the first.

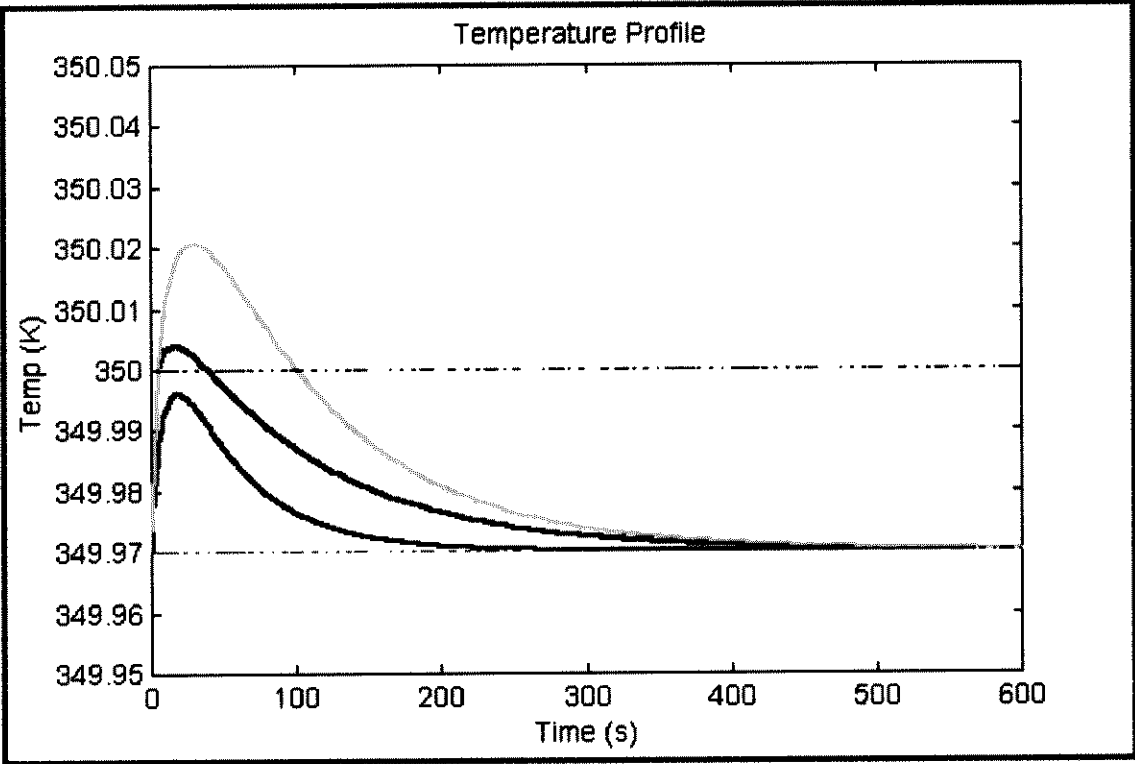


Figure 4.1a Temperature Response (First Operating Condition)

(Green: PI controller; Red: DMC with $qq = 0$; Yellow: DMC with $qq = 10$)

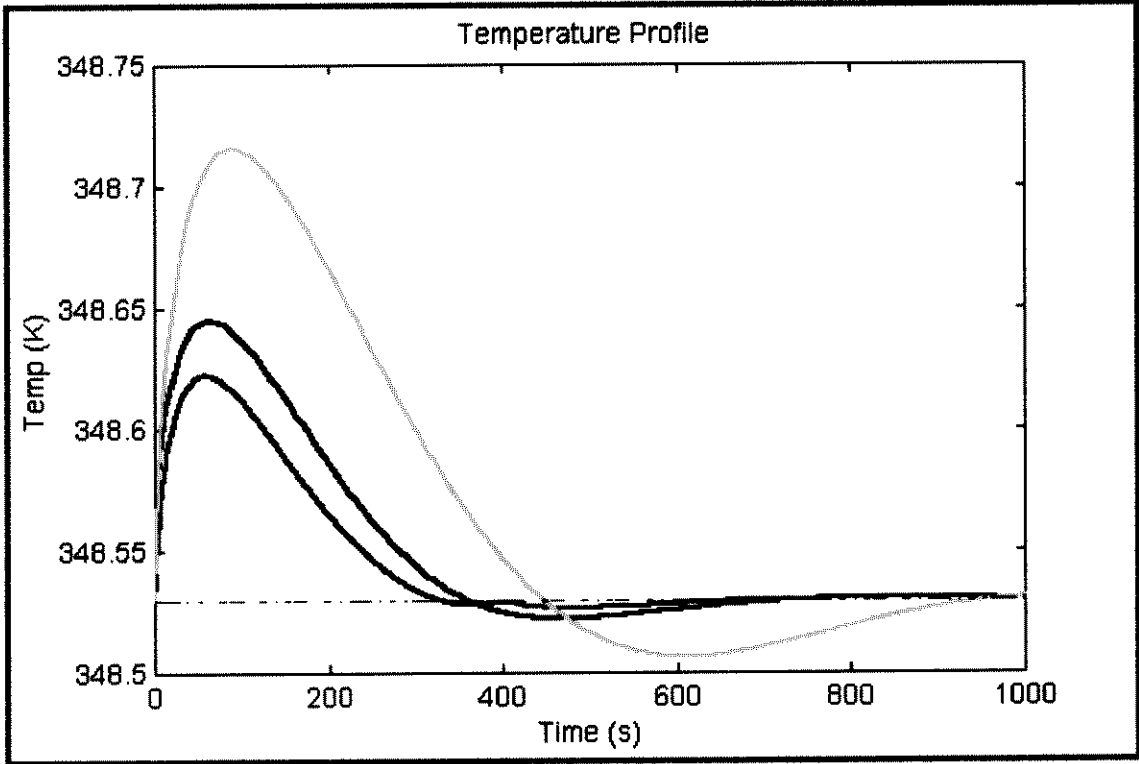


Figure 4.1b Temperature Response (Final Operating Condition)

(Green: PI controller; Red: DMC with $qq = 0$; Yellow: DMC with $qq = 15$)

As the value of qq is increased from 0 to 10 or 15, the temperature in case (a) and the coolant rate in case (b) (see Figure 4.2a) exceed the constraints. Increasing the weighting for the manipulated variable obviously degrades the controlled variable performance. Tuning parameters can be adjusted to satisfy these constraints. The temperature overshoot in this case can be reduced, if necessary, by backing-off a little further. In other words a lower operating temperature is required. A direct method to satisfy constraint on manipulated variables is adding the constraints explicitly in the algorithm to limit the control move. This method can only be used if it does not cause constraint violation on controlled variables. Figure 4.2b shows this feature. The yellow curve is plotted from the simulation of an unconstrained dynamic problem; the red one is the solution of the optimization problem, which explicitly includes constraints on control moves. Setting bounds on control actions is an advantage of DMC over PI and PID controllers. However, in many cases reducing the variability of the manipulated variable would degrade the controlled variable performance; then NLPC is the option to be considered.

Figures 4.3a and b demonstrate the circumstances in which qq should be increased to improve the robustness of the closed-loop plant. Since there is no information on current disturbances, DMC tuning parameters are designed to handle the worst situation ($T_{in} = 300 \rightarrow 305$; $T_{ci} = 283 \rightarrow 286$) and the configuration is written again:

$$\Delta t = 5; V = 40; U = 1; ww = 1; qq = 0$$

However, using this configuration the DMC does not work if disturbances approach their lower bounds ($T_{in} = 300 \rightarrow 298$; $T_{ci} = 283 \rightarrow 280$). The variability of the coolant flowrate has to be reduced by selecting a higher value for qq . In Figure 4.3a, green curves are temperature and coolant responses of the plant, operating at the first state, using DMC with $qq = 0$. Increasing the value of qq to 10 results in more robust responses represented by red curves. For a higher throughput to the plant (final operating condition, $Q_{in} = 0.657$), a higher value of qq is required. The temperature response of the plant operating at the final condition and the corresponding manipulated variable, using DMC with $qq = 15$ are plotted in Figure 4.3b.

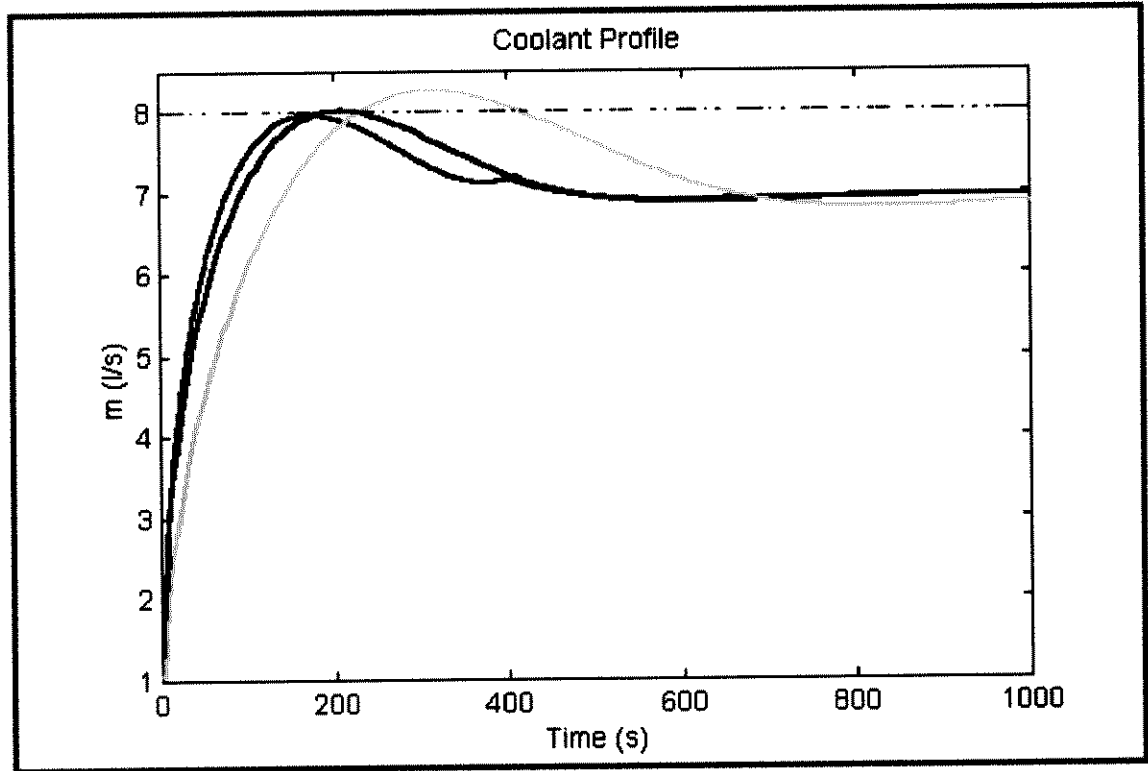


Figure 4.2a Coolant Profile (Final Operating Condition)

(Green: PI controller; Red: DMC with qq = 0; Yellow: DMC with qq = 15)

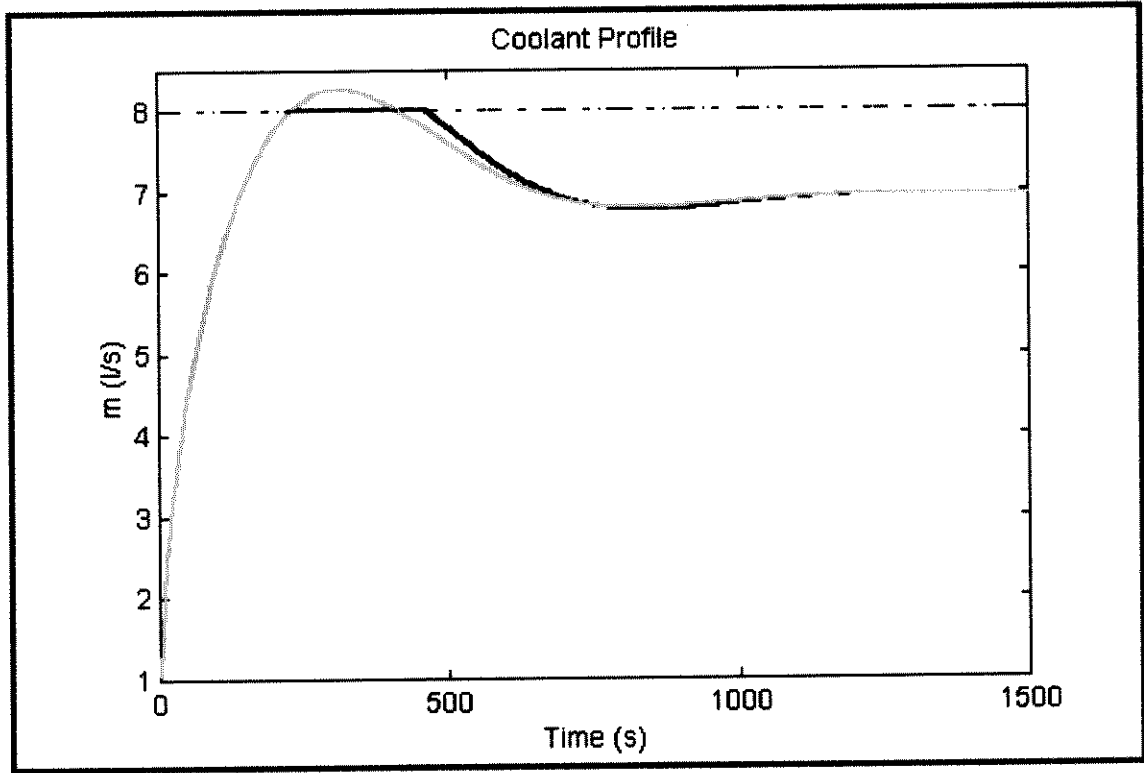


Figure 4.2b Coolant Profile (Final Operating Condition)

(Green: Constraint on manipulated variable; Yellow: No constraint)

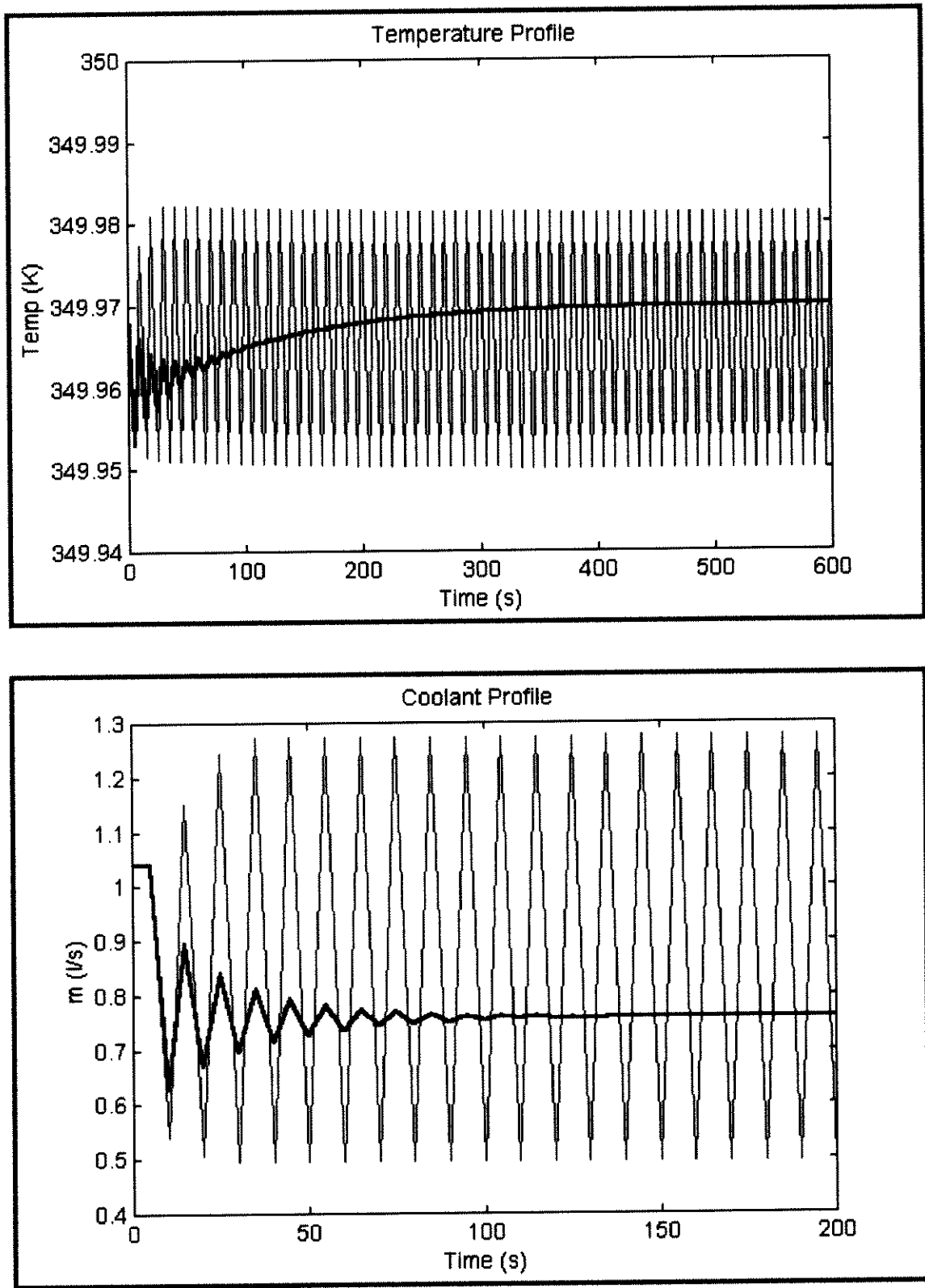


Figure 4.3a Temperature and Corresponding Coolant Profiles
(First Operating Condition)
(Green: DMC with $qq = 0$; Red: DMC with $qq = 10$)

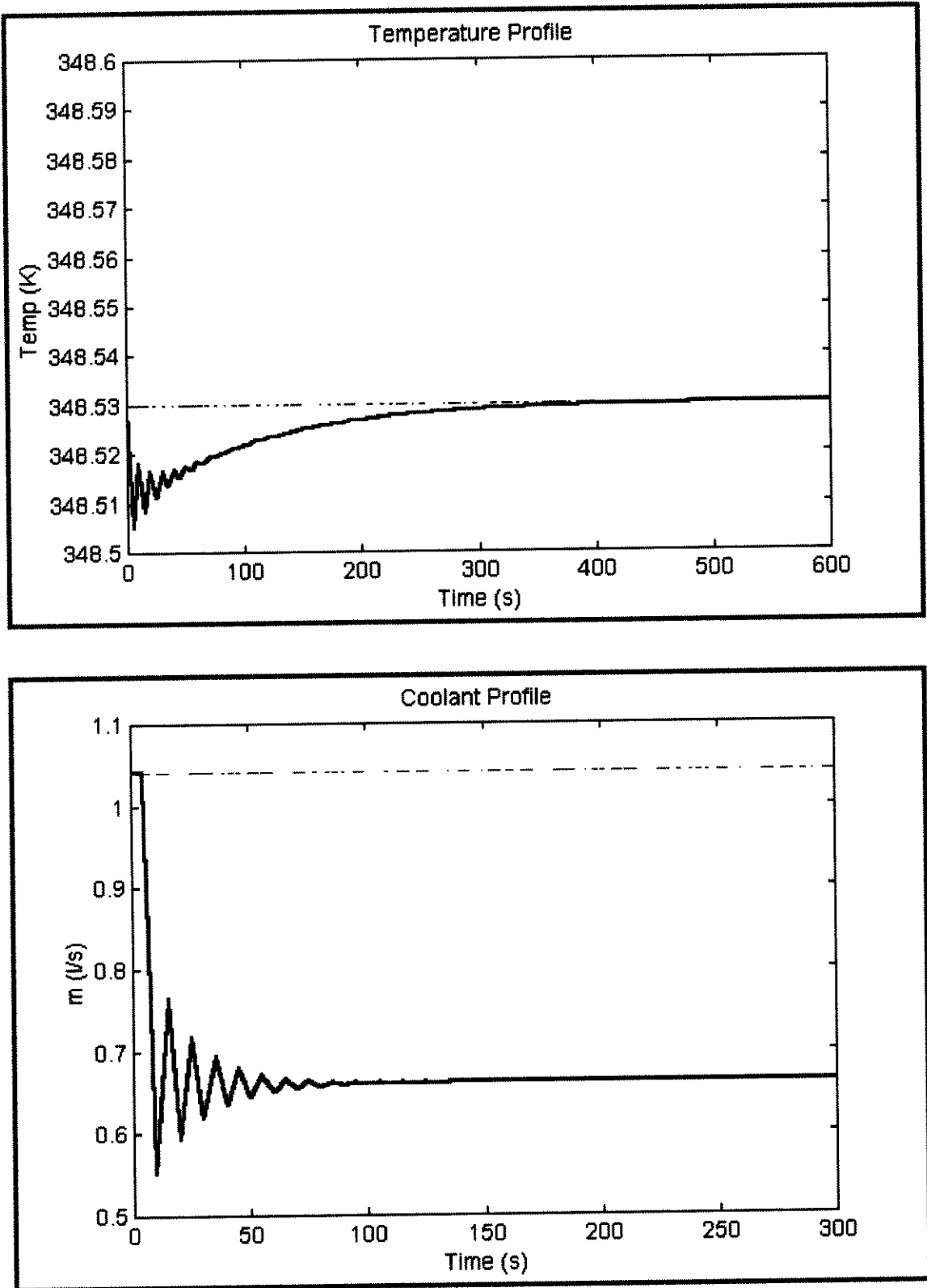


Figure 4.3b Temperature and Corresponding Coolant Profiles
(Final Operating Condition)
(DMC with $qq = 15$)

The selection of the control horizon (U) also affects the robustness of the DMC. A small value of U in this case study leads to a robust controller. However, for the MIMO case shown later, to improve the control performance it is sometimes required to use higher values of U . Figure 4.4 plots the responses of controlled and manipulated variables using DMC with different values of U and qq . Red curves represent responses with $U = 2$, $qq = 1$. Green curves are for $U = 1$, $qq = 0$, yellow curves for $U = 1$, $qq = 1$ and cyan ones for $U = 1$, $qq = 10$. The figures indicate relatively minor influences of qq on manipulated and controlled variables. However, the control horizon U has a major impact on the control action. The effect of U and qq on the control performance is similar to that of gain and reset time of a PI controller.

Finally, another issue should be considered before presenting the switching problem. Since the process dynamic model is known, the convolution model is not used to predict the output over the prediction horizon, but this linear model is still required in the calculation of control moves. An important assumption has been made that the dynamic coefficient matrix A is constant. That allows using the gain matrix K_{DMC} in computing the control action without solving the optimization problem. Figure 4.5, plotting temperature response to a unit step change in coolant flowrate, would prove the validity of the above assumption. The graph actually plots temperature difference (or temperature deviation, $\Delta T = T - T_{initial}$) rather than temperature T against time. Figure 4.5 shows:

- ❖ Disturbances do not have a significant effect on temperature difference responses. Whether the disturbances approach the upper values or the lower values, the response curves are very similar (green and red ones are similar, blue and magenta ones are similar).
- ❖ Throughput has a great impact on temperature difference responses. The blue and green curves are subject to the same disturbances but the responses are different, because the throughputs (Q_{in}) are different. Similarly, the responses represented by the magenta and red curves are different.

Since the construction of the dynamic coefficient matrix A is based on these response curves (see Appendix 4A), similar conclusions can be made. Disturbances have an insignificant impact on the coefficient matrix A , but throughputs do affect A .

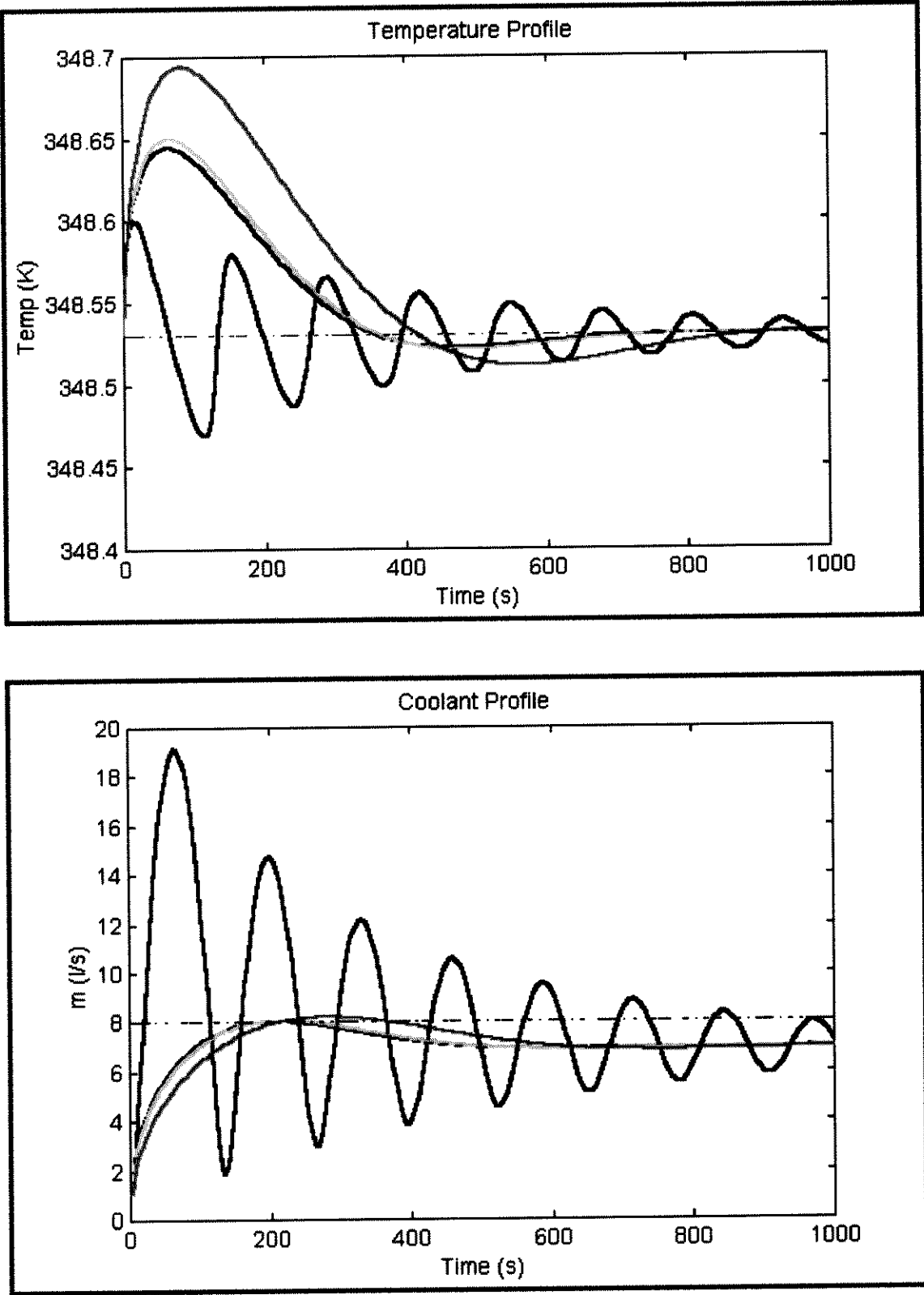


Figure 4.4 Temperature and Corresponding Coolant Profiles

(Final Operating Condition)

(Green: $U = 1$, $qq = 0$; Red: $U = 2$, $qq = 0$)

(Yellow: $U = 1$, $qq = 1$; Cyan: $U = 1$, $qq = 10$)

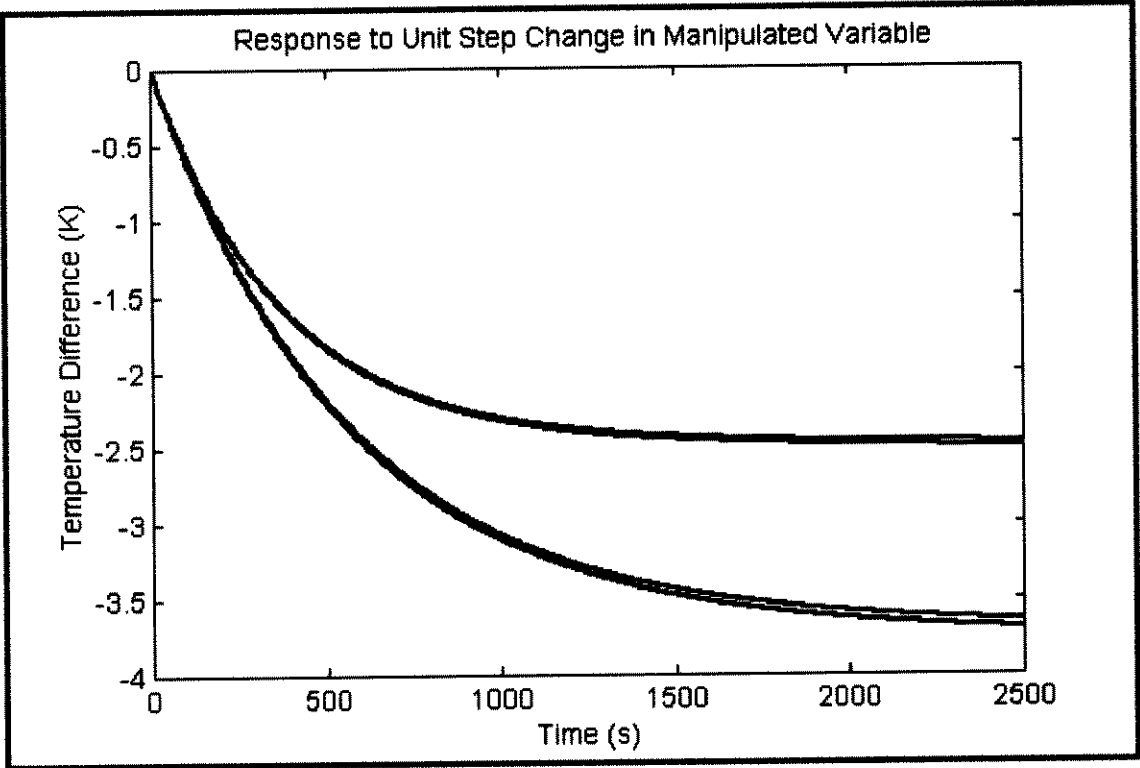


Figure 4.5 Temperature Difference Response to Unit Step Change in Coolant Flowrate

(Blue: $Q_{in} = 0.657$, $T_{in} = 300$, $T_{ci} = 283$; Magenta: $Q_{in} = 0.657$, $T_{in} = 305$, $T_{ci} = 286$)
(Green: $Q_{in} = 0.342$, $T_{in} = 300$, $T_{ci} = 283$; Red: $Q_{in} = 0.342$, $T_{in} = 305$, $T_{ci} = 286$)

The assumption of a constant matrix A is valid for a control problem that only involves disturbances on feed and coolant temperatures. The coefficient matrix A needs to be updated in a switchability problem, which deals with both changes in flowrate and disturbances on temperature. That necessity will be discussed next.

3.1.2. Switchability problem with DMC

As shown in Table 4.1, for a step change in feed concentration and possible step changes in disturbances, the switchability problem finds the optimal profiles of feed flowrate change, temperature set point change and in some cases even inventory change.

$C_{in} = 20 \rightarrow 15$	Step change (input)
$T_{in} = 300 \rightarrow 305$	Step change (input)
$T_{ci} = 283 \rightarrow 286$	Step change (input)
$Q_{in} = 0.342 \rightarrow 0.657$	Optimal trajectory (solution)
$Stpt = 349.97 \rightarrow 348.53$	Step change (input) or optimal trajectory (solution)

A level control loop must be introduced to the plant, since the problem deals with flowrate change. The switching problem now is highly nonlinear, with interactions between controlled variables. Temperature and concentration changes do not affect inventory. However, inventory change may affect other state variables. No attempt is made using NLPC to solve this problem on-line for two reasons:

1. The speed of solving the optimization problem is slower than the dynamics of the problem.
2. There is no guarantee of finding a feasible solution at all time steps that can satisfy the set of constraints on pages 3.24 - 3.25.

It is always safer to solve the switching problem off-line first, as demonstrated in Chapter 3. Although PI controllers are used in the formulation of the problem, the control technique is nonlinear and all path constraints on variables are explicitly handled. Then the optimal feed flowrate profile obtained from solving the switching problem can be implemented on-line with the DMC. The liquid level is still adjusted by the PI controller. Using this strategy, without having to solve the optimization problem on-line, the computational time is small and the problem has solutions at all time steps.

Furthermore this control scheme allows the incorporation of future set point changes in the control algorithm, using current information of disturbances and measured variables. The interaction between manipulated variables and/or controlled variables are also taken into account. The solutions obtained from solving the switching problem are presented in the first graph of Figure 4.6. Two cases are solved. The first problem assumes a step change in temperature set point. The green curve plots the optimal feed profile of this first case. The second problem solves for the optimal temperature set point profile as well. The red curve plots the feed profile for the second problem. The second graph of Figure 4.6 shows trajectories of temperature set point for both cases.

The necessity of updating the coefficient matrix A at each or some time steps is being considered now. Figure 4.5 shows that the response curves are similar up to 200 seconds. After that the deviation is significant. Consequently, it is not necessary to update the coefficient matrix A during this time, although the flowrate changes. Figure 4.6a shows that after 200 seconds, the feed flowrate (Q_{in}) almost reaches the final steady state value. Therefore, if the coefficient matrix A is constructed on the response curve evaluated at the final steady-state value of Q_{in} (blue and magenta curves in Figure 4.5), the assumption of the constant matrix A is valid at all time steps. Thus a constant gain matrix K_{DMC} can be used to calculate the control move during the transition.

The switchability problem with DMC is now ready to be run on-line, but the following simulations are performed off-line under the worst situation. Feasibility tests are carried out to cover other situations that might occur. Dynamic simulations with PI controllers can be performed in MATLAB or in SPEEDUP, since computational time and results obtained from these packages are similar. However, it is much simpler and faster to run dynamic simulations with DMC using MATLAB, because the package can easily handle all matrix operations in the calculations of control moves. Figures 4.7a, b and c plot temperature, coolant and cooling profiles, respectively. Further details of the plots include:

- ❖ Blue curves plot the solution obtained from solving the nonlinear dynamic problem, a mixture of control and switching problems using simultaneous optimization and integration technique (GAMS with MINOS optimizer).
- ❖ Green curves plot the simulation results from SPEEDUP. The optimal feed flowrate trajectory, solution of the nonlinear dynamic problem, is fed back as input to

perform dynamic simulations in SPEEDUP. The configurations of the PI controllers are temperature reset time = 100, temperature gain = 0.8, level reset time = 100, level gain = 40. The temperature controller is not robust, but these configurations give feasible solutions when disturbances approach their lower bounds ($T_{in} = 300 \rightarrow 298$; $T_{ci} = 283 \rightarrow 280$) or upper bounds ($T_{in} = 300 \rightarrow 305$; $T_{ci} = 283 \rightarrow 286$). If a higher value of temperature gain is used, there is no feasible solution. That is one main disadvantage of using PI controllers in this case.

- ❖ Red and yellow curves in Figure 4.7 are also simulation results but from MATLAB, and the temperature PI controller is replaced by the DMC having the configuration $\Delta t = 5$; $V = 40$; $U = 1$; $ww = 1$; $qq = 10$ (yellow curve) or 15 (red curve).

In Figure 4.7a, the temperature output with PI controllers (green) is different from the NL solution response (blue), although PI controllers are used in the formulation of the NLP dynamic problem as well as in SPEEDUP simulations, to test the results afterwards. However, only a low value of temperature gain and a high value of reset time can be used in the simulations to avoid constraint violations. That does not lead to a robust controller. With the DMC, upper and lower bounds on the manipulated variable can be included in the control algorithm. As a result, controlled, manipulated and other variables approach their final steady-state values faster while satisfying path constraints (Figures 4.7b and c). These figures also show that the control performance is not sensitive to the weighting for the manipulated variable (qq). Red and yellow curves are similar. However, a higher value of qq is selected to cover the case requiring suppression of control move, as discussed before (see Figures 4.3a and b). The NLP dynamic problem and the dynamic simulation are designed for the worst situation. Therefore, feasibility tests must be carried out for other situations, in which disturbances approach their lower limits. Figures 4.8a, b and c plot temperature, coolant and cooling profiles, respectively, when feed and coolant temperatures decrease ($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$). In this situation a high value of qq is very useful to avoid too much oscillation. Red curves in the plots are for DMC and green curves are for PI controllers.

The NLP dynamic problem presented above assumes a step change in the temperature set point. The solution of the second NLP problem including the best temperature set point policy is considered next.

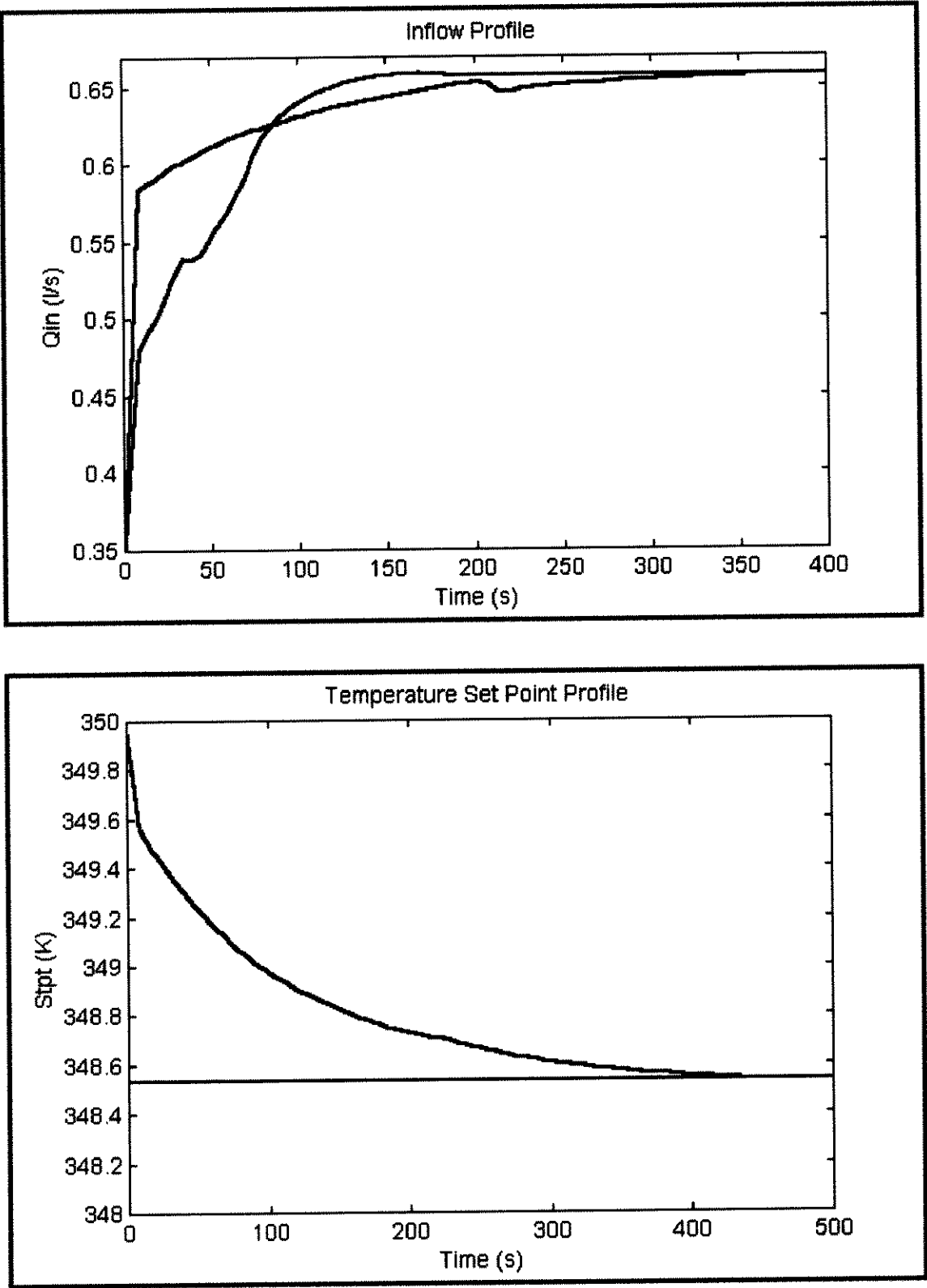


Figure 4.6 Optimal Feed Flowrate Profile and Corresponding Temperature Set Point Trajectory

(Green: Step change in temperature set point)
(Red: Temperature set point following optimal trajectory)

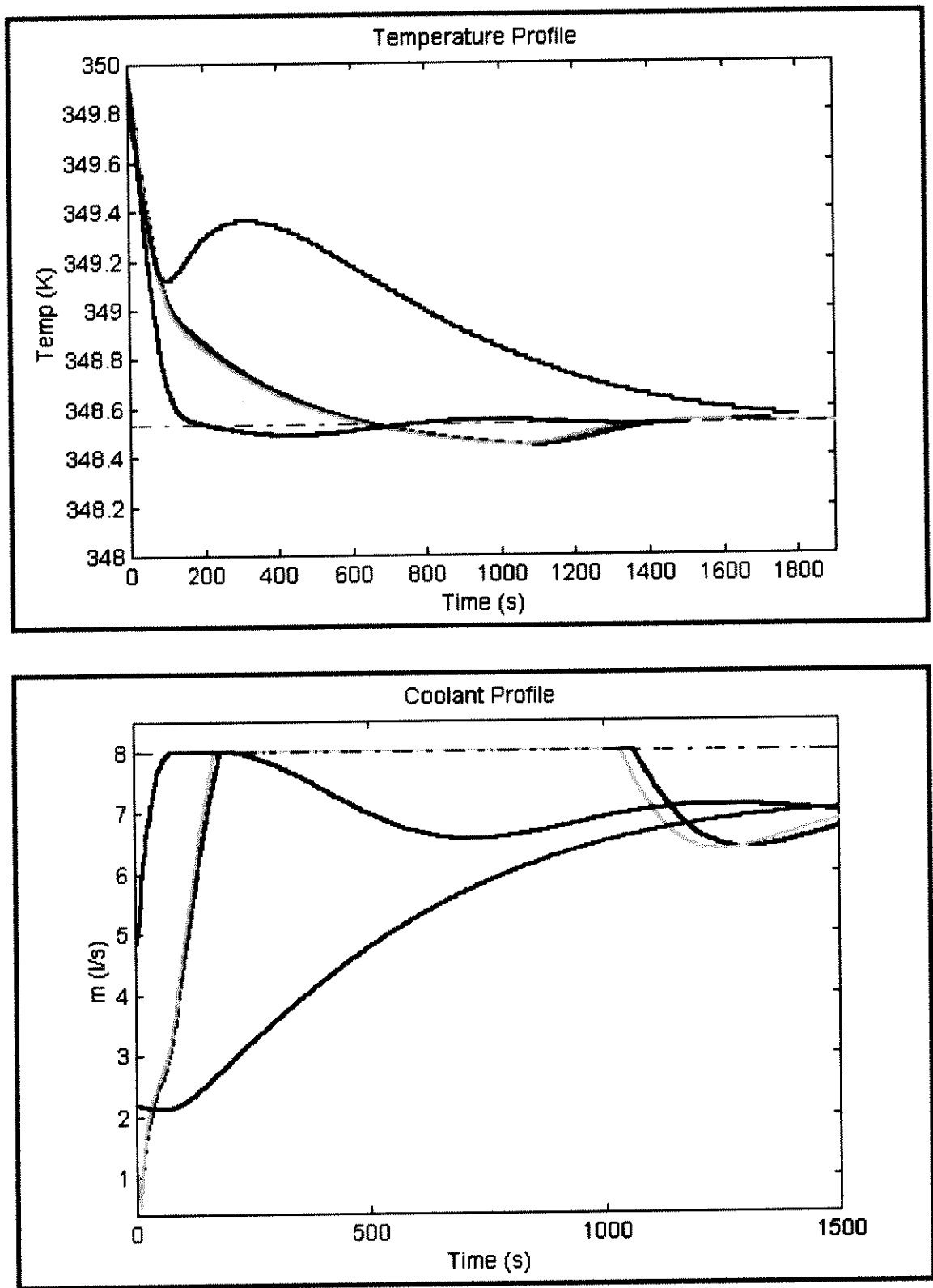


Figure 4.7a, b Temperature and Coolant Profiles

(Controlled and Manipulated Variables)

(Blue: Solution of NL problem; Green: Simulation result with PI controllers)

(Red: DMC with $qq = 15$; Yellow: DMC with $qq = 10$)

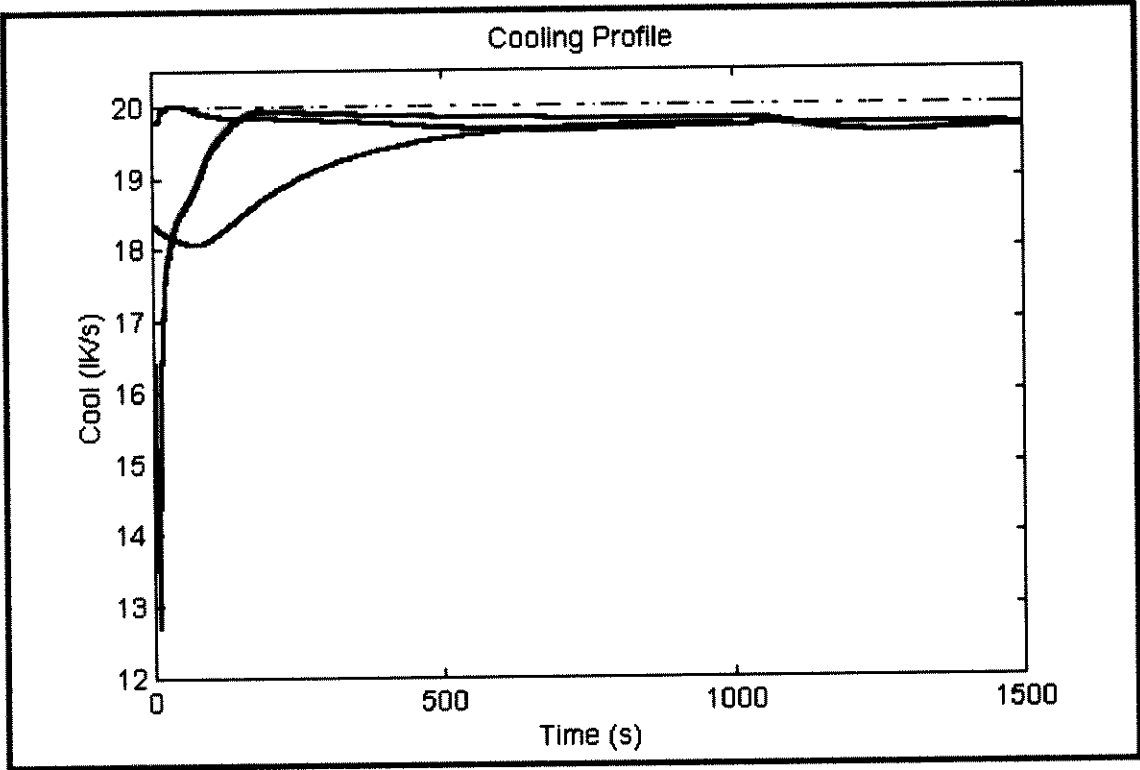


Figure 4.7c Cooling Profile

(Blue: Solution of NL problem; Green: Simulation result with PI controllers)
(Red: DMC with $qq = 15$; Yellow: DMC with $qq = 10$)

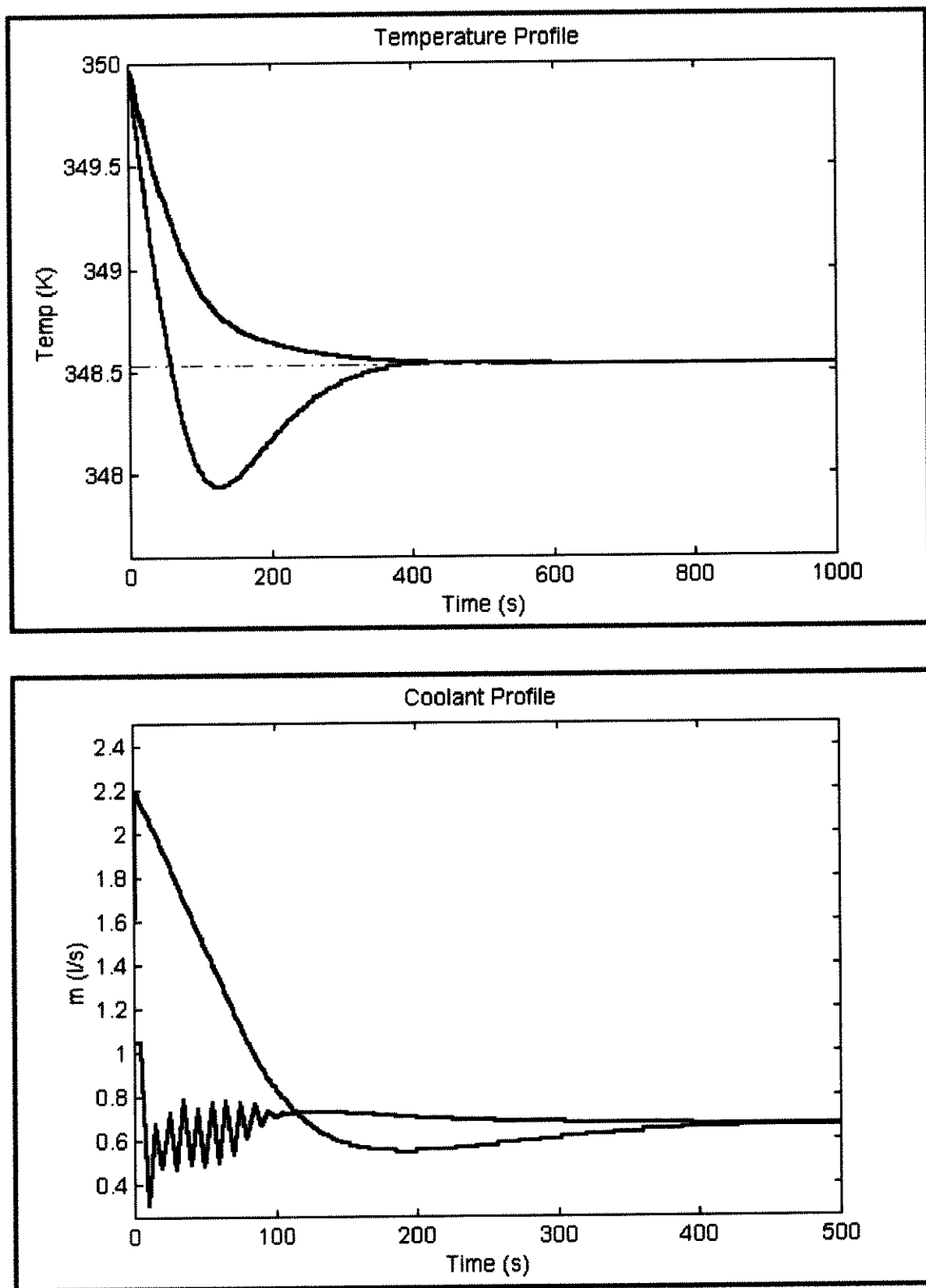


Figure 4.8a, b Temperature and Coolant Profiles

(Controlled and Manipulated Variables)

(Green: Simulation result with PI controllers; Red: Simulation result with DMC)

($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$)

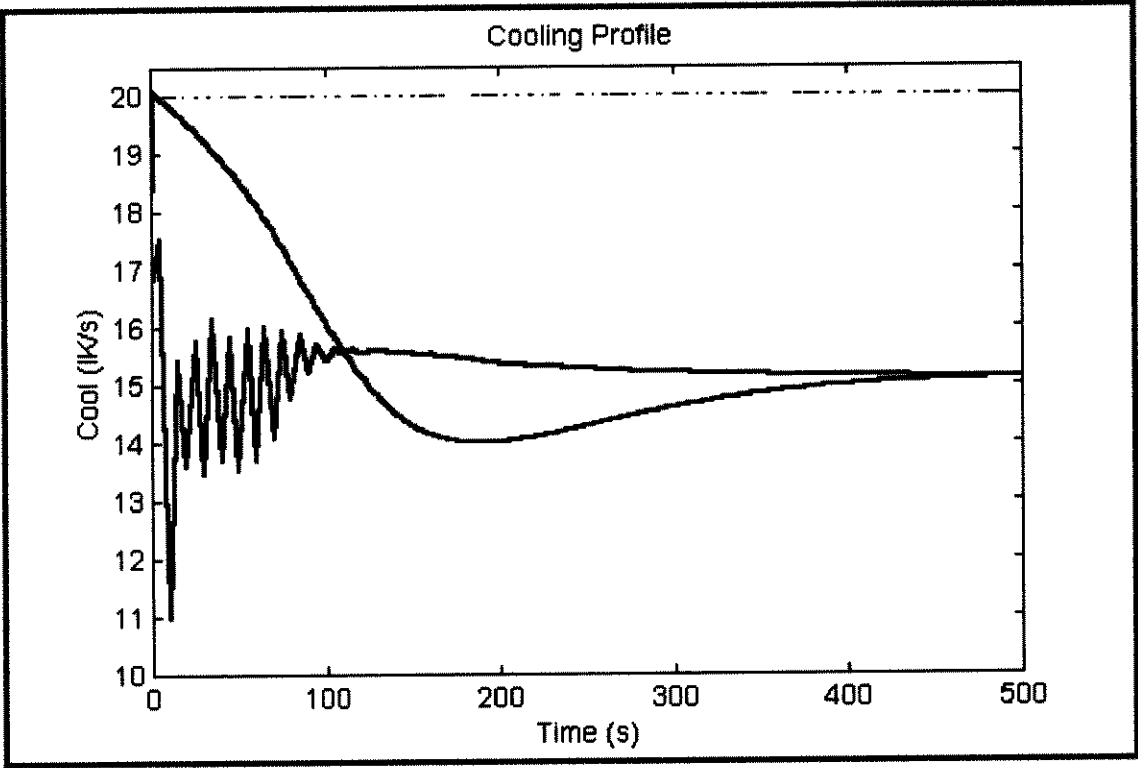


Figure 4.8c Cooling Profile

($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$)

(Green: Simulation result with PI controllers; Red: Simulation result with DMC)

The optimal feed flowrate profile obtained from this second NLP problem is fed back as input to perform dynamic simulations in SPEEDUP (with PI temperature controller) and in MATLAB (with DMC). The temperature set point policy is only introduced to PI controllers not to DMC, since the latter naturally deals with the set point change. Outputs are plotted in Figure 4.9. For comparison the similar color arrangement in Figure 4.7 is used in Figure 4.9. Blue is for the solution of the NLP dynamic problem, green for SPEEDUP and red for MATLAB simulations. Introducing the optimal policy of temperature set point to replace the step change policy cannot improve the PI performance. The PI configuration used in the formulation of the NLP problem is gain = 30, reset time = 60. However, only a small value of gain or a high value of reset time can be used in the simulation with PI controllers, if constraints on the manipulated variables are not explicitly handled in the control algorithm. Consequently, all green response curves are very sluggish. The DMC performance is better in this case and even better than the original solution in some aspects. In Figure 4.9a, the temperature response of DMC is similar to the solution response (red and blue curves). These two responses are different in the first case (Figure 4.7a), in which the NLP dynamic problem does not include the temperature set point policy in its solution. This demonstrates one of the most advantageous features of DMC over PI controllers. DMC naturally updates the set-point vector. Furthermore Figures 4.9b and c prove that the cooling and coolant responses of DMC are even better than solutions of the NLP problem. These solutions give fluctuating coolant and cooling rates for the first 400 seconds compared to very smooth responses from DMC (red curves compared to blue curves). Finally, Figure 4.10 shows coolant and cooling profiles when feed and coolant temperatures decrease ($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$).

In this SISO case study, the application of the well-tuned DMC to a mixture of regulator and servo problems has been proved to be more advantageous than that of a PI controller. The DMC approach in the MIMO case study is discussed next.

3.2. Case study 2: Two CSTRs in series

The second case study is the problem of two CSTRs in series shown in Chapter 3. This problem is solved again with the same set of disturbances as in the first case study (page 4.7) with $U_a = 0.35$. The equality constraints describing the model and the inequality constraints are found on page 3.46.

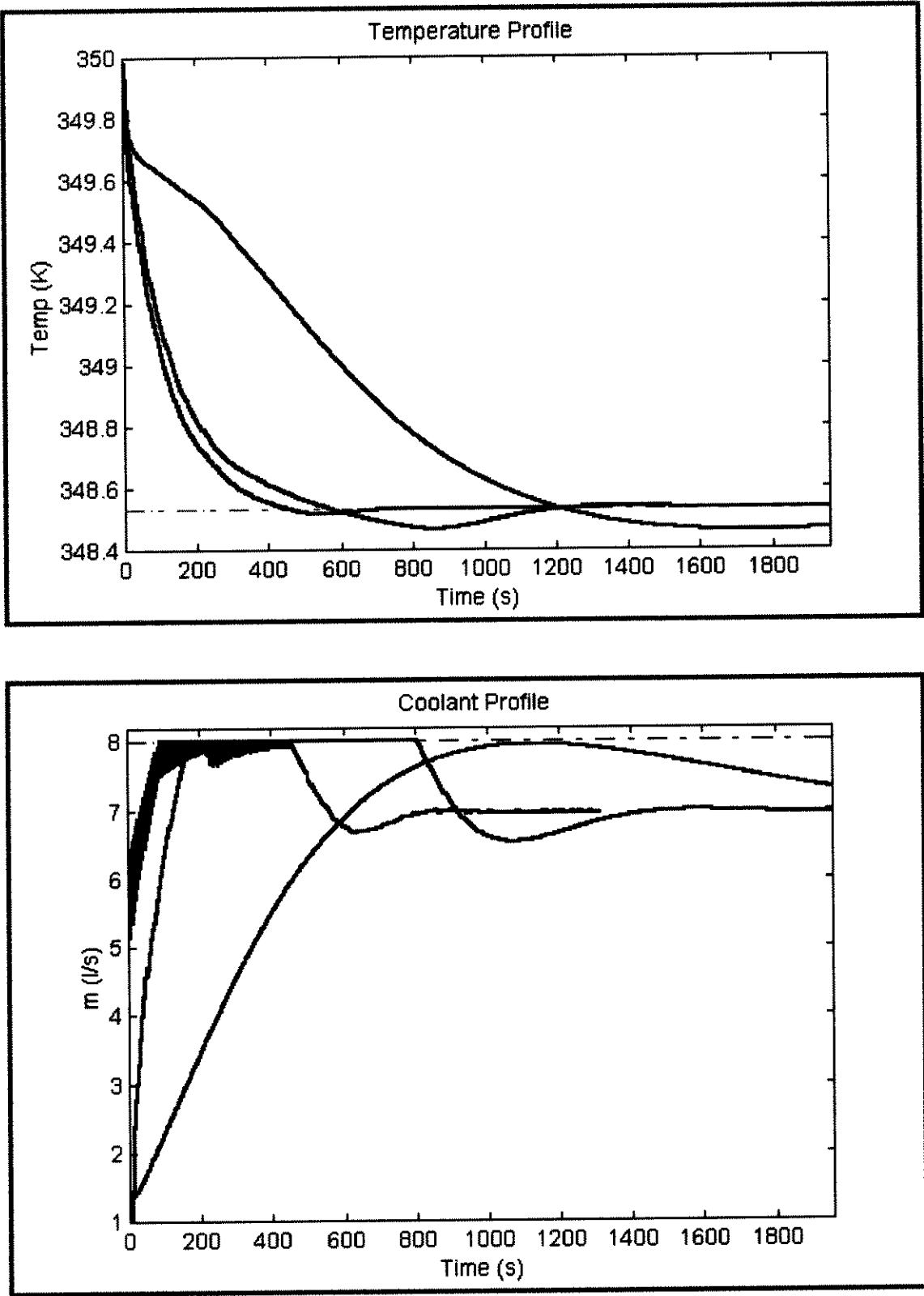


Figure 4.9a, b Temperature and Coolant Profiles

(Controlled and Manipulated Variables)

(Blue: Solution of NL problem, Green: Simulation result with PI controllers)

(Red: Simulation with DMC, $qq = 15$)

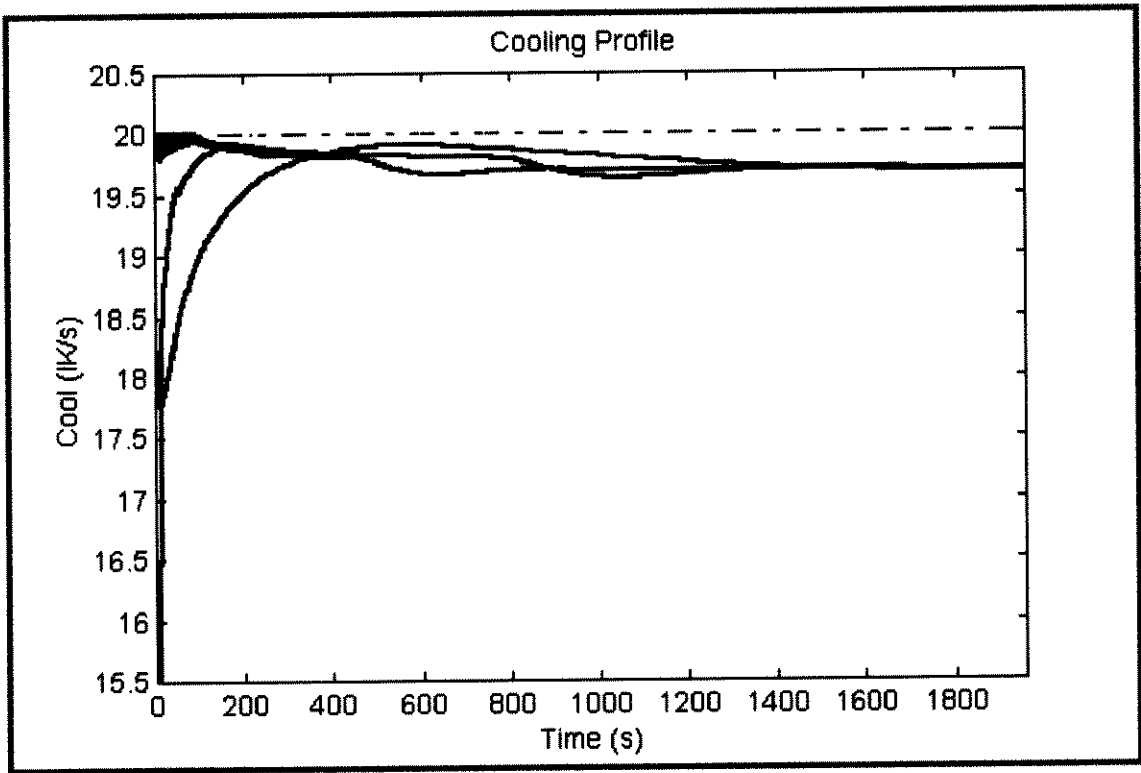


Figure 4.9c Cooling Profile

(Blue: Solution of NL problem, Green: Simulation result with PI controllers)

(Red: Simulation with DMC, $qq = 15$)

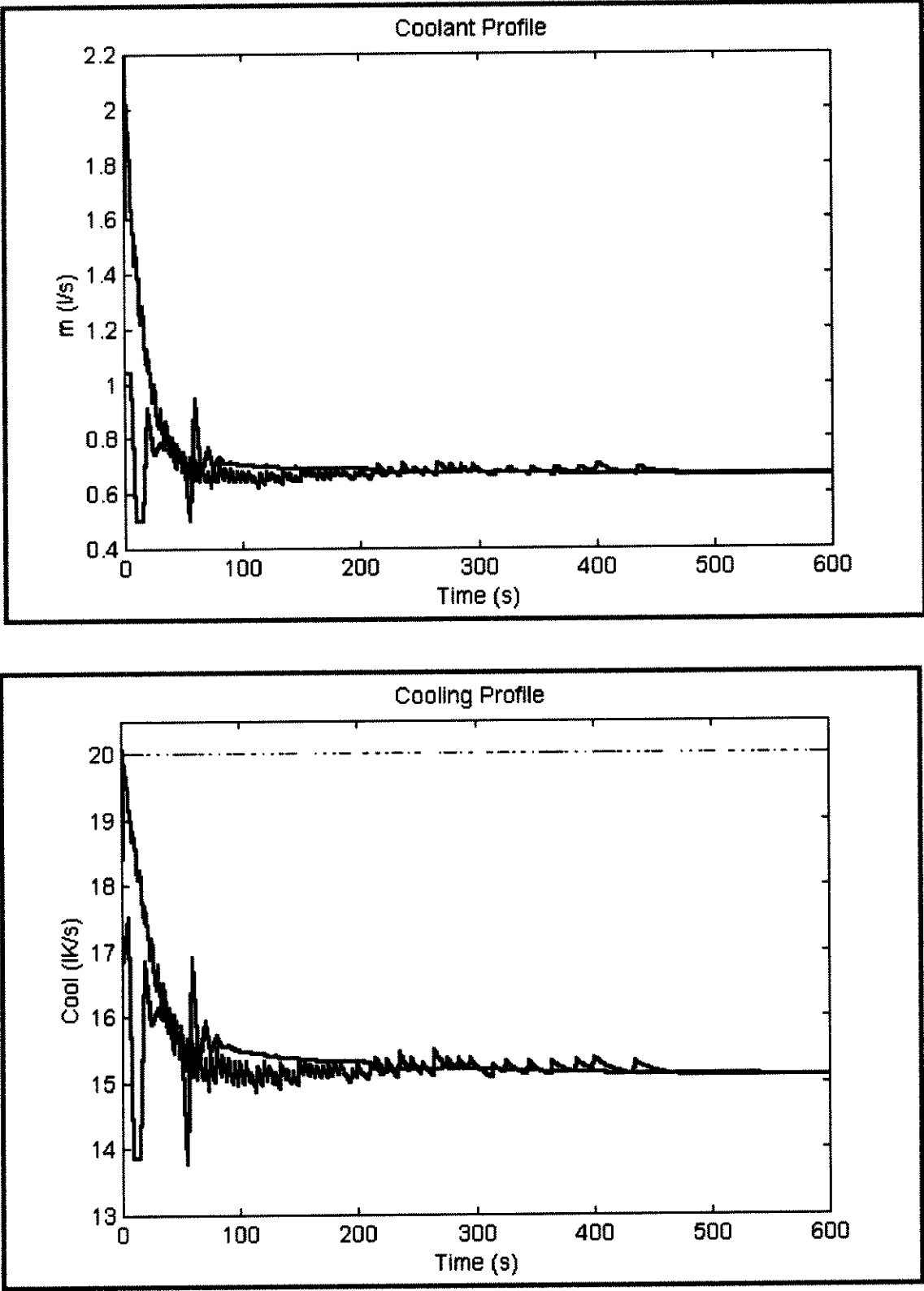


Figure 4.10 Coolant and Cooling Profiles

$(T_{in} = 300 \rightarrow 298, T_{ci} = 283 \rightarrow 280)$

(Green: Simulation result with PI controllers; Red: Simulation result with DMC)

3.2.1. Dynamic closed-loop back-off problem with DMC

The results shown in Table 4.2 are solutions of the dynamic closed-loop back-off problem with the two PI temperature controllers. The tuning parameters are $K_{c1} = 0.2$, $K_{c2} = 0.14$, $\tau_1 = \tau_2 = 10$. The inventory is fixed at $V_1 = V_2 = 360$ l.

Feed Condition	Q^1 (l.s ⁻¹)	Q^2 (l.s ⁻¹)	Stpt ₁ (K)	Stpt ₂ (K)
$T_{in} = 300 \rightarrow 305$ $T_{ci} = 283 \rightarrow 286$ $C_{in} = 20$	0.531	0.134	349.5	335.4
$T_{in} = 300 \rightarrow 305$ $T_{ci} = 283 \rightarrow 286$ $C_{in} = 15$	0.750	0.050	340.2	328.2

Table 4.2 Dynamic Closed-Loop Back-Off Operating Conditions (Two CSTRs)

The above conditions are also used in the switching problem as the first and final steady-state conditions. The DMC in this case is extended for two inputs and two outputs to replace two temperature PI controllers. Equations (4.1) and (4.5) are used to calculate the gain matrix K_{DMC} . The dynamic coefficient matrix A is now composed of four matrices.

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

Matrices A_{11} and A_{12} represent the effect of the first manipulated on the first and the second controlled variables, respectively. Similarly, matrices A_{21} and A_{22} represent the effect of the second manipulated on the first and the second controlled variables, respectively. In this case, matrix A_{21} is zero, since the coolant flow in the second reactor does not affect the temperature in the first reactor. These matrices are constructed using four response curves plotted in Figure 4.11. The zero yellow line proves $A_{21} = 0$. Since the diagonal matrices $[WW]$ and $[QQ]$ are also blocks of matrices, the number of adjustable parameters are enormously increased. These parameters should be well tuned off-line first to provide an effective controller.

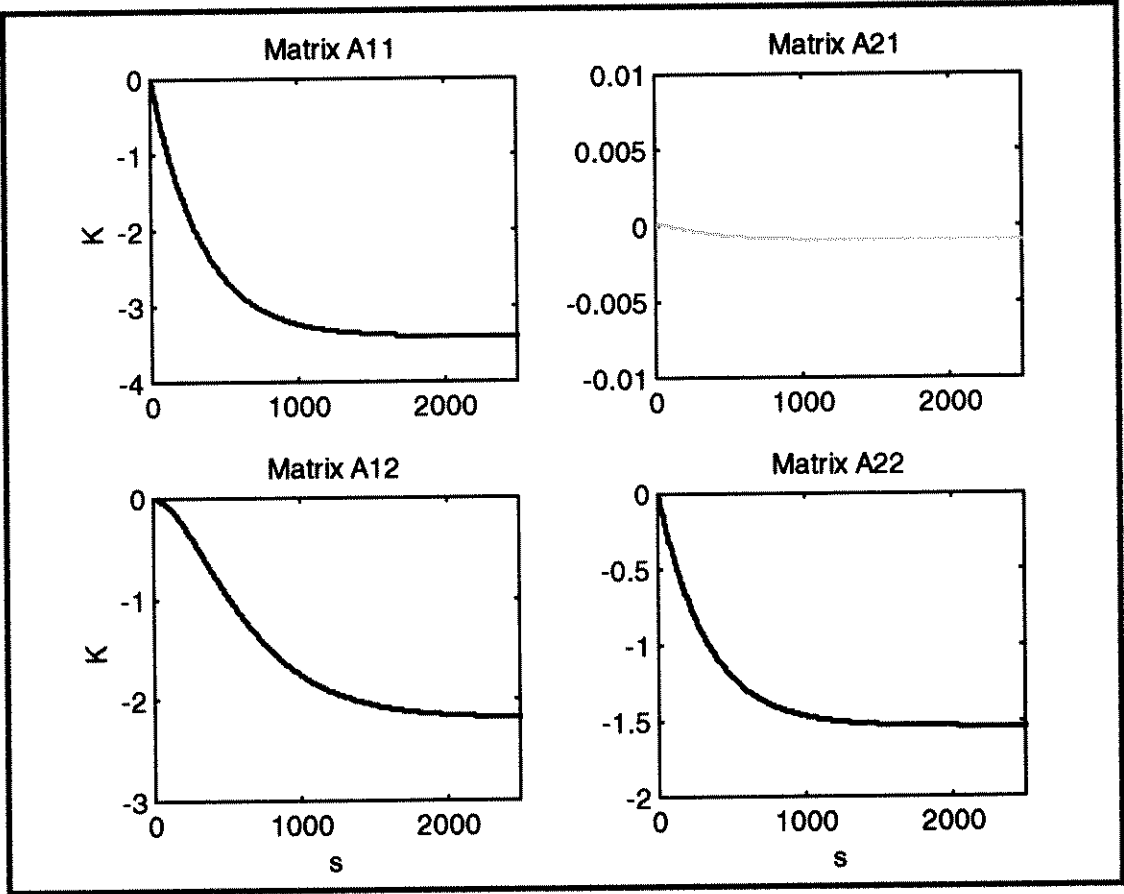


Figure 4.11 Temperature Difference Responses in First and Second CSTRs to Unit Step Change in Coolant flowrate
(Green and yellow: First CSTR; Red and blue: Second CSTR)

DMC does not offer a significant advantage in either SISO or MIMO regulator problems. The following section focuses on the selection of tuning parameters, which can be used in a mixture of regulator and servo problems. In general, small values of control horizon (U) and weighting for manipulated variables (qq) lead to the robust DMC. However, in some circumstances presented in the SISO case, high values of qq are essential to reduce the variability of manipulated variables. Similarly, high values of U are required in the MIMO case to improve the robustness of the control performance. To avoid an over-designed controller using the DMC technique, the adjustable parameters are tuned with the set of disturbances that produces the most constraint violation, but qq is generally selected with the set which produces the least violation. Then feasibility tests are carried out with other possible combinations of disturbances. The configuration of the DMC to replace temperature PI controllers is $\Delta t = 5$, $V = 40$, $U = 2$, $ww_1 = ww_2 = 1$, $qq_1 = qq_2 = 1$. The selection of U and qq has a great impact on coolant and cooling rates. Some selected outputs are shown in Figure 4.12. Green curves represent responses using DMC with $U = 1$, $qq_1 = qq_2 = 1$, red ones with $U = 2$, $qq_1 = qq_2 = 1$ and yellow ones with $U = 1$, $qq_1 = qq_2 = 3$. When feed and coolant temperatures approach their lower limits, cooling rates in both reactors (at the first operating state) violate the constraints, if the control horizon $U = 1$ is selected (Figure 4.12a, green curves). Increasing the value of weighting ($qq = 3$) reduces the variability of manipulated variables but is still not as good as increasing the value of control horizon ($U = 2$). Similarly, at the final operating state, the cooling rate in the second reactor violates the constraint (see green curves in Figure 4.12b), if $U = 1$ is selected. Figure 4.13 plots temperature, corresponding coolant and cooling profiles, when feed and coolant temperatures approach their upper limits. Responses of the plant using PI controllers are also shown in the same graphs (blue curves) for reference.

3.2.2. Switchability problem with DMC

As shown before in Table 4.2, for a step change in feed concentration and possible step changes in disturbances the switchability problem finds the optimal profiles of two feed flows and temperature set points in two reactors.

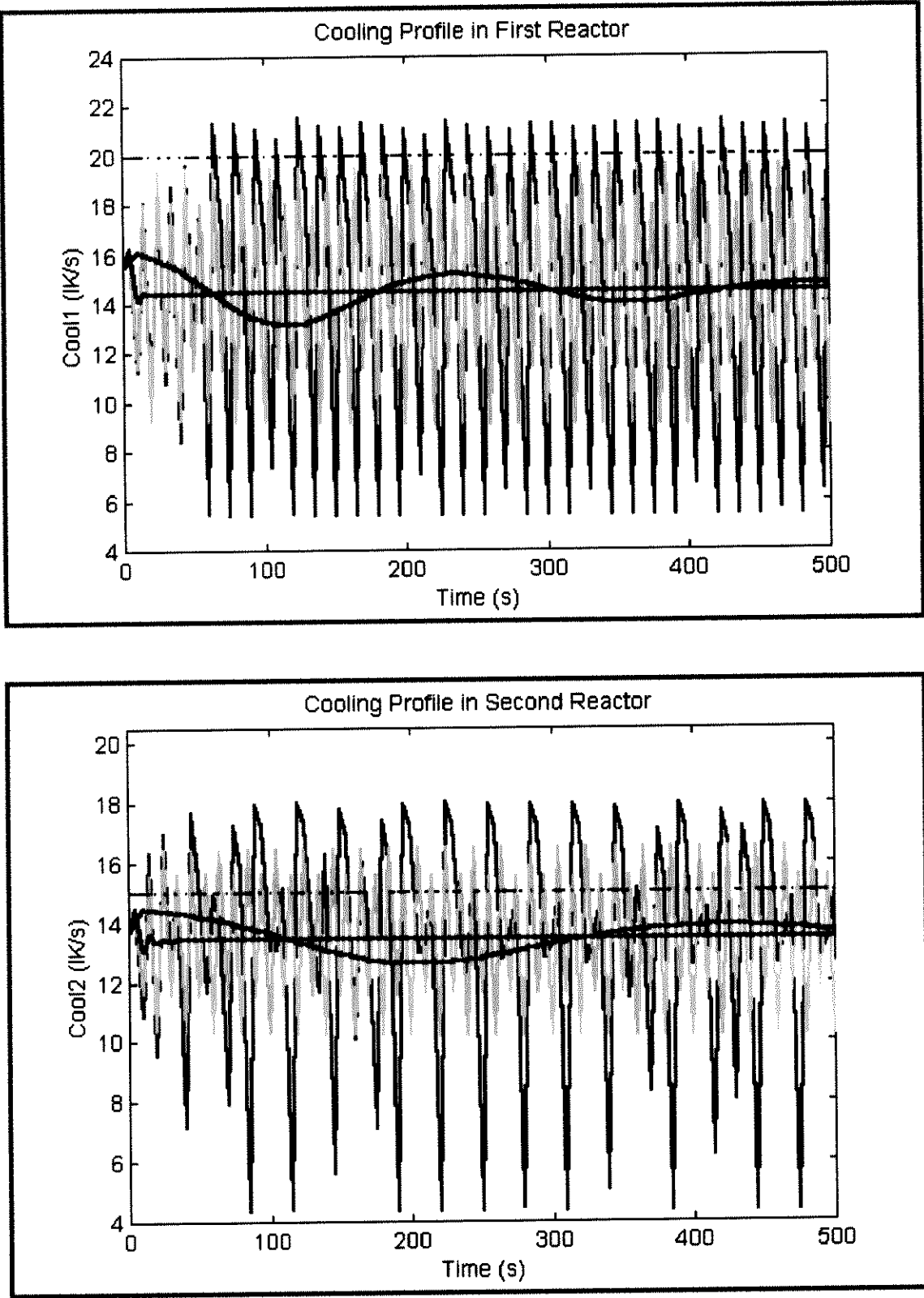


Figure 4.12a Cooling Profile in Reactors (First Operating Condition)

($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$)

(Green: $U = 1$, $qq_1 = qq_2 = 1$; Red: $U = 2$, $qq_1 = qq_2 = 1$; Yellow: $U = 1$, $qq_1 = qq_2 = 3$)

(Blue: PI controllers)

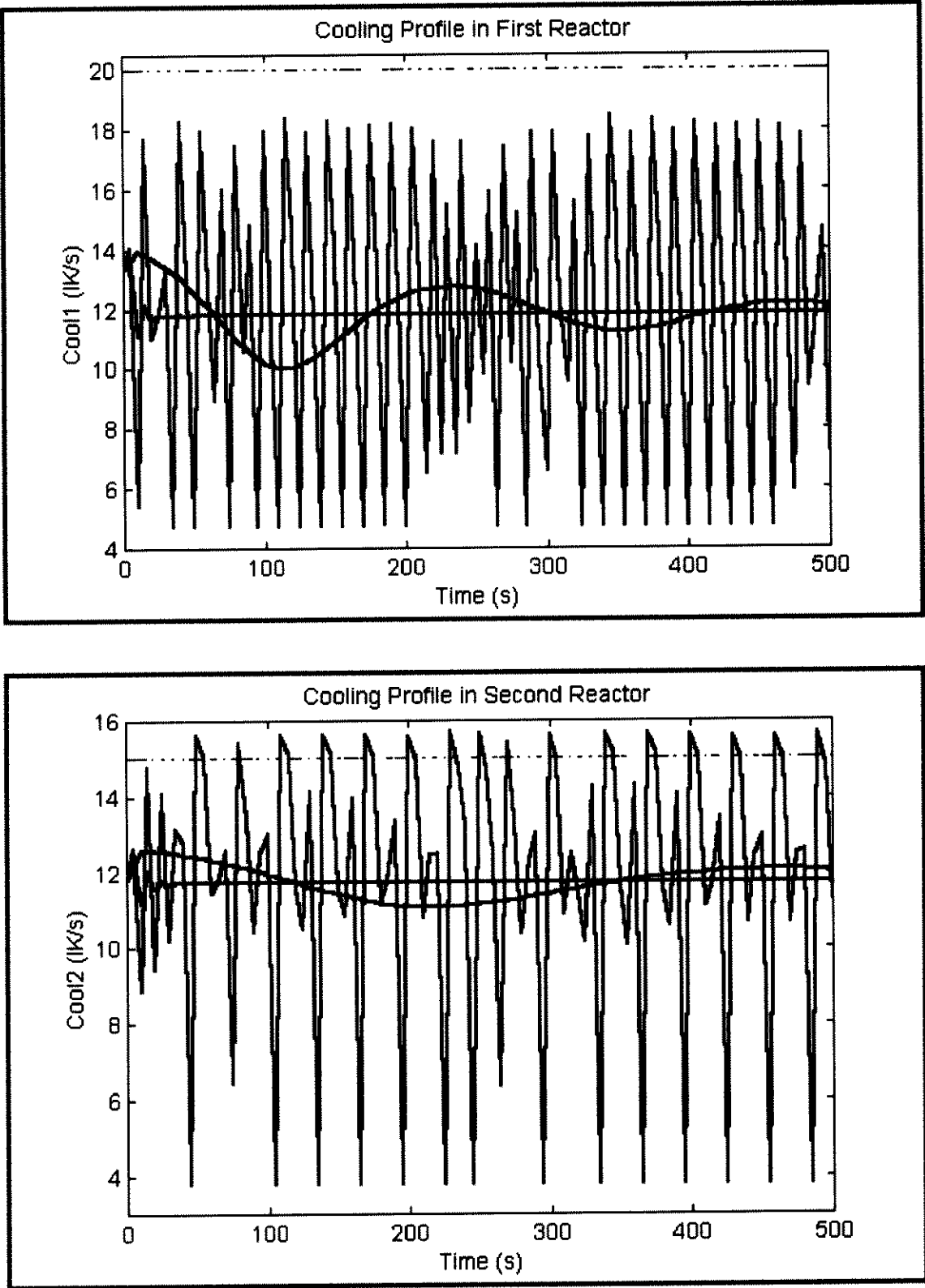


Figure 4.12b Coolant Profile in Reactors (Final Operating Condition)

($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$)

(Green: $U = 1$, $qq_1 = qq_2 = 1$; Red: $U = 2$, $qq_1 = qq_2 = 1$)

(Blue: PI controllers)

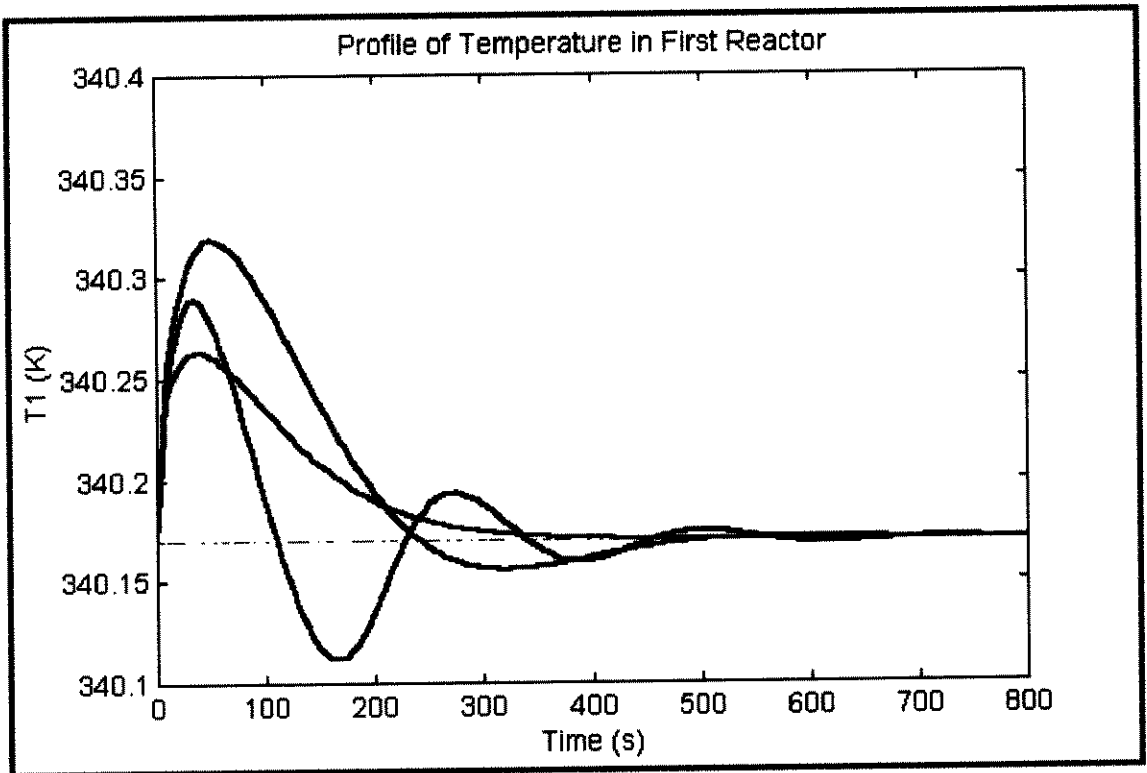
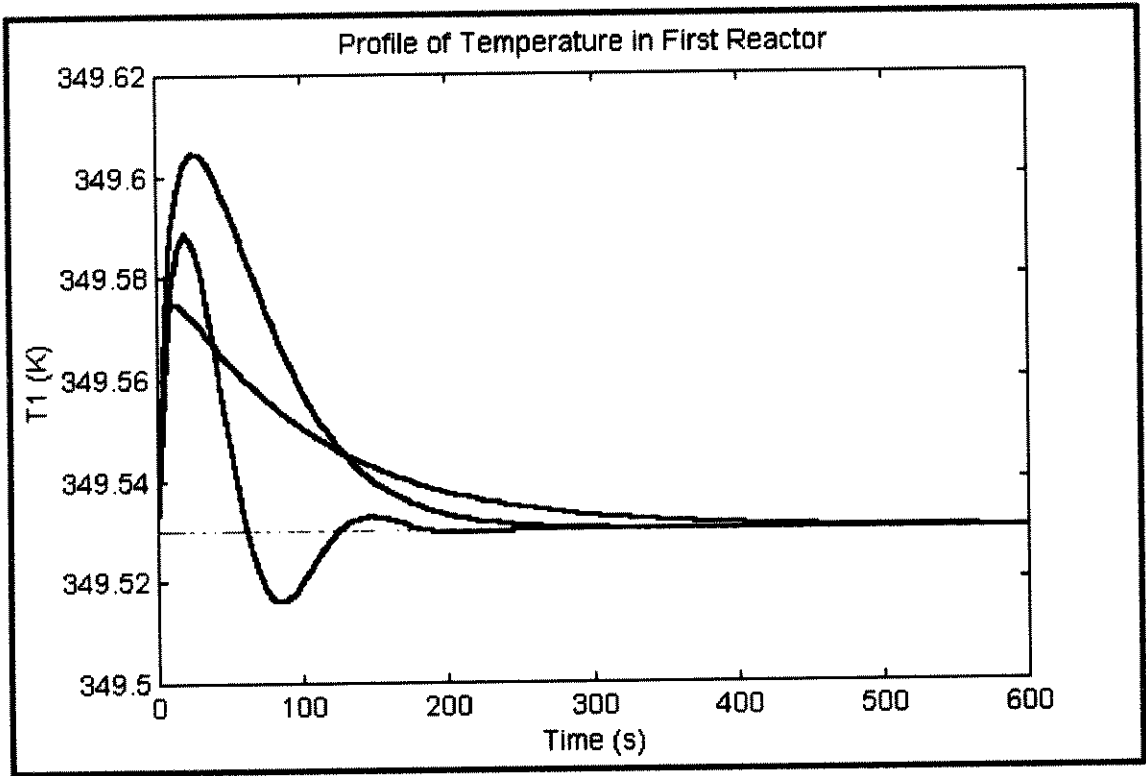


Figure 4.13a Temperature Profiles at First and Final Operating Conditions
(First Reactor)

($T_{in} = 300 \rightarrow 305$, $T_{ci} = 283 \rightarrow 286$)

(Green: $U = 1$, $qq_1 = qq_2 = 1$; Red: $U = 2$, $qq_1 = qq_2 = 1$; Blue: PI controllers)

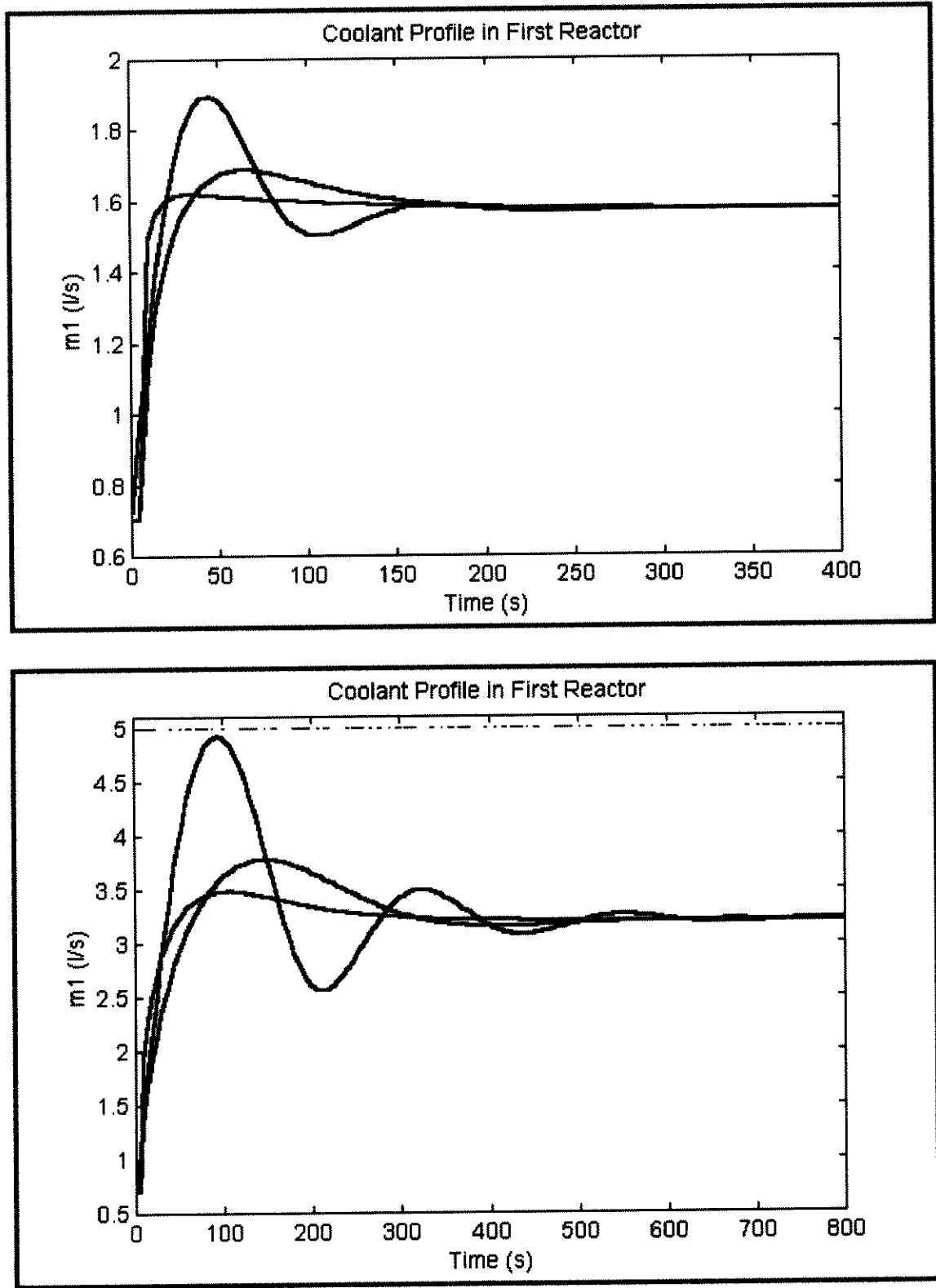


Figure 4.13b Coolant Profiles at First and Final Operating Conditions
(First Reactor)

($T_{in} = 300 \rightarrow 305$, $T_{cl} = 283 \rightarrow 286$)

(Green: $U = 1$, $qq_1 = qq_2 = 1$; Red: $U = 2$, $qq_1 = qq_2 = 1$; Blue: PI controllers)

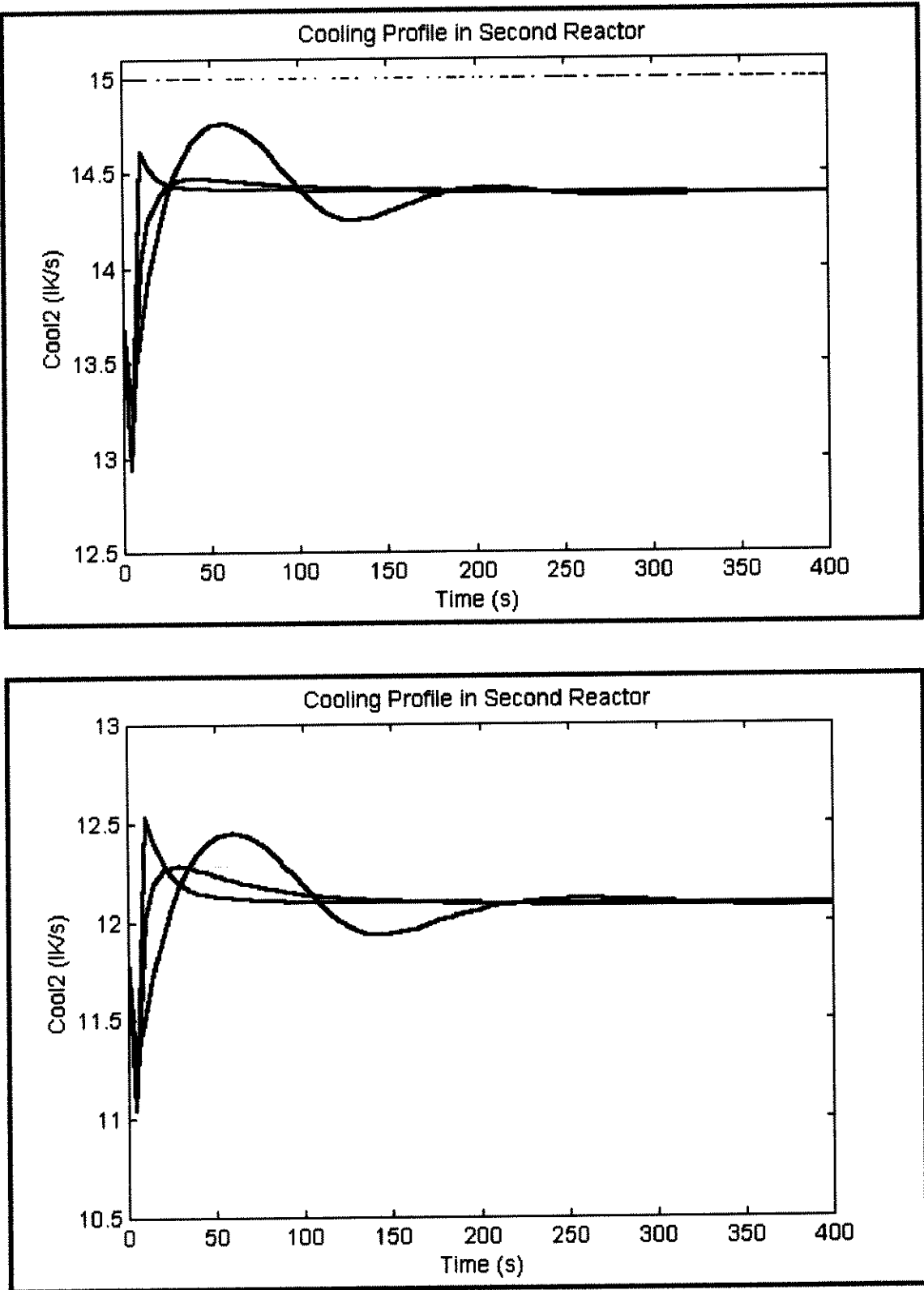


Figure 4.13c Cooling Profiles at First and Final Operating Conditions
(Second Reactor)

($T_{in} = 300 \rightarrow 305$, $T_{ci} = 283 \rightarrow 286$)

(Green: $U = 1$, $qq_1 = qq_2 = 1$; Red: $U = 2$, $qq_1 = qq_2 = 1$; Blue: PI controllers)

The plant has two level and two temperature control loops. Since it is very complicated to solve the NLP problem on-line, the required optimal trajectories are obtained from solving the switchability problem off-line first. There is no feasible solution for the regulator and servo problem, if the temperature set points drop more than seven degrees as shown in Table 4.2. The two-step switching policy in Table 4.3 is considered instead. The profiles found (see Figure 4.14) are then implemented on-line with DMC replacing PI temperature controllers.

❖ <u>First Step</u>	
$C_{in} = 20 \rightarrow 15$	Step change (input)
$T_{in} = 300 \rightarrow 305$	Step change (input)
$T_{ci} = 283 \rightarrow 286$	Step change (input)
$Q^1 = 0.531 \rightarrow 0.750$	Optimal trajectory (solution)
$Q^2 = 0.134 \rightarrow 0.050$	Step change (input)
$Stpt_1 = 349.5 \rightarrow 347.5$	Optimal trajectory (solution)
$Stpt_2 = 335.4 \rightarrow 333.4$	Optimal trajectory (solution)
❖ <u>Second Step</u>	
$Stpt_1 = 347.5 \rightarrow 340.2$	Step change (input) or optimal trajectory (solution)
$Stpt_2 = 333.4 \rightarrow 328.2$	Step change (input) or optimal trajectory (solution)

Table 4.3 Two Step Switching Policy

As discussed in the SISO case, it is not necessary to update the coefficient matrix A during the transition if four blocks A_{11} , A_{12} , A_{21} and A_{22} are constructed on the response curves evaluated at the final steady state. Figures 4.14 and 4.15 prove the validity of the assumption, which keeps the matrix A constant. The response curves used to develop matrices A_{11} and A_{22} in Figure 4.15 show significant deviation after 100 seconds. However, Figure 4.14 shows that after 100 seconds the feed flowrate (Q^1_{in}) almost reaches the final steady state value. Thus the constant gain matrix K_{DMC} can be used to calculate the control move in the MIMO case study.

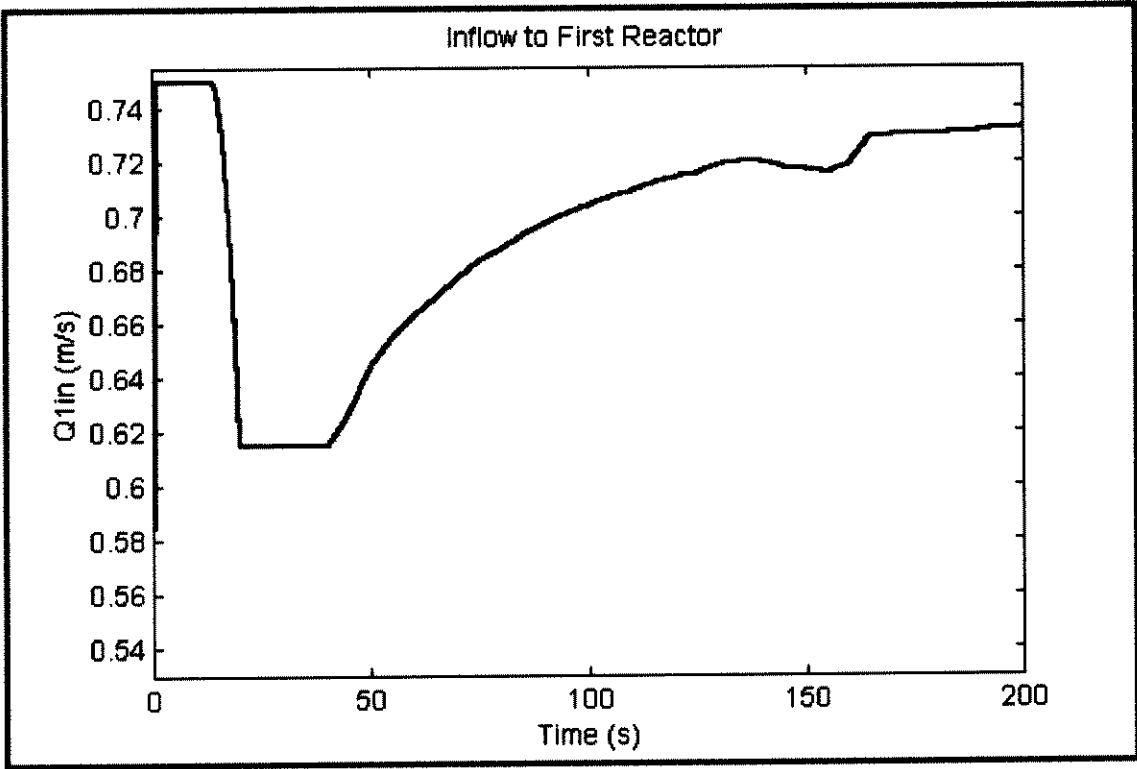
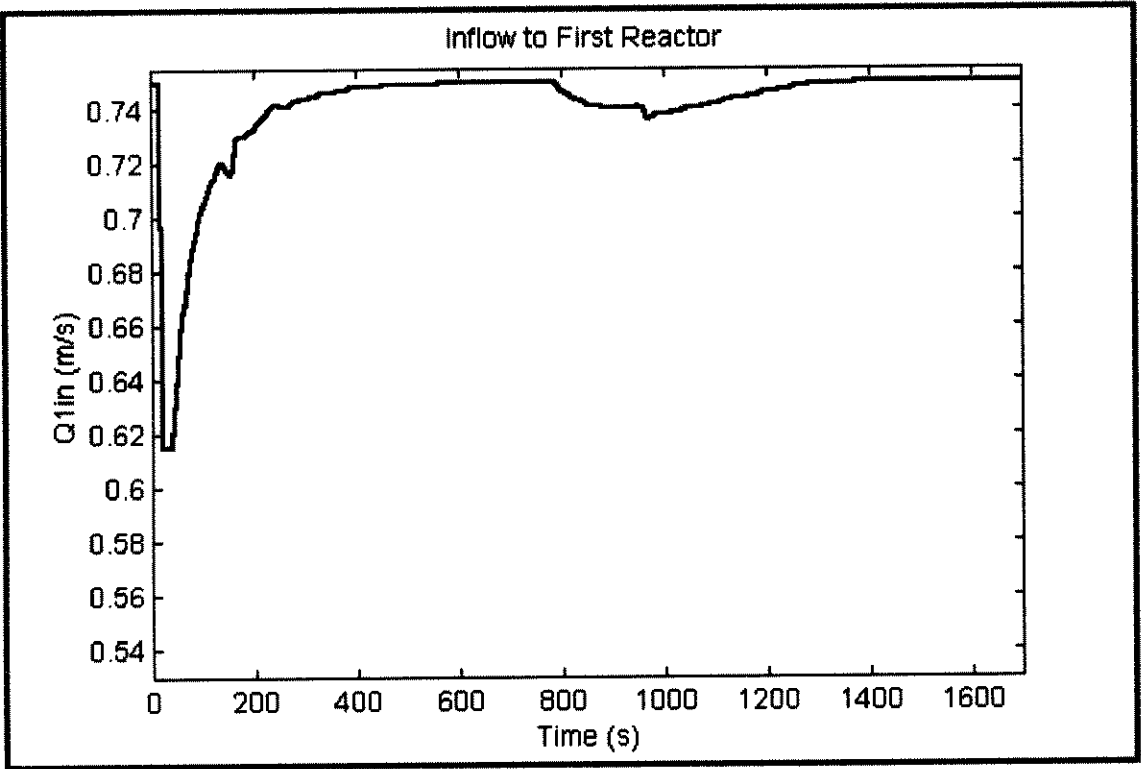


Figure 4.14 Optimal Flowrate Profile (Feed to First Reactor)

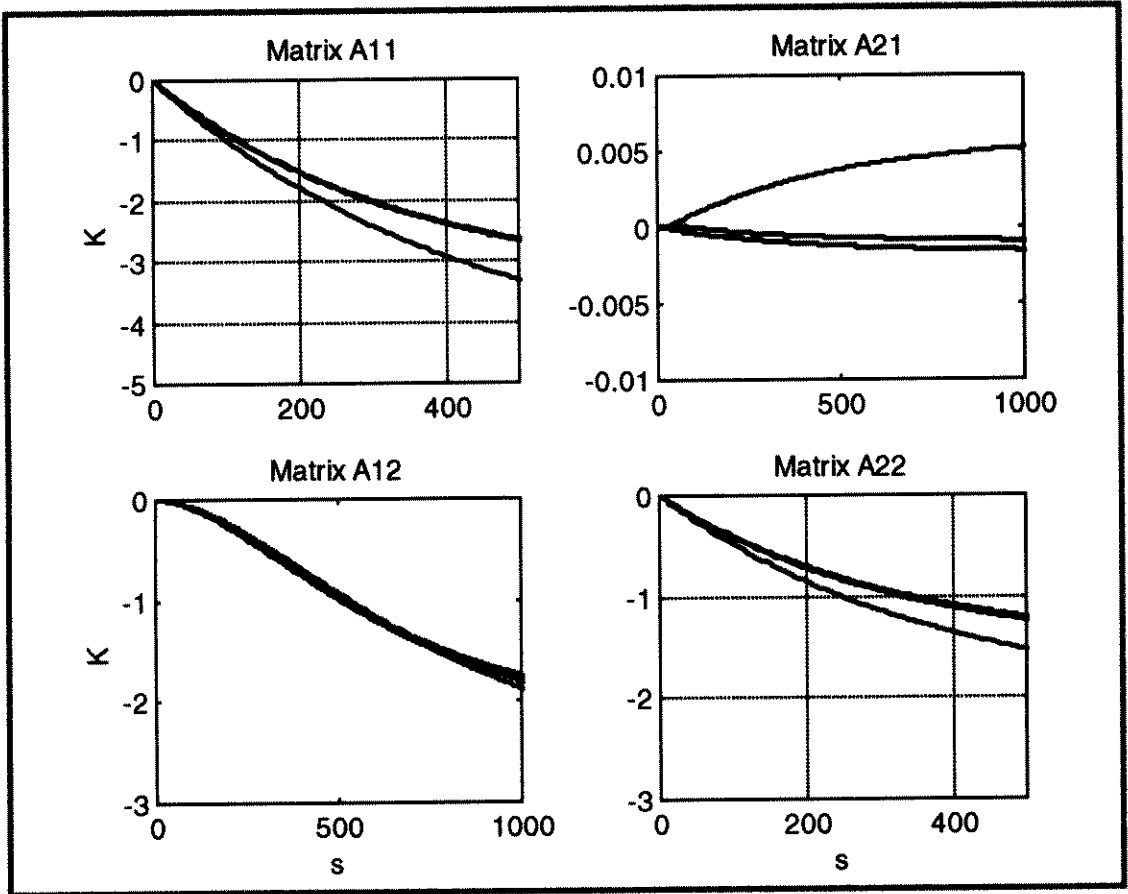


Figure 4.15 Temperature Difference Responses to Unit Step Change in Coolant

Flowrate

(Blue: $Q_{in} = 0.750$, $T_{in} = 300$, $T_{ci} = 283$);

(Green: $Q_{in}^1 = 0.531$, $T_{in} = 300$, $T_{ci} = 283$)

(Red: $Q_{in} = 0.750$, $T_{in} = 305$, $T_{ci} = 286$)

The switchability problem with DMC designed for the MIMO case is now ready to be run on-line. The following simulations are performed off-line under the worst situation, then feasibility tests are carried out afterwards. Figure 4.16 shows that the constraint on cooling rate in the second reactor is violated, when feed and coolant temperatures decrease ($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$). As discussed in Chapter 3, to find a feasible solution that satisfies all constraints under disturbance effects, the switchability problem must be solved for two or more systems of two CSTRs in series. Each system is subject to a different situation described by a corresponding row of the matrix of disturbance and uncertainty.

$$d^n = \begin{vmatrix} T_{in} & T_{ci} \\ 300 & 283 \\ 305 & 286 \\ 305 & 280 \\ 298 & 286 \\ 298 & 280 \end{vmatrix}$$

Because of the complexity of the problem and the size limitation of the solver and the software, there is no guarantee of a feasible solution. A simpler remedy is used as before. The NLP problem using PI controllers is solved again with a time delay ($\theta \geq 100$ s) posed on the temperature set point of the second reactor. For the switching problem using DMC, tuning parameters can be adjusted until all constraints are satisfied. The configuration of the DMC used to construct the red curve in Figure 4.16 is:

$$\Delta t = 5, V = 40, U = 8, qq_1 = 5, qq_2 = 20, ww_1 = 1, ww_2 = 1.$$

The green curve is constructed from the solution of the NLP problem. Both curves violate the path constraint $Cool_2 \leq 15$. In Figure 4.17 time delay is included in the NLP problem and the configuration of the DMC is changed to:

$$\Delta t = 5, V = 40, U = 8, qq_1 = 5, qq_2 = 20, ww_1 = 1, ww_2 = 0.05.$$

Both cases satisfy the path constraint $Cool_2 \leq 15$.

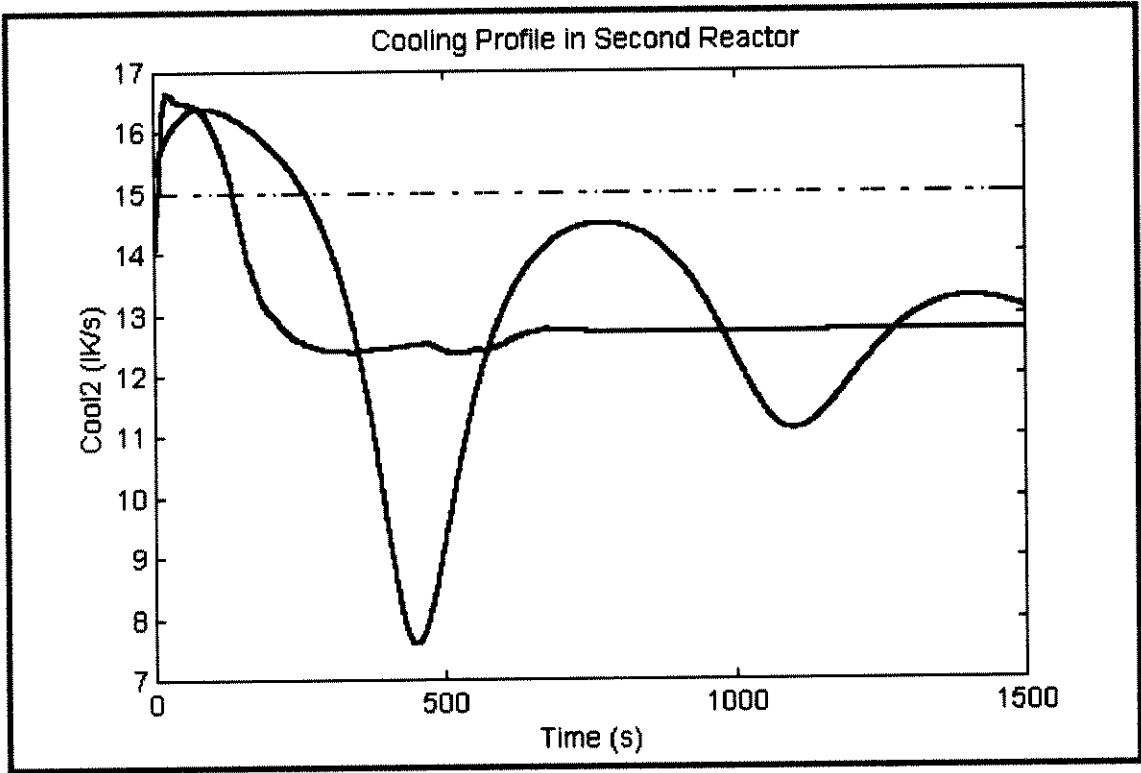


Figure 4.16 Cooling Profile in Second Reactor (Constraint Violation)

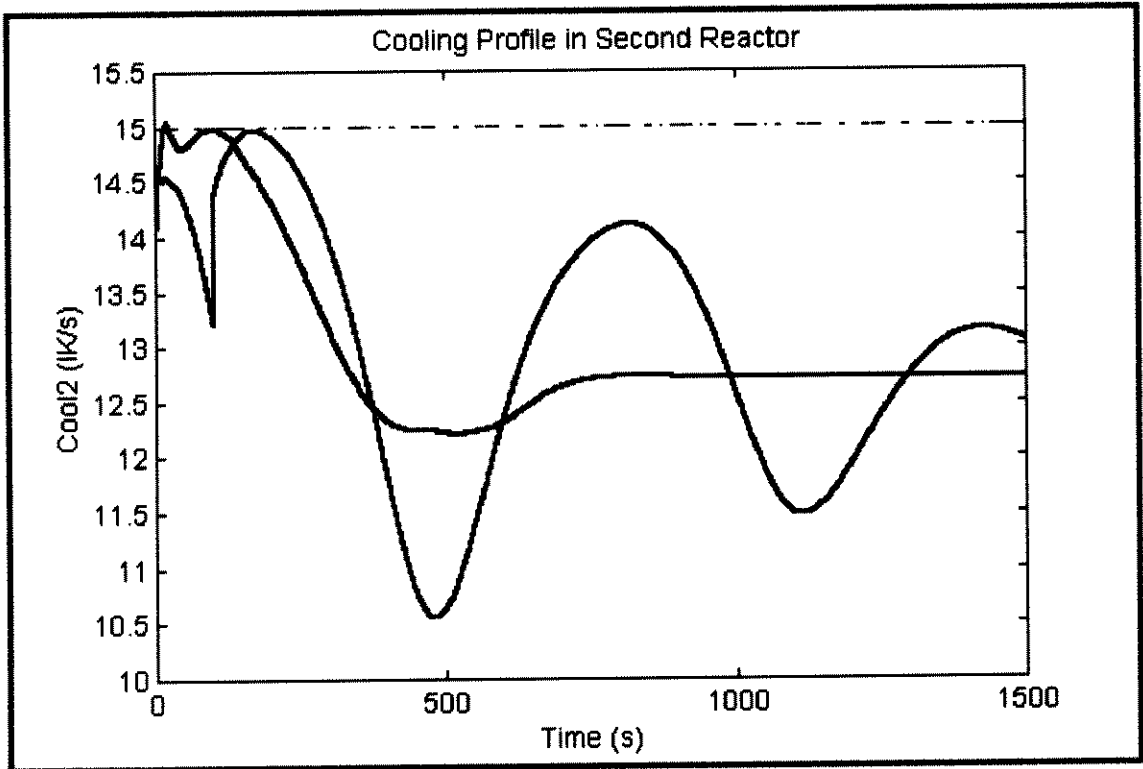


Figure 4.17 Cooling Profile in Second Reactor (Constraint Satisfaction)

($T_{in} = 300 \rightarrow 298$, $T_{ci} = 283 \rightarrow 280$)

(Green: Solution of NLP problem with PI controllers, Red: Simulation with DMC)

Figure 4.18 is similar to 4.17 but the feed and coolant temperatures approach their upper limits ($T_{in} = 300 \rightarrow 305$, $T_{ci} = 283 \rightarrow 286$). The corresponding temperatures in the reactors are shown in Figures 4.18a and b. Blue curves are constructed from the original solutions of the NLP problem using PI controllers. These solutions are not feasible when tested with disturbances approaching their lower limits. Green curves are from NLP solutions including the time delay on the temperature set point of the second reactor. Red curves are results of DMC simulations with the weighting for the controlled variable deviation from set point ww_2 much smaller than ww_1 .

The second step is also a servo plus regulator problem with the temperature set point change. The configuration of DMC used in this step is:

$$\Delta t = 5, V = 40, U = 1, qq_1 = 20, qq_2 = 40, ww_1 = 0.01, ww_2 = 0.01.$$

The above parameters are compared with the DMC configuration used in the first step, which is:

$$\Delta t = 5, V = 40, U = 8, qq_1 = 5, qq_2 = 20, ww_1 = 1, ww_2 = 0.05.$$

It shows that the second step policy requires robust DMC (U is eight times smaller) but more suppression of control move (higher values of qq and smaller values of ww) to satisfy the path constraints $Cool_1 \leq 20$ and $Cool_2 \leq 15$. However, this configuration results in sluggish responses of the second reactor. Another option is to include a policy for the temperature set point change in each reactor as shown in Figure 4.19. A smaller qq_1 and a higher ww_1 ($qq_1 = ww_1 = 1$) can be selected for this alternative. Responses in the first reactor are faster but those in the second are not improved. In the following figures, green curves represent the step-change set-point policy and DMC with $qq_1 = 20$, $ww_1 = 0.01$. Red curves represent the optimal set-point policy and DMC with $qq_1 = ww_1 = 1$. Both manipulated and controlled variables in the first reactor respond faster with a smaller qq_1 and a higher ww_1 . Figures 4.20 a, b and c plot coolant, cooling and corresponding temperature profiles in the first reactor. Using DMC, there is also a possibility to combine two steps shown in Table 4.2 into one. The selection of the configuration for one step policy must satisfy path constraint during the whole transition. As shown in Figure 4.16, constraint violations occur at the beginning of the trajectory. The parameters selected to satisfy these constraints at the early stage

would give a sluggish control performance at the other stage of the transition. The two-step policy creates a chance to update the DMC configuration required at each stage of the switch.

4. Conclusion

The performance of the DMC based on a convolution model has been compared with PI controllers through several examples. In a regulator control problem designed for the SISO case, DMC does not offer significant advantages over a PI controller. In more complicated control and switchability problems such as servo plus regulator switching problems designed for the MIMO case, well-tuned DMC can handle much better these situations, which sometimes cannot be solved by a PI controller. Compared to a PI controller, DMC is more flexible in dealing with disturbance variation since the latter controller has a greater number of adjustable parameters, all of which influence the control performance. However, the selection of these parameters is a time consuming job as there is no tuning methodology except some guidelines discussed before. It is sometimes possible to include tuning parameters of a conventional controller as decision variables in minimizing the Integral Square of the Error (ISE), but it is impossible to include DMC adjustable parameters in the same optimization problem. As a result, DMC is more practical for multivariable systems, especially for distillation columns, which will be discussed further in Chapter 6.

Without information of on-line measurement, this chapter cannot demonstrate full capabilities of the MPC techniques. However, the case studies have shown that a good performance is achievable with a large number of design and implementation decisions. Some major tuning issues have also been discussed. Although DMC is designed for on-line implementation, the parameters should be tuned off-line with care first under the worst situation. Feasibility tests are then carried out to cover other situations.

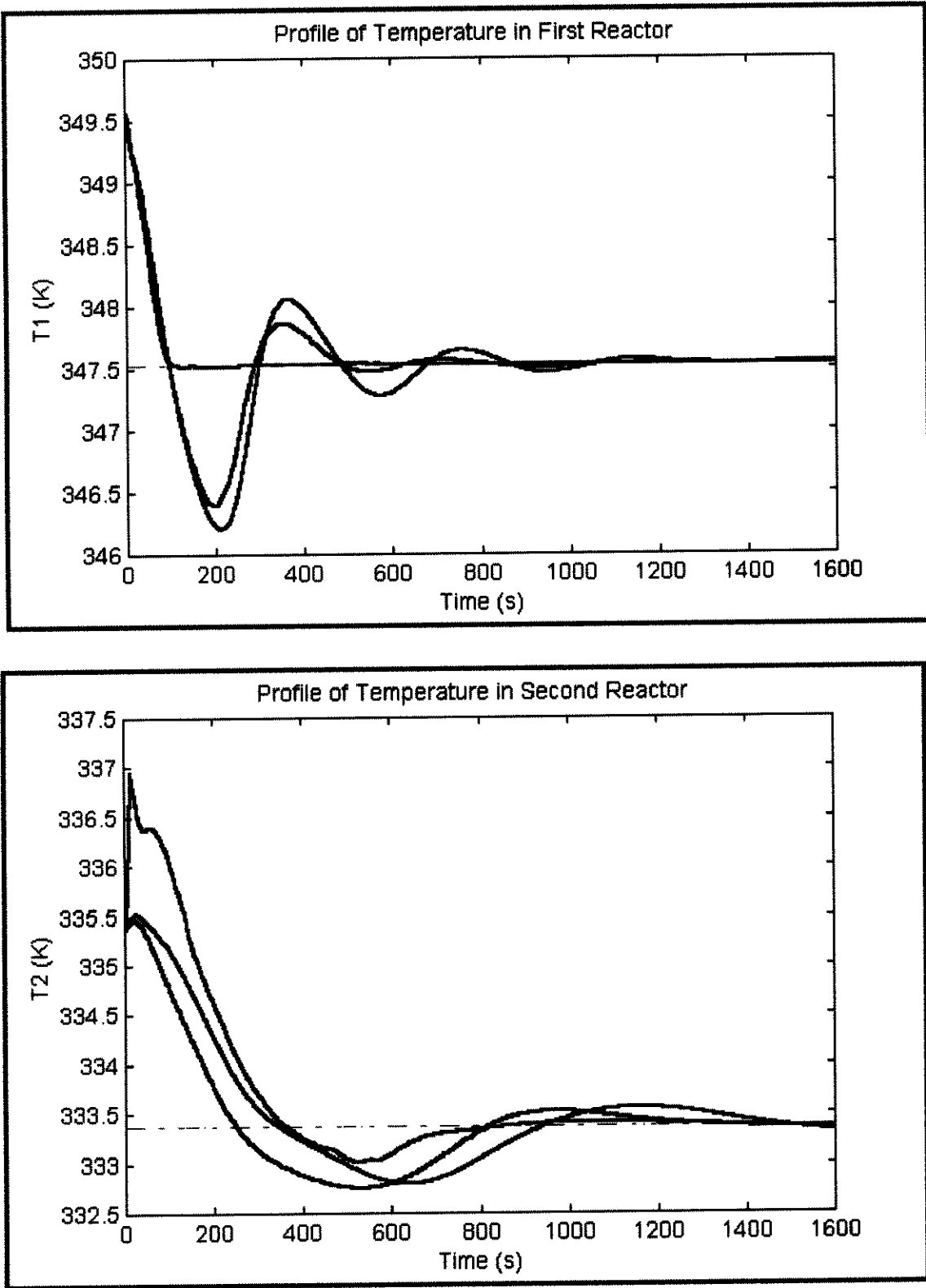


Figure 4.18a Temperature Profiles in Reactors

($T_{in} = 300 \rightarrow 305$, $T_{ci} = 283 \rightarrow 286$)

(Blue: Solution of NLP problem with PI controllers)

(Green: PI controllers with time delay on temperature set point)

(Red: DMC configuration $U = 8$, $qq_1 = 5$, $qq_2 = 20$, $ww_1 = 1$, $ww_2 = 0.05$)

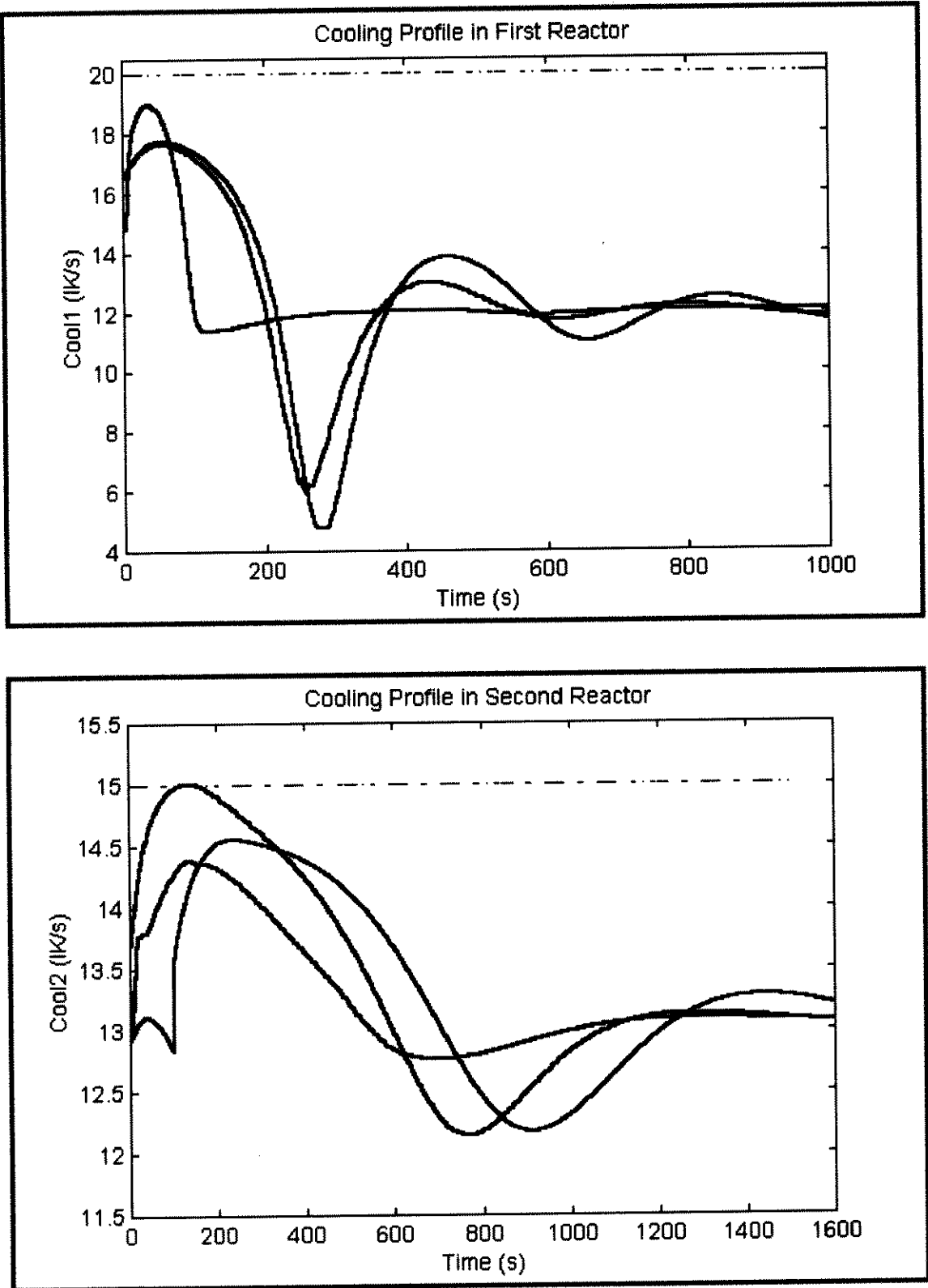


Figure 4.18b Corresponding Cooling Profiles in Reactors

($T_{in} = 300 \rightarrow 305$, $T_{ci} = 283 \rightarrow 286$)

(Blue: Solution of NLP problem with PI controllers)

(Green: PI controllers with time delay on temperature set point)

(Red: DMC configuration $U = 8$, $qq_1 = 5$, $qq_2 = 20$, $ww_1 = 1$, $ww_2 = 0.05$)

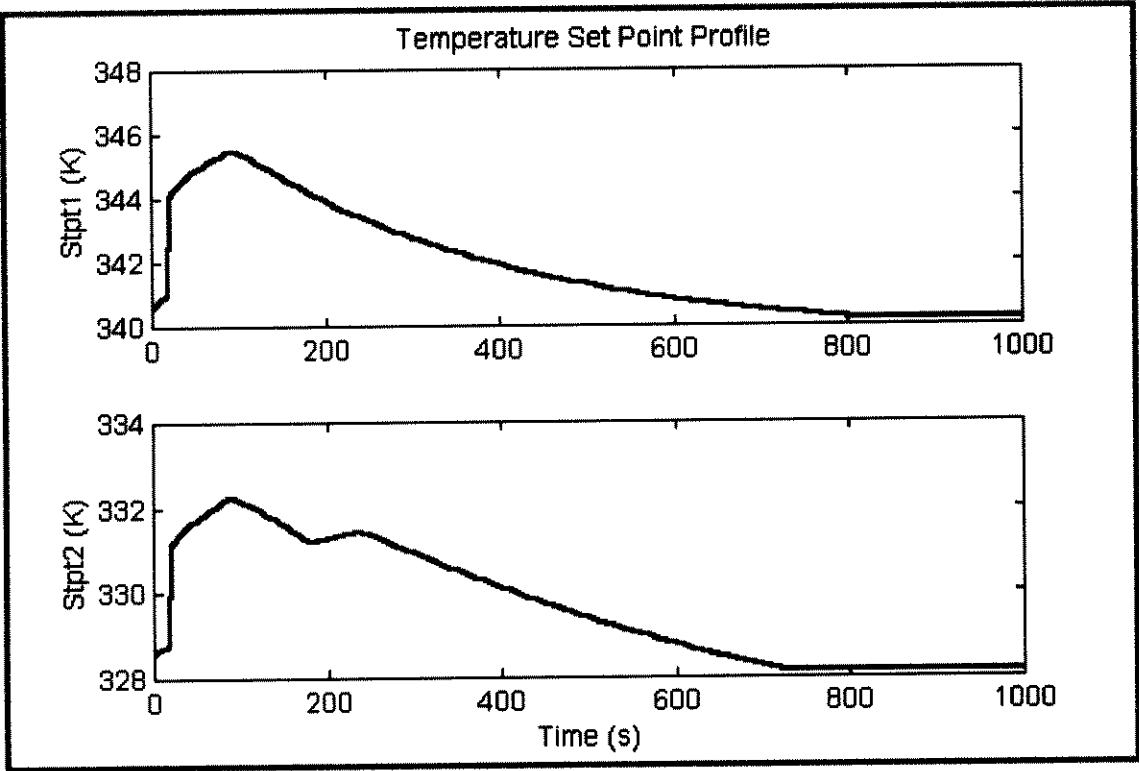


Figure 4.19 Temperature Set Point Policies in First and Second Reactors

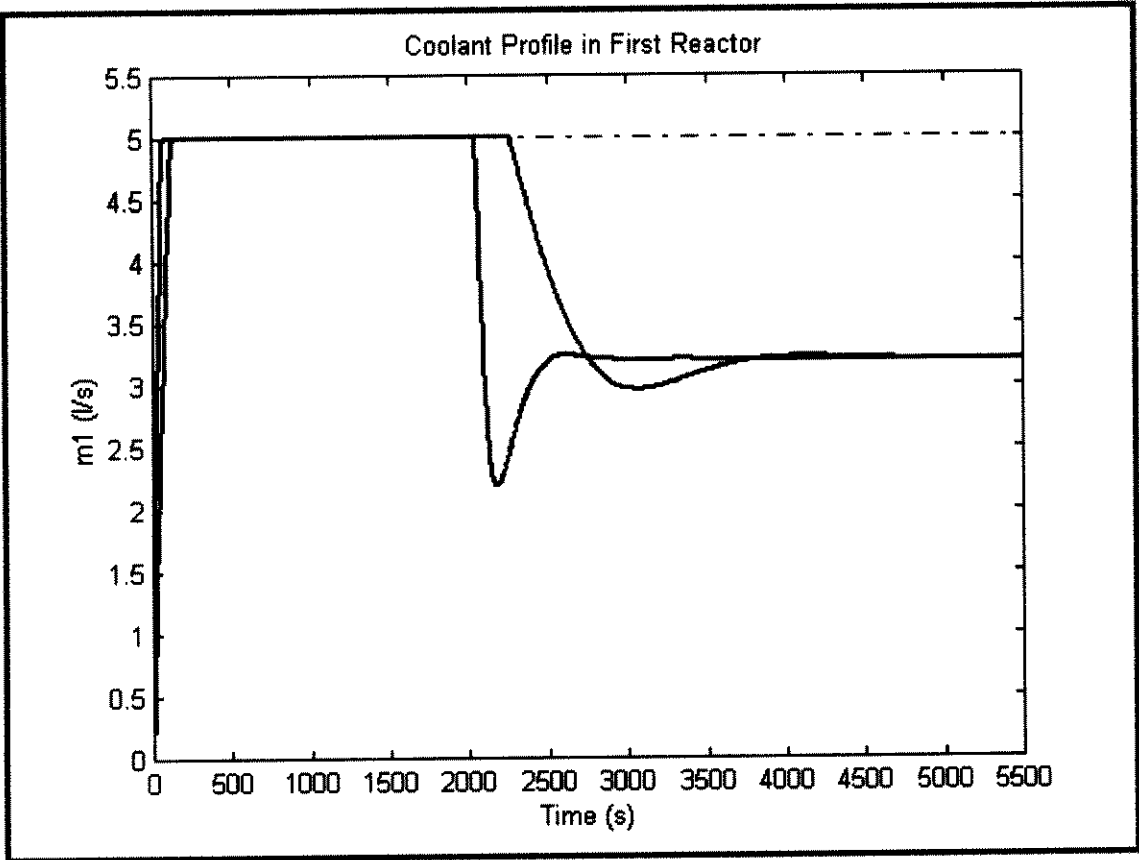


Figure 4.20a Coolant Profile in First Reactor

(Green: Step-change set-point policy; Red: Optimal set-point policy)

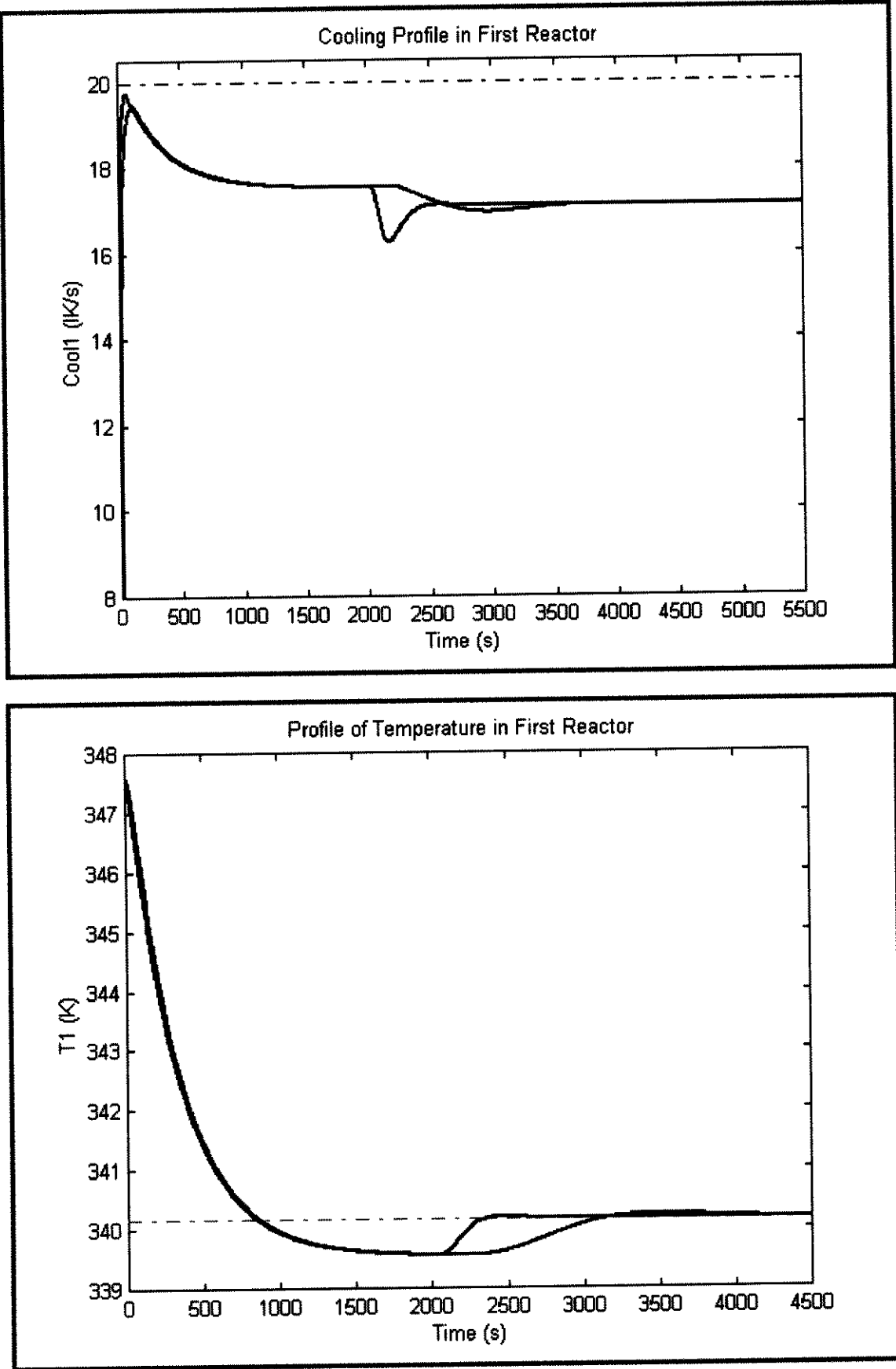


Figure 4.20 b, c Cooling and Temperature Profiles in First Reactor
(Green: Step-change set-point policy; Red: Optimal set-point policy)

5. Nomenclature

a_i	: Coefficients of step response. $a_i = 0$ for $i \leq 0$
A	: Dynamic matrix (see Appendix 4a)
cool	: Removal heat from the reactor to the cooling jacket, $l.Ks^{-1}$
d_k	: Difference between prediction and measurement
d^n	: Matrix of disturbances and uncertainties
E	: Matrix of closed-loop predicted error (see Appendix 4A)
E'	: Matrix of open loop predicted error (see Appendix 4A)
h_i	: Coefficients of impulse response. $h_i = a_i - a_{i-1}$, $i = 1, 2, \dots, T$
F	: Objective function or flexibility index
I_V, I_U	: Identity matrix of size V and U , respectively
K_{DMC}	: Gain vector
N :	: Model horizon. $N\Delta t$ is the settling time for the process (open loop) to reach 99% completion
qq	: Adjustable parameter (≥ 0), weighting the adjustments of the manipulated variable (move suppression factor)
[QQ]	: Diagonal weighting matrix = $qq * I_U$
Δt	: Sampling period
Δu	: Change in input
U	: Control horizon
V	: Prediction horizon
ww	: Adjustable parameter (≥ 0), weighting the controlled variable deviation from set point
[WW]	: Diagonal weighting matrix = $ww * I_V$
y	: Output

6. References

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Appendix 4A

Figure 4.a1 shows the typical open-loop response. The values of the unit step response are given by $a_0, a_1, a_2, \dots, a_N$ and the impulse response by $h_1, h_2, \dots, h_N$. The relationship between a_i and h_i is shown by equation (4a.1). S and P are defined by equations (4a.2) and (4a.3), respectively.

$$a_i = \sum_{j=1}^i h_j \quad (4a.1)$$

$$S_m = \sum_{i=m+1}^N h_i \Delta u_{k+m-i} \quad (m = 1, 2, \dots, V) \quad (4a.2)$$

$$P_i = \sum_{m=1}^i S_m \quad (i = 1, 2, \dots, V) \quad (4a.3)$$

$$y_{k+j}^c = y_{k+j-1}^c + \sum_{i=1}^N h_i \Delta u_{k+j-i} \quad (i = 1, 2, \dots, V) \quad (4a.4)$$

Equation (4a.4) can be written in a more convenient vector-matrix form:

$$\begin{bmatrix} y_{k+1}^c \\ y_{k+2}^c \\ y_{k+3}^c \\ \vdots \\ y_{k+V}^c \end{bmatrix} = \begin{bmatrix} a_1 & 0 & 0 & \dots & 0 \\ a_2 & a_1 & 0 & \dots & 0 \\ a_3 & a_2 & a_1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_V & a_{V-1} & a_{V-2} & \dots & a_{V-U+1} \end{bmatrix} * \begin{bmatrix} u_k \\ u_{k+1} \\ u_{k+2} \\ \vdots \\ u_{k+U-1} \end{bmatrix} + \begin{bmatrix} y_k + P_1 \\ y_k + P_2 \\ y_k + P_3 \\ \vdots \\ y_k + P_V \end{bmatrix} \quad (4a.5)$$

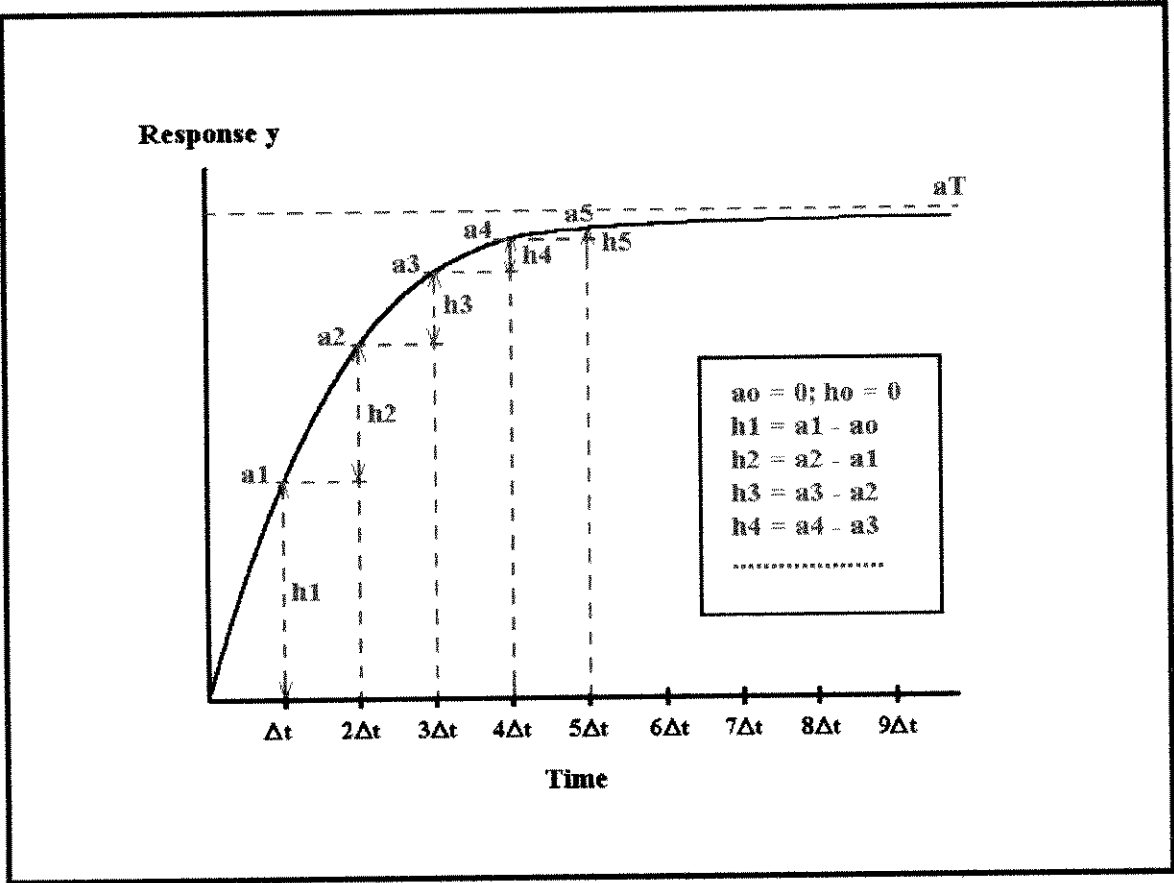


Figure 4a.1 Open-Loop Response Curve

The coefficient matrix A is defined by equation (4a.6). The matrices of closed-loop (E) and open loop (E') predicted error are shown by equations (4a.7) and (4a.8), respectively.

$$A = \begin{bmatrix} a_1 & 0 & 0 & 0 & . & . & . & 0 \\ a_2 & a_1 & 0 & 0 & . & . & . & 0 \\ a_3 & a_2 & a_1 & 0 & . & . & . & 0 \\ a_4 & a_3 & a_2 & a_1 & . & . & . & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ a_V & a_{V-1} & a_{V-2} & . & . & . & . & a_{V-U+1} \end{bmatrix}$$

(4a.6)

$$E = \begin{bmatrix} y_{k+1}^d - y_{k+1}^c \\ y_{k+2}^d - y_{k+2}^c \\ y_{k+3}^d - y_{k+3}^c \\ . \\ . \\ . \\ y_{k+V}^d - y_{k+V}^c \end{bmatrix} \quad (4a.7)$$

$$E' = \begin{bmatrix} E_k - P_1 \\ E_k - P_2 \\ E_k - P_3 \\ . \\ . \\ . \\ E_k - P_V \end{bmatrix} \quad (4a.8)$$

The diagonal weighting matrices [WW] and [QQ] are defined as:

$$[WW] = ww^* = \begin{bmatrix} 1 & 0 & . & . & 0_V \\ 0 & 1 & . & . & 0 \\ 0 & . & 1 & . & 0 \\ 0 & . & . & 1 & 0 \\ 0_V & . & . & 0 & 1_V \end{bmatrix} \quad (4a.9)$$

$$[QQ] = qq^* = \begin{bmatrix} 1 & 0 & . & 0_U \\ 0 & 1 & 0 & . \\ . & 0 & 1 & 0 \\ 0 & . & 0 & 1_U \end{bmatrix} \quad (4a.10)$$

Appendix 4B

The dynamic coefficient matrix A for the two inputs and two outputs is composed of four matrices A_{11} , A_{12} , A_{21} and A_{22} . These four matrices are constructed on four response curves similar to that shown in Figure 4a.1. A unit-step change in one input gives two output responses. The matrix A is now defined as:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad (4b.1)$$

where:

$$A_{11} = \begin{bmatrix} a_{11}^1 & 0 & 0 & . & . & . & 0 \\ a_{11}^2 & a_{11}^1 & 0 & . & . & . & 0 \\ a_{11}^3 & a_{11}^2 & a_{11}^2 & . & . & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ a_{11}^V & a_{11}^{V-1} & a_{11}^{V-2} & . & . & . & a_{11}^{V-U+1} \end{bmatrix} \quad (4b.2)$$

Similarly, the diagonal weighting matrices $[WW]$ and $[QQ]$ become:

$$[WW] = \begin{bmatrix} [WW]_1 & 0 \\ 0 & [WW]_2 \end{bmatrix} \quad [QQ] = \begin{bmatrix} [QQ]_1 & 0 \\ 0 & [QQ]_2 \end{bmatrix} \quad (4b.3)$$

$$[WW]_1 = ww_1 * \begin{bmatrix} 1 & 0 & 0 & . & 0 \\ 0 & 1 & 0 & . & 0 \\ 0 & 0 & 1 & . & 0 \\ . & . & . & . & . \\ 0_V & 0_V & 0_V & . & 1_V \end{bmatrix} \quad [QQ]_1 = qq_1 * \begin{bmatrix} 1 & 0 & 0 & . & 0 \\ 0 & 1 & 0 & . & 0 \\ 0 & 0 & 1 & . & 0 \\ . & . & . & . & . \\ 0_U & 0_U & 0_U & . & 1_U \end{bmatrix} \quad (4b.4)$$

Chapter 5

Solution Method for Operability and Switchability Analysis

1	Introduction.....	5.1
2	Open loop back-off calculations.....	5.2
2.1	Reactor problems.....	5.2
2.2	Distillation problems.....	5.7
3	Dynamic closed-loop back-off calculations.....	5.11
4	Switchability calculations.....	5.14
5	Nonlinear Model Predictive Control (NLPC) calculations..	5.20
6	Conclusion.....	5.22
7	Nomenclature.....	5.25
8	References.....	5.25
	Appendix 5A.....	5.26

Many software packages now available in the market can perform steady-state, dynamic, optimization simulations and even deal with optimal control problems, which require more knowledge of programming. Chapter 5 discusses the application of three packages: SPEEDUP, GAMS and MATLAB with SIMULINK in solving optimization problems generated by the flexibility, switchability and controllability analysis. Each package has its own advantages and disadvantages. The selection of software and technique to approach the optimization problems affects the computational time, convergence and accuracy. These factors will be considered in the case studies solved in the thesis.

1. Introduction

Up to this stage, solutions of normal and dynamic optimization problems have been obtained from three packages SPEEDUP, GAMS with MINOS 5.2 (updated version 5.4) optimizer and MATLAB. The algorithm developed for the steady-state flexibility study finds solutions of normal optimization problems, which include an appropriate objective function to be optimized, subject to a set of algebraic equality and inequality constraints. The algorithm developed for the dynamic flexibility, switchability and controllability study requires the minimum of a cost or an integral error objective function, subject to a set of mixed algebraic and differential equations (ADEs). These optimal control problems can be solved by two sophisticated mathematical techniques: sequential optimization and simultaneous integration and optimization approaches.

- ❖ The first technique spends most of the computational time in solving the ADEs, evaluating the objective function and constraints, and calculating their gradients. Consequently, it strongly depends on the selection of and interfacing to the optimizer. SPEEDUP can do the integration and provide the information required by the optimizer through the External Data Interface (EDI) mechanism because it cannot use its own optimizer within the dynamic environment. MATLAB is simpler to use, thus requires less time to do the same job, since it is possible to use the optimization toolbox while performing dynamic simulations. However, SPEEDUP is more advantageous over MATLAB and GAMS in optimizing the whole flowsheet, which includes many operation units. A further discussion on this feature will be given later through the examples.

- ❖ The simultaneous integration and optimization technique converts the ODEs to algebraic equations using Orthogonal Collocation on Finite Elements (OCOFE) approximating method. Then the approximated problem becomes a normal NLP problem, which can be solved by any existing optimization technique. GAMS with MINOS 5.4 optimizer has been used through all case studies. This approach provides a promising research area but it still cannot be used for complicated problems due to the size limitation of the package and the solver itself.

A thorough comparison between solution methods and software package usage in flexibility, switchability and controllability analysis will be presented in the following sections.

2. Open Loop Back-Off Calculations

The algorithm developed for open-loop back-off calculations reviewed in Chapter 2 is an iterative dual level optimization. The outer and inner levels search for the optimality at all iterations until the algorithm reaches the permanent feasible region. The optimization problems in both levels aim to different objectives but share a similar mathematical structure, which can be solved easily by any optimizer. However, for a chemical process involving physical and thermodynamic properties such as distillation process, the package that can supply these properties are more favorable. Distillation problems will be solved later in this and the following chapters.

2.1. Reactor Problems

Since the reactor problems do not require properties, any package having an optimization simulator can be used for open loop back-off calculations. SPEEDUP is selected to solve the case studies in Chapter 2. At some steps of the back-off algorithm, the number of unit operations might become double or triple but SPEEDUP needs only one model or one set of equations to describe more than one unit operations of the same type. Moreover the solution of the units is not dependent on the order of the equations or the units in the program. SPEEDUP is thus very handy for model development or design, especially when dealing with the flowsheet. MATLAB, on the contrary is sequential modular or equation order-dependent. Although the execution time is quite fast when handling each unit operation individually, it is very complicated or even

impossible to model several units connected by streams in MATLAB. The optimality of the solutions found by the optimization simulators should also be looked at when selecting the solver. The first case study on page 2.16 is solved as an example, using GAMS, SPEEDUP and MATLAB. The objective function and the set of inequality constraints are written as:

Obj (\$/time) = pv*Q_{in}*(C_{in} - C_o) - mc* Q_{in} - cc*Cool

(5.1)

$$T \leq 350 \text{ K}$$

Constraint 1

$$200 \text{ l} \leq V \leq 300 \text{ l}$$

Constraint 2

$$C \leq 0.3 \text{ mol/l}$$

Constraint 3

Two highlighted constraints (1 and 3) are active. For comparison three solvers start with the same initial guesses. Table 5.1 shows results of the first iteration (nominal case).

Solver	Initial V	Obj. Value	Q _{in}	V	Active
GAMS	220	71.0549	0.3618	245.16	Constraints 1 & 3
	240	71.0549	0.3618	245.16	Constraints 1 & 3
	260	71.0549	0.3618	245.16	Constraints 1 & 3
	280	71.0549	0.3618	245.16	Constraints 1 & 3
SPEEDUP	220	71.0549	0.3618	245.16	Constraints 1 & 3
	240	71.0549	0.3618	245.16	Constraints 1 & 3
	260	70.9903	0.3611	259.99	Constraint 1
	280	70.9145	0.3604	279.99	Constraint 1
MATLAB	245	71.0032	0.3615	250.97	Constraint 1
	245.1	71.0549	0.3618	245.16	Constraints 1 & 3
	250	71.0260	0.3611	248.34	Constraints 1
	280	70.7793	0.3604	279.84	Constraint 1

Table 5.1 Results from First Iteration (Nominal Case, Single CSTR)

The problem is solved for two decision variables: feed flowrate Q_{in} and liquid inventory V . The latter variable is not explicitly seen in the objective function but it is related to the outlet concentration (constraint 3). The residence time increases, the concentration decreases if a bigger tank is used, which means the fixed cost is increased. As GAMS is specially designed for optimization problems, it has many powerful solvers. Starting with four different initial values of V , the solver gives only one true solution, which is the intersection point of two active constraints. The optimization problem is fully constrained, as the numbers of decision variables and active constraints are equal. Starting with two different initial values of V , which are smaller than the optimal values, SPEEDUP gives the same solution as GAMS. However, with two initial values of V greater than the optimal values, SPEEDUP does not change the value of the second decision variable. The iteration is terminated before the problem becomes fully constrained. The solution found is slightly different from the true optimum. MATLAB cannot find the solution with two smaller initial values and only gives the true optimal values, if the solver starts with values close to the optimum.

Table 5.2a shows the results from two CSTRs case study. The problem is solved for three decision variables: two feed flowrates (Q^1_{in} , Q^2) and inventory ($V_1 = V_2 = V$). Table 5.2b presents the case solved for four decision variables ($V_1 \neq V_2$). The objective function and constraints of this problem are:

$$\text{Obj}(\$/\text{time}) = p_v \cdot Q_f \cdot (C_f - C_o) - m_c \cdot Q_f \cdot C_f - c_{c1} \cdot \text{Cool}_1 - c_{c2} \cdot \text{Cool}_2$$

(5.2)

$Q_{in} \leq 50 \text{ m}^3/\text{s}$	Constraint 1
$200 \text{ l} \leq V \leq 400 \text{ l}$	Constraint 2
$C_o \leq 0.3 \text{ mol/l}$	Constraint 3
$\text{Cool}_1 \leq 20 \text{ l.K.s}^{-1}$	Constraint 4
$\text{Cool}_2 \leq 15 \text{ l.K.s}^{-1}$	Constraint 5

Solver	Initial V	Obj. Value	Q^1_{in}	Q^2	V	Active
GAMS & SPEEDUP	220	141.43	0.5511	0.2442	273.38	Constraints 1, 3, 5
	250	141.43	0.5511	0.2442	273.38	Constraints 1, 3, 5
	300	141.43	0.5511	0.2442	273.38	Constraints 1, 3, 5
	350	141.43	0.5511	0.2442	273.38	Constraints 1, 3, 5
MATLAB	220	129.86	0.5580	0.1754	226.69	Constraints 1, 3
	250	141.43	0.5511	0.2440	273.38	Constraints 1, 3, 5
	300	141.01	0.5482	0.2450	299.98	Constraints 1, 5
	350	140.40	0.5440	0.2460	349.99	Constraints 1, 5

Table 5.2a Results from First Iteration (Nominal Case, Two CSTRs)

The highlighted constraints (1, 3 and 5) are active. As three active constraints lead to three decision variables, the problem is also fully constrained. GAMS and SPEEDUP find the true optimal solution with different initial values of V. MATLAB only gives the optimum with the initial value $V = 250$. With other initial values of V, MATLAB terminates when two constraints 1 and 3 or 1 and 5 are active. Figures 5.1 and 5.2 show the fully constrained problems plotted in two and three dimensions. In both cases the optimum is the intersection point of the active constraints. If the problem is solved for four decision variables but only three constraints are active, the optimal objective value and the total feed remain constant while the optimal values of feeds and inventories vary with initial values of V_1 and V_2 . Table 5.2b presents the results given by GAMS for four decision variables.

Initial V_1 and V_2	Obj. Value	Q^1_{in}	Q^2	$Q_t = Q^1_{in} + Q^2$	V_1	V_2
220	141.43	0.5563	0.2389	0.7953	236.20	269.69
250	141.43	0.5543	0.2410	0.7953	249.30	271.13
300	141.43	0.5603	0.2350	0.7953	214.87	266.92
350	141.43	0.5604	0.2348	0.7953	214.06	266.80

Table 5.2b Results from First Iteration (Two CSTRs, Four Decision Variables)

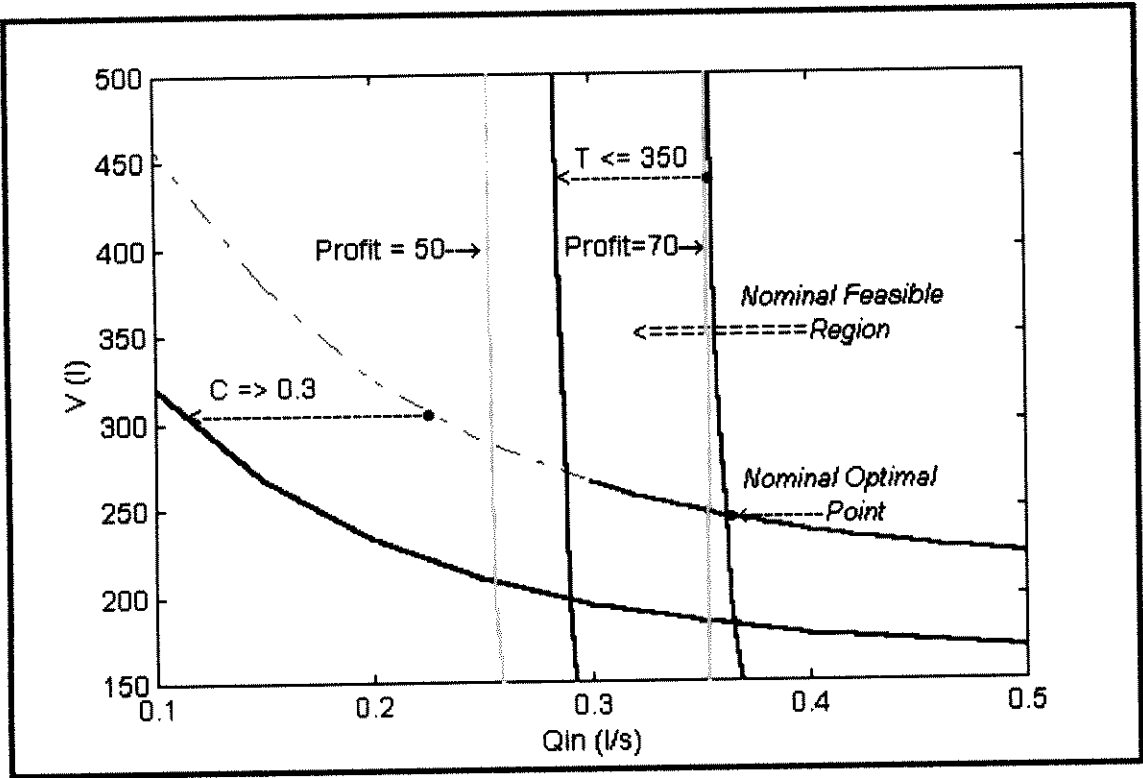


Figure 5.1 Optimal Solution (2 Decision Variables & 2 Active Constraints)

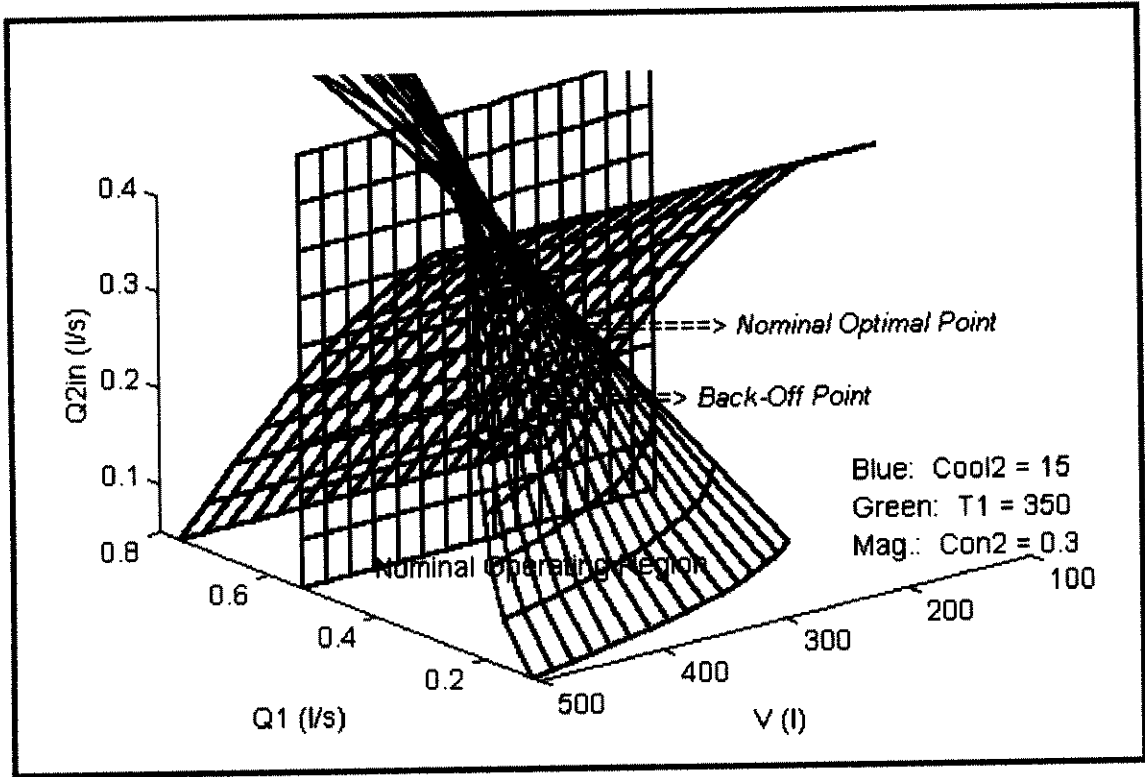


Figure 5.2 Optimal Solution (3 Decision Variables & 3 Active Constraints)

2.2. Distillation Problems

Almost all petroleum and other chemical industries involve in one of the most important processes: distillation. Some software packages, such as PROCESS, HYSIM, ASPEN, etc are specially designed for column simulations, which can provide physical property data or estimate the property of an uncommon component. Some packages that do not have the databank must interface to or use the information from other sources. Using ASPEN in open loop back-off calculations for distillation columns is, therefore, more advantageous than using GAMS, MATLAB or SPEEDUP. As the latter packages cannot provide physical property data, they must interface to or use the information provided by ASPEN. Large size columns, over fifty trays are very common in petroleum industries. A rigorous model for an industrial column can be developed in ASPEN with reliable thermodynamic data. In tray-by-tray calculation the number of equations to be solved simultaneously is so enormous that the solver of GAMS, MATLAB or SPEEDUP cannot handle. In this situation the compartmental model usually replaces the rigorous model with some errors within acceptable limits. However, ASPEN can be used only for open loop back-off calculations, which are steady-state optimization problems. Other packages that extract property data from ASPEN perform dynamic closed-loop back-off and switching calculations. Figure 5.3 shows the flowsheet of the purification column at the final step of the algorithm to search for the permanent feasible operating region. Three identical columns operate at different feed conditions, as shown in the following matrix:

	<i>B1</i>	<i>B2</i>	<i>B3</i>
<i>Feed (kg/hr)</i>	4809	4580	4351
<i>EA (ppm)</i>	45	30	45
<i>MA (ppm)</i>	20	15	20
<i>Q_{REB} (kW)</i>	1750	1660	1750

These three columns produce the same distillate rates and the same base product rates, as well. However, the side product rates are different and the compositions of the impurities in each product vary with three columns.

The flowsheet and more details of the purification column are actually presented in Chapter 6. This section and the following paragraph only show the final step

involving three identical columns, subject to three different sets of disturbances d^n , d^1 and d^2 . The problem is solved for two decision variables: the distillate and the side stream coming from tray 11 (from top to bottom, including the condenser as the first tray). The column has 85 trays plus a condenser and a reboiler. The feed contains one main component with two impurities. Tray-by tray calculations must give solution for more than a thousand variables. Therefore, the rigorous problem is only solved using ASPEN. Chapter 6 will solve the same problem with the compartmental model replacing the rigorous one. Results of the final step dealing with three identical columns and all streams, flowing to and leaving the columns, under different disturbance effects are shown on page 5.10. The ASPEN input file used in this final step is included in Appendix 5A for reference. The following samples are extracted from ASPEN results.

DESCRIPTION

OPTIMIZATION OF THE PURIFICATION COLUMN: FEED FLOW RATE IS 110 TONS/DAY. DISTURBANCES ARE IN FEED RATE, COMPOSITION AND REBOILER DUTY.

OPTIMIZATION AND CONSTRAINTS SUMMARY

OPTIMIZATION BLOCK IS MIXPRO
FINAL OBJECTIVE ERROR = 0.18190E-11
OBJECTIVE FUNCTION = 12186

BLOCK STATUS

```
*****
*                                     *
* CALCULATIONS WERE COMPLETED NORMALLY                                     *
*                                     *
* ALL UNIT OPERATION BLOCKS WERE COMPLETED NORMALLY
*                                     *
* ALL STREAMS WERE FLASHED NORMALLY                                         *
*                                     *
* ALL CONVERGENCE BLOCKS WERE COMPLETED NORMALLY
*                                     *
```

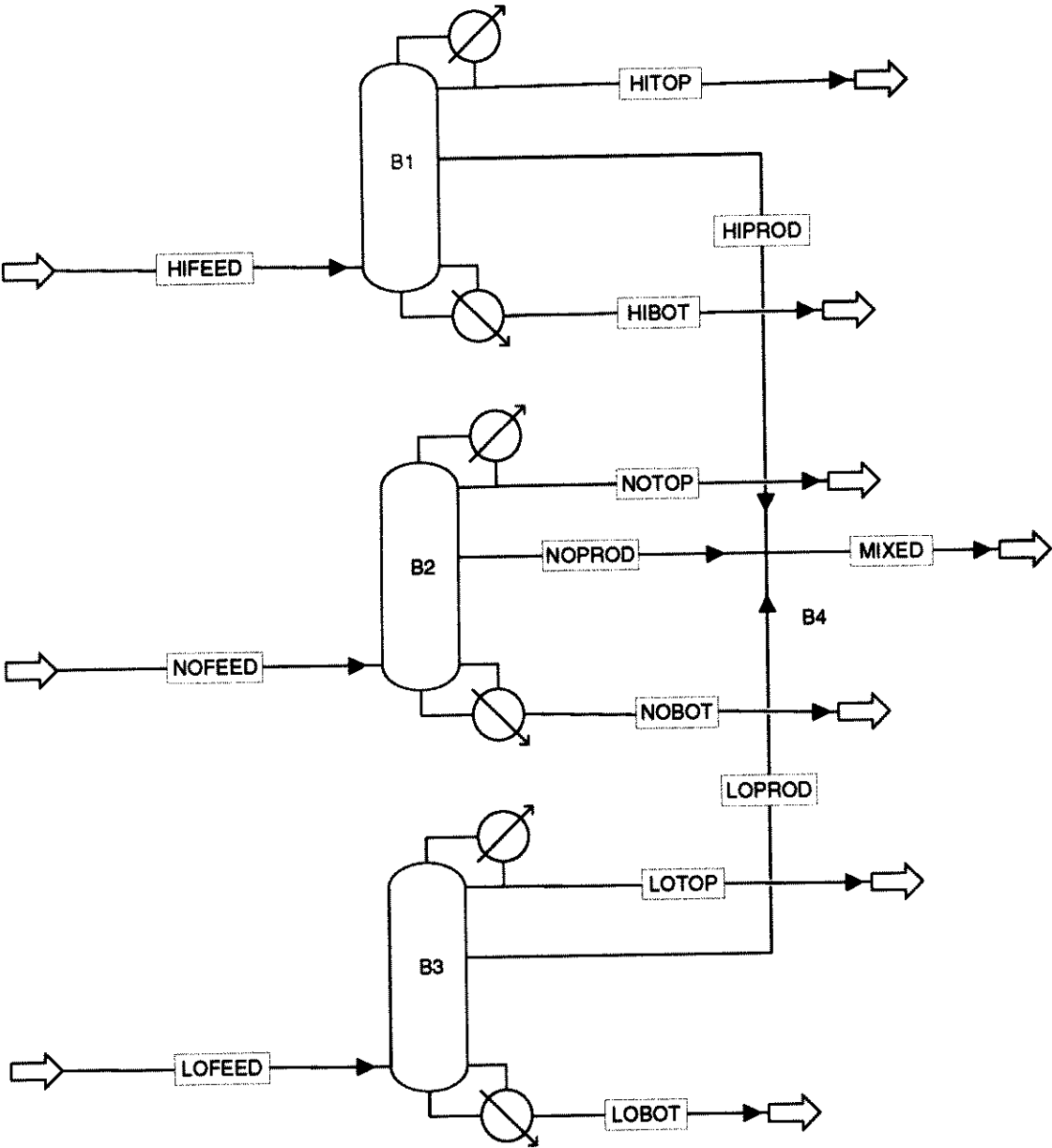


Figure 5.3 Flowsheet of Purification Columns

STREAM ID	HIBOT	HIFEED	HIPROD	HITOP
PHASE	L	L	L	L
COMPONENTS: MASS FRAC				
EO	0.9984	0.9999	0.9999	0.9998
EA	1.5392-03	4.4999-05	1.4509-05	5.4981-07
MA	2.7147-13	2.0000-05	3.9016-06	1.9000-04
TOTAL FLOW:				
KMOL/HR	2.2699	109.1645	97.4031	9.4914
KG/HR	99.9998	4809.0000	4290.9099	418.0902
CUM/HR	0.1222	5.9416	5.1989	0.5059

STREAM ID	LOBOT	LOFEED	LOPROD	LOTOP
PHASE	L	L	L	L
COMPONENTS: MASS FRAC				
EO	0.9984	0.9999	0.9999	0.9998
EA	1.5506-03	4.4999-05	1.0583-05	4.0121-07
MA	2.5056-13	2.0000-05	3.6016-06	1.7512-04
TOTAL FLOW:				
KMOL/HR	2.2699	98.7679	87.0066	9.4913
KG/HR	99.9998	4351.0000	3832.9099	418.0902
CUM/HR	0.1222	5.3758	4.6440	0.5059

STREAM ID	NOBOT	NOFEED	NOPROD	NOTOP
PHASE	L	L	L	L
COMPONENTS: MASS FRAC				
EO	0.9990	0.9999	0.9999	0.9998
EA	9.7607-04	3.0000-05	9.7580-06	3.7463-07
MA	2.0591-13	1.5000-05	2.9359-06	1.3580-04
TOTAL FLOW:				
KMOL/HR	2.269910	3.9660	92.2048	9.4911
KG/HR	100.0003	4580.0000	4061.9094	418.0902
CUM/HR	0.1222	5.6587	0.5059	4.9214

Table 5.3 Purification Column - Stream Section

3. Dynamic Closed-Loop Back-Off Calculations

The algorithm developed for closed-loop back-off calculations is exactly the same as for steady state open loop case except that the dynamic model is used instead of the steady state one. Consequently, some of the equality constraints are ordinary differential equations and the involving problem can be solved by two different techniques as reviewed in the introduction section. The solutions found in the following examples are dependent on both solution techniques and solvers. The case study on page 3.21 is solved as an example. The objective function and the set of inequality constraints are written as:

$$\text{Obj (\$/time)} = p_v * Q_{in} * (C_{in} - C_o) - m_c * Q_{in} - c_c * \text{Cool} \quad (t = 0) \quad (5.3)$$

$$T \leq 380 \text{ K}$$

Constraint 1

$$200 \text{ l} \leq V \leq 380 \text{ l}$$

Constraint 2

$$C_s \leq 0.3 \text{ mol/l}$$

Constraint 3

$$\text{Cool} \leq 20 \text{ LKJ/s}$$

Constraint 4

The sequential technique is applied in MATLAB, then in SPEEDUP to solve the problem for two decision variables: feed flowrate (Q_{in}) and operating temperature or temperature set point (Stpt). The inventory is fixed. Since SPEEDUP cannot perform optimization within the dynamic simulation environment, SPEEDUP must interface to OPT (Biegler, 1985). MATLAB, on the contrary, includes the optimization toolbox in its package. The execution time of the same problem in SPEEDUP interfacing to OPT is about ten times larger than in MATLAB.

The simultaneous integration and optimization technique is applied in GAMS to solve the problem again. Table 5.4 compares results obtained from GAMS and MATLAB. GAMS gives the true optimal solution, independent on initial values of decision variables. Solutions obtained from MATLAB vary with initial values and are not true optimum, since the solver stops before all active constraints are found.

Similarly, Table 5.5 shows results of the same problem with three decision variables: Q_{in} , $Stpt$ and V . GAMS finds as many active constraints as possible before the iteration terminates. The error from approximating the ODEs, using orthogonal collocation approaches zero, if the number of collocation points increases. However, due to the size limitation of the software, only two collocation points are used in each finite element. Consequently, the results obtained from the simultaneous technique may slightly be different from the sequential method. Although it cannot be used for complex problems, the application of the simultaneous technique together with MINOS optimizer is a powerful tool for dynamic optimization problems. The problem of two CSTRs in series is solved for four, five and then six decision variables (DV). The objective value and the number of active constraints (AC) increase as the number of DV increases. Table 5.6 compares execution times in GAMS for these calculations. For comparison, execution times given in Tables 5.5, 5.6, and 5.7 are measured in the same personal computer.

Number of Its	Bounds	Initial Value	Obj. Value	Q_{in}	$Stpt$	Active Constraints
GAMS						
59 Iter. in 78 sec	0.2 - 0.4 340 - 350	0.30 347.8	70.882	0.3609	349.87	1 & 4
60 Iter. in 84 sec	0.2 - 0.4 340 - 350	0.30 347.8	70.882	0.3609	349.87	1 & 4
MATLAB						
106 Iter. in 212 sec	0.3 - 0.4 348 - 350.2	0.345 349.98	70.851	0.3607	349.89	1
92 Iter. in 182 sec	0.2 - 0.4 340 - 350	0.300 348.98	68.309	0.3478	349.92	1
63 Iter. in 129 sec	0.2 - 0.4 340 - 350	0.350 349.98	70.716	0.360	349.89	1

Table 5.4 Results of Dynamic Closed-Loop Back-Off Calculations

(A single CSTR, two decision variables)

Number of Iterations	Bounds & Initial Value	Obj. Value	Q_{in}	Stpt	V	Active Constraints
GAMS 60 Iter. in 110 sec	0.20 - 0.40 0.30 340 - 350 347.8 200 - 380 300	71.687	0.3650	349.85	249.75	1 & 3 & 4
MATLAB 83 Iter. in 174 sec	0.27 - 0.45 0.37 348 - 350.2 349.8 230 - 330 249.7	58.924	0.3443	349.70	249.86	1
78 Iter. in 172 sec	0.27 - 0.45 0.355 348 - 350 349.8 230 - 330 249.6	71.813	0.3659	349.87	250.13	1

Table 5.5 Results of Dynamic Closed-Loop Back-Off Calculations

(A single CSTR, three decision variables)

N ^o of Its	CPU Time (s)	Obj. Value	No of DV	No of AC
92	344	124.40	4	3
93	393	130.69	5	4
103	436	140.42	6	4

Table 5.6 Execution Times of Dynamic Back-Off Calculations in GAMS

(Two CSTRs in series)

4. Switchability Calculations

The objective function of the closed-loop back-off problem is commonly a cost or a profit index evaluated at a specific time such as at the beginning or by the end of a dynamic response. The solution of this problem is the optimal operating condition at the back-off point. The switchability problem selects the integral quadratic function as its objective function and the solution is the optimal control trajectory. However, the solution techniques and optimization simulators in section 3 can be applied to the switching problems. To avoid lengthy calculations, the reactor application problem is selected as a switchability example solved by different techniques and different solvers. Details of the flowsheet will be given later in Chapter 6. The application is brought up in this section in order to compare computational times and solutions obtained from different solvers and methods. The problem is solved for the optimal feed policy when the inlet flowrate changes from 0.75 to 1.8 l.min^{-1} . Two path constraints require that the outflow from each reactor is less than 2.1 l.min^{-1} and the level does not exceed 80% of the maximum inventory in the tank. For comparison, the simultaneous integration and optimization technique is applied in GAMS and the sequential technique in SPEEDUP to solve the problem. SPEEDUP can interface to different solvers, which are more appropriate for the problem than the only solver included in MATLAB optimization toolbox.

The optimal feed profiles obtained from GAMS are presented in Figure 5.4. The plot shows the effect of time delay on these profiles. The green trajectory is dead time free and the red one is with time delay. Figure 5.4 includes the blue profile, which is obtained from SPEEDUP plus OPT using sequential optimization technique. The shapes of these profiles, using different solution methods are similar. However, the blue trajectory is suboptimal compared to the red one. The true optimal trajectory is rather a curve than a series of steps as shown in the plot. Discretizing the control profile requires extra finer steps but these steps would enormously increase the computational time. Responses of the second tank plotted in Figure 5.5 satisfy path constraints. The figures also prove that dead time is an important element in mathematical modeling of chemical processes and controller design. The model equations including the time delay will be presented in Chapter 6. A large time delay means the system is closer to the verge of instability, which creates more oscillation in the responses (red curves compared to green curves in Figure 5.5). They truly represent real plant responses.

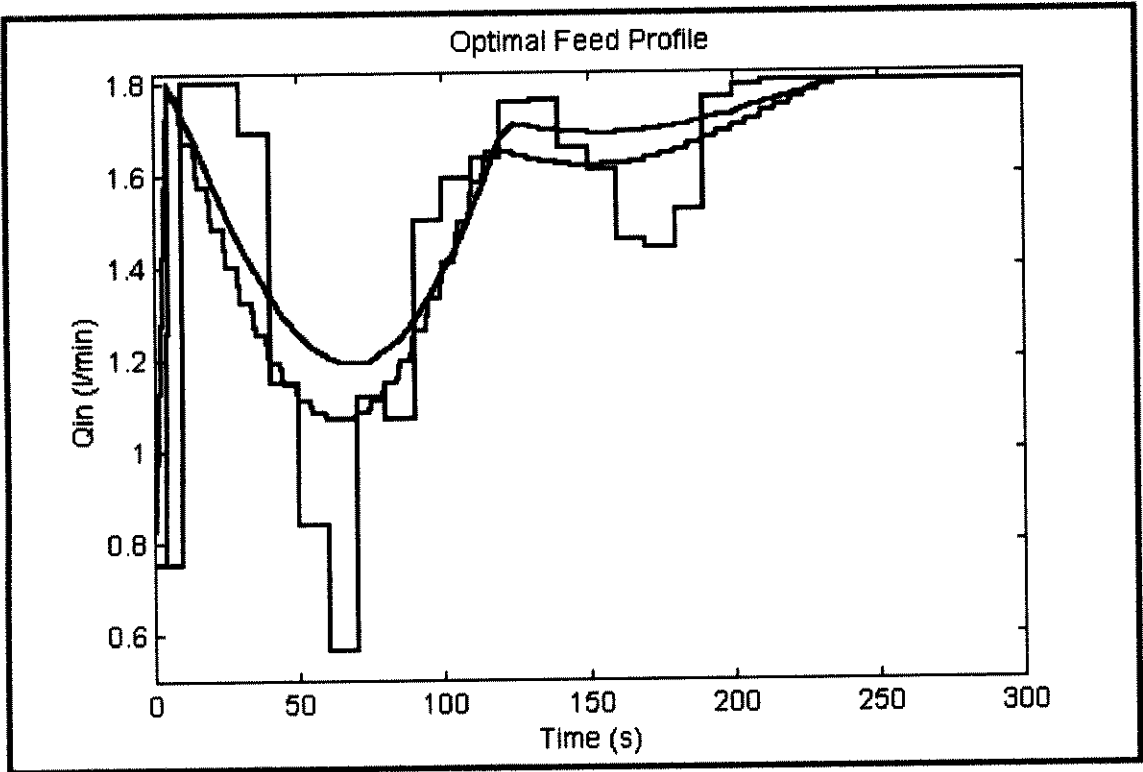


Figure 5.4 Optimal Feed Profile

(Green curve: No time delay, GAMS and simultaneous technique)

(Red curve: Under effect of time delay, GAMS and simultaneous technique)

(Blue curve: Under effect of time delay, SPEEDUP and sequential technique)

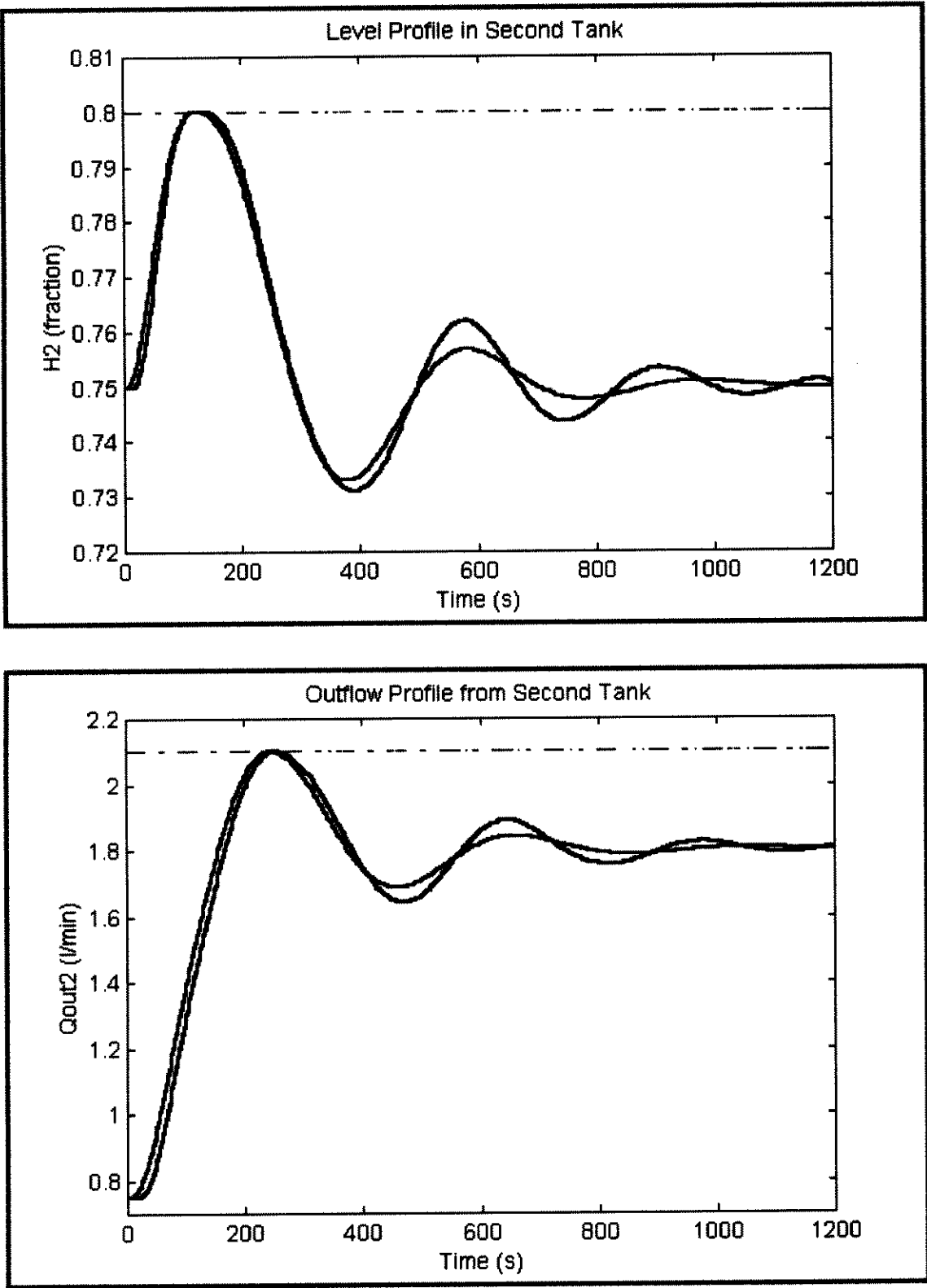


Figure 5.5 Responses from Second Tank

(Green curve: No time delay, GAMS and simultaneous technique)
(Red curve: Under effect of time delay, GAMS and simultaneous technique)

An effort to reduce computational time when applying the sequential technique is using large Kuhn-Tucker error tolerance to get the rough solution first. This solution will be used as the initial guess in the following run using smaller Kuhn-Tucker error tolerance to get the fine solution. Table 5.7 shows the computational time against the error tolerance. Applying the simultaneous technique in GAMS decreases the execution time by sevenfold (67 min CPU). Figure 5.6 plots three optimal feed policies dependent on values of Kuhn-Tucker (KT) error tolerance. The corresponding responses for level in the second tank are not much different (see Figure 5.7).

Computational Time (min CPU)	Kuhn-Tucker Error	Initial Value	Max. Constraint Violation
480	0.296e-02	Randomly guessed	0.21e-02
186	0.596e-02	Randomly guessed	0.68e-02
186	0.488e-02	Solution from previous run	0.12e-02

Table 5.7 Computational Time against KT Error (Sequential technique-SPEEDUP)

This section has proved that the simultaneous integration and optimization technique in GAMS plus MINOS is one of the best tools to solve optimal control problems. Unfortunately this tool cannot be used for complex processes, so the sequential technique is applied in SPEEDUP plus OPT to deal with these cases. The second case study in Chapter 3 is brought back. As discussed on page 3.57, the solution under the worst situation is not feasible when it is tested with other combinations of disturbances. The switchability problem must be solved again with the updated matrix of disturbances. A similar procedure has been presented in Chapter 2 but in this case the problems must be solved for two systems of two CSTRs in series, using dynamic optimization techniques. Each system is subject to a different situation described by a corresponding row of the uncertain matrix. The problem of four CSTRs and eight controllers is solved in SPEEDUP using the sequential technique. Results are shown in Figure 5.8.

$$d^n = \begin{vmatrix} 305 & 286 \\ 305 & 280 \end{vmatrix}$$

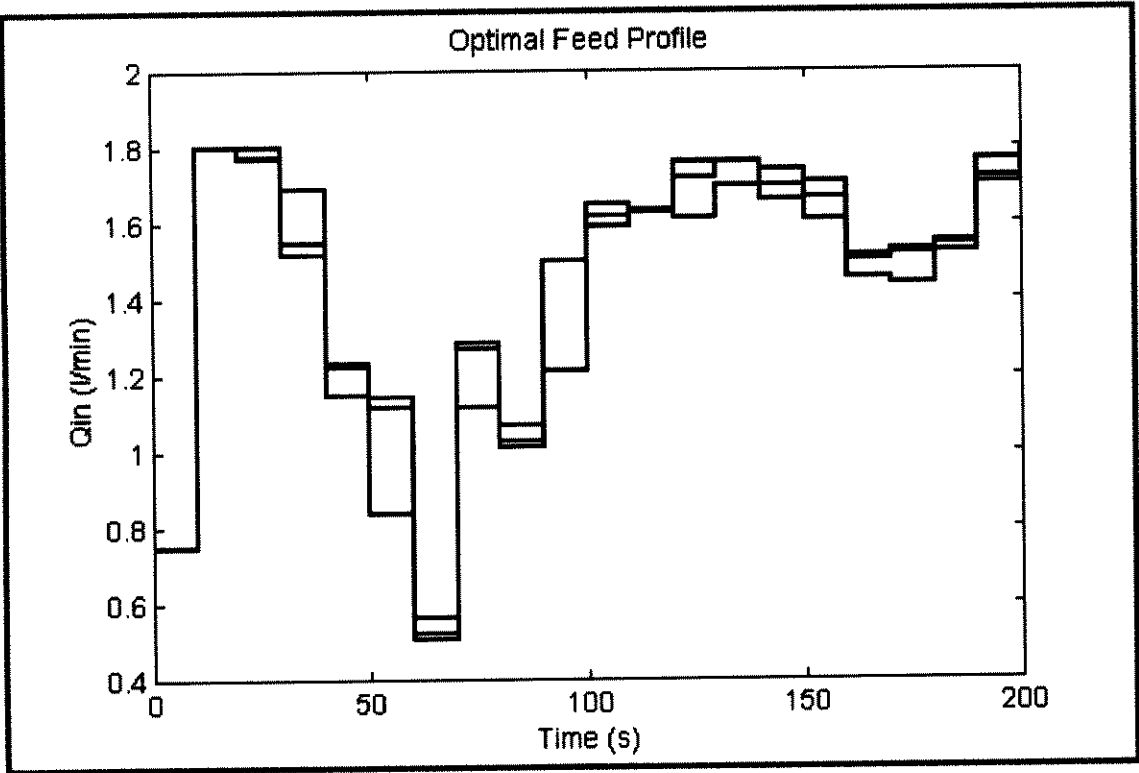


Figure 5.6 Optimal Feed Profile (SPEEDUP and sequential technique)
(Blue curve: Kuhn-Tucker error = $0.488e-02$)
(Green curve: Kuhn-Tucker error = $0.596e-02$)
(Red curve: Kuhn-Tucker error = $0.296e-02$)

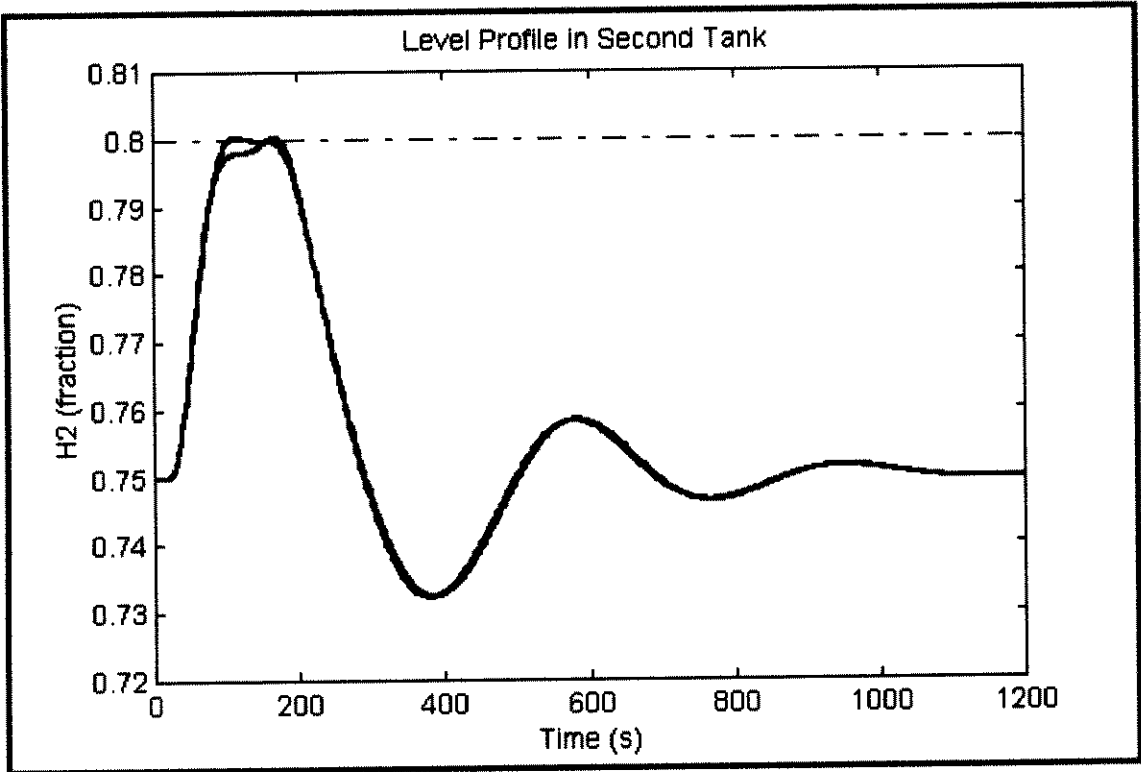


Figure 5.7 Corresponding Level Responses

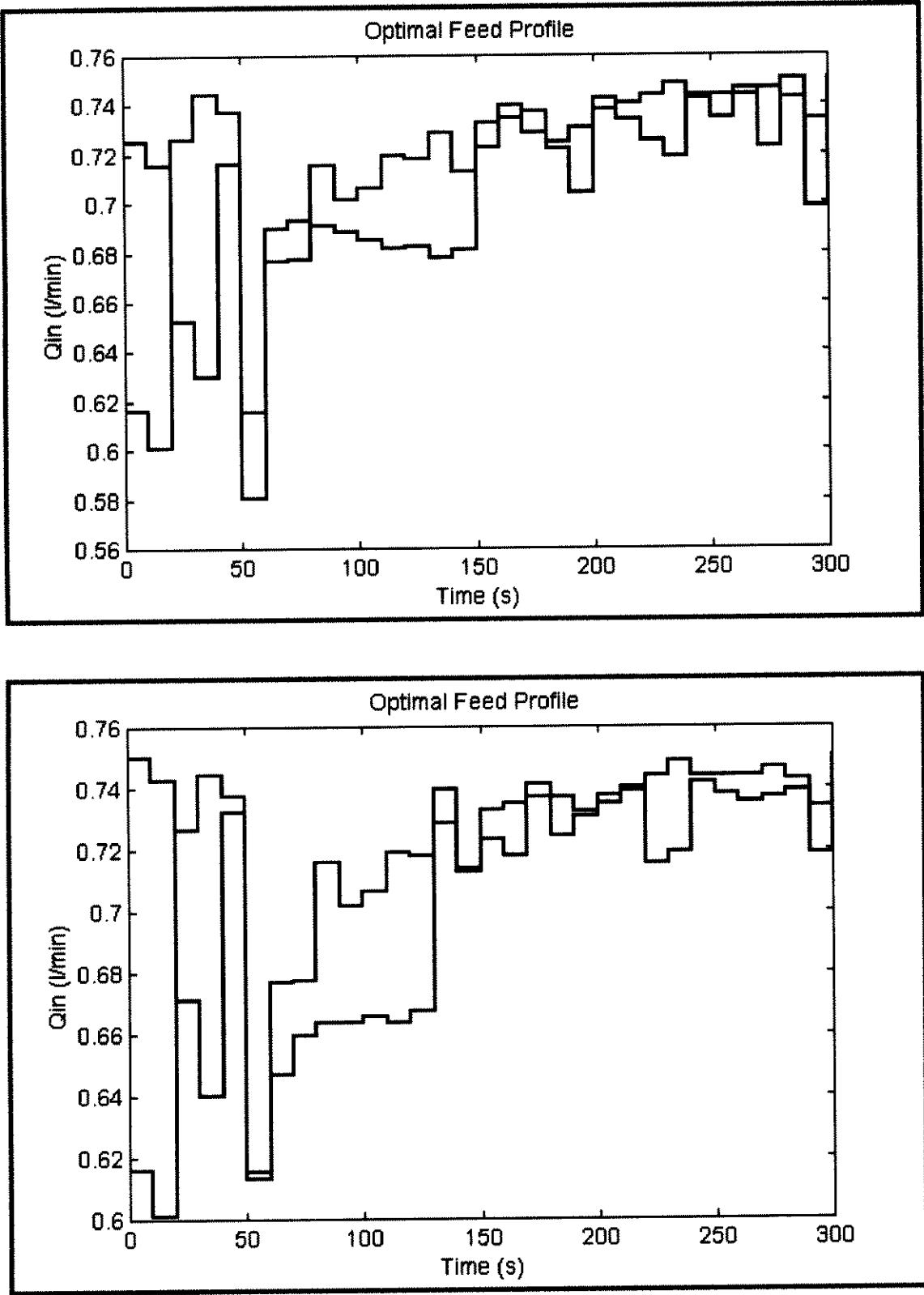


Figure 5.8 Optimal Feed Profile (SPEEDUP and sequential technique)
(Green: Two systems of two CSTRs, subject to different sets of disturbance)
(Blue: One system of two CSTRs with time delay)
(Red: One system of two CSTRs without time delay)

5. Nonlinear Model Predictive Control (NLPC) Calculations

The previous chapter did not present any example on NLPC. As mentioned before, the formulation of NLPC is very similar to that of a switchability problem. Instead of using a linear convolution model to estimate the control actions, NLPC method uses a nonlinear dynamic process model. The aim is to select a set of future control moves (control horizon), in order to minimize a function based on a desired output trajectory over a prediction horizon. The objective function is the integral squared deviation of the model-predicted outputs from the set point values over the prediction horizon V . Equations (4.6) and (4.7) are written as:

Minimize:

$$F = \sum_{i=k+1}^{k+V} (y(i) - y(i)_{sp})^2 \quad (5.4)$$

Subject to:

$$\begin{aligned} (dy/dt) &= f[y(t), u(t), m(t), p, d^n] & x_0 &= x(0) \\ c_i[y(t), u(t), m(t), p, d^n] &= 0 & i &\in E \\ g_j[y(t), u(t), m(t), p, d^n] &\leq 0 & j &\in I \\ u^L &\leq u(t) \leq u^U \end{aligned}$$

As in DMC, although the optimization is based on a control horizon, only the first control action is implemented. Plant output is measured, compensation of plant and model mismatch is performed and the optimization problem is solved again.

NLPC can explicitly handle path constraints on manipulated and controlled variables but it also faces some problems. The major disadvantage is in solving the optimization problem. There is no guarantee of convergence and robustness at all time steps. Computational time is an issue as well with complex models that have relatively fast dynamics. The simultaneous integration and optimization approach can certainly solve the optimal control problem better and faster than the sequential optimization technique. On the other hand, MATLAB is the best package for MPC. Therefore, in the following example the optimization problem is solved in GAMS for the optimal set of control actions. Only the first control action is implemented in MATLAB to perform the dynamic simulation. Without information of on-line measurement and disturbance,

it is assumed that the nonlinear dynamic process model is perfect. The effects of the manipulated variable on the real plant and the model are identical. Then the feedback signal is equal to the effect of the disturbance on the controlled variable. The simulations are performed under the worst situation as an example. Feasibility tests are not required, since in real plant implementation the optimization problem with updated information is solved again at every time step. As a result, the path constraints are satisfied at all time steps. Another advantage of NLPC over DMC is that NLPC does not require either tuning parameter or set point change policy. Tuning methodology is unnecessary in this case and NLPC provides a more robust performance than DMC. This feature is proved in the final example of Chapter 4. The problem on page 4.38 is solved again using NLPC technique.

$$Q^1 = 0.750; Q^2 = 0.05$$

$$T_{in} = 300 \rightarrow 305$$

$$T_{ci} = 283 \rightarrow 286$$

$$Stpt_1 = 347.5 \rightarrow 340.2$$

$$Stpt_2 = 333.4 \rightarrow 328.2$$

Figure 5.9 also plots responses of DMC (green curves) for comparison. Red curves are NLPC responses, with time step $\Delta t = 20$ seconds and prediction horizon $V = 10$. The optimization problem is solved in GAMS, using 4 collocation points and 10 finite elements. The length of each element is 20 seconds. Blue curves plot solutions of the same optimization problem with 70 finite elements, which cover the whole trajectory. The red and blue curves are similar in this example, since on-line measurement information is not available and current values of outputs and disturbances cannot be updated. In real plant implementation, feed temperature (T_{in}), coolant temperature (T_{ci}) (disturbances) and temperatures in each reactor (outputs) should be updated at each time step. The red curve in that case plots responses to updated data so it must be different from the blue one. The optimization problem, however, should be solved off-line first with a long prediction horizon, which covers the whole trajectory. The result might be different from those solved on-line with a shorter prediction horizon but it can be stored as backup data. At any time step, if the on-line optimization problem is infeasible, the backup data can be used (replacing the missing solution) to update the current outputs, then the problem can be solved again after time moves one step forward. The DMC responses are very sluggish, compared to NLPC (green curves

compared to red ones). As discussed above, DMC requires many tuning parameters. To satisfy path constraints under possible disturbance effects, the problem requires suppression of control move, which means, high values of the move suppression factor (qq) should be selected. Such configurations result in sluggish responses especially in the second reactor. Meanwhile NLPC avoids the selection of adjustable parameters and also the sluggish control performance during the transition. Figures 5.9 and 5.10 show better performances of NLPC than those of DMC.

6. Conclusion

This chapter reviews the usage of software packages and solution techniques to solve standard and dynamic optimization problems generated by the flexibility, switchability and controllability analysis.

Standard optimization problems such as those in the outer loop and inner loop of the steady state back-off calculations can be solved easily by GAMS, MATLAB or SPEEDUP. The first package is designed specially for optimization problems so it has the most powerful optimizer. SPEEDUP is a handy package for model development or design and MATLAB for controllability problems. When the process requires physical and thermodynamic properties, ASPEN is more advantageous than other packages, since it can provide reliable property information.

Dynamic optimization requires more sophisticated solving techniques. The simultaneous integration and optimization technique applied in GAMS is a promising tool for optimal control problems. Unfortunately it cannot be used for large and complicated problems due to the size limitation of the package and the solver. The sequential optimization technique applied in SPEEDUP together with an optimizer can be used in optimizing the whole flowsheet, which includes many operation units.

An example of nonlinear model predictive control is solved, using GAMS to find a set of control moves. The first control action is implemented in MATLAB to perform the dynamic simulation. It is proved that NLPC provides a better control performance than DMC. The disadvantage is found in the interfacing of software packages to reduce computational time and guarantee of convergence and robustness at all times steps.

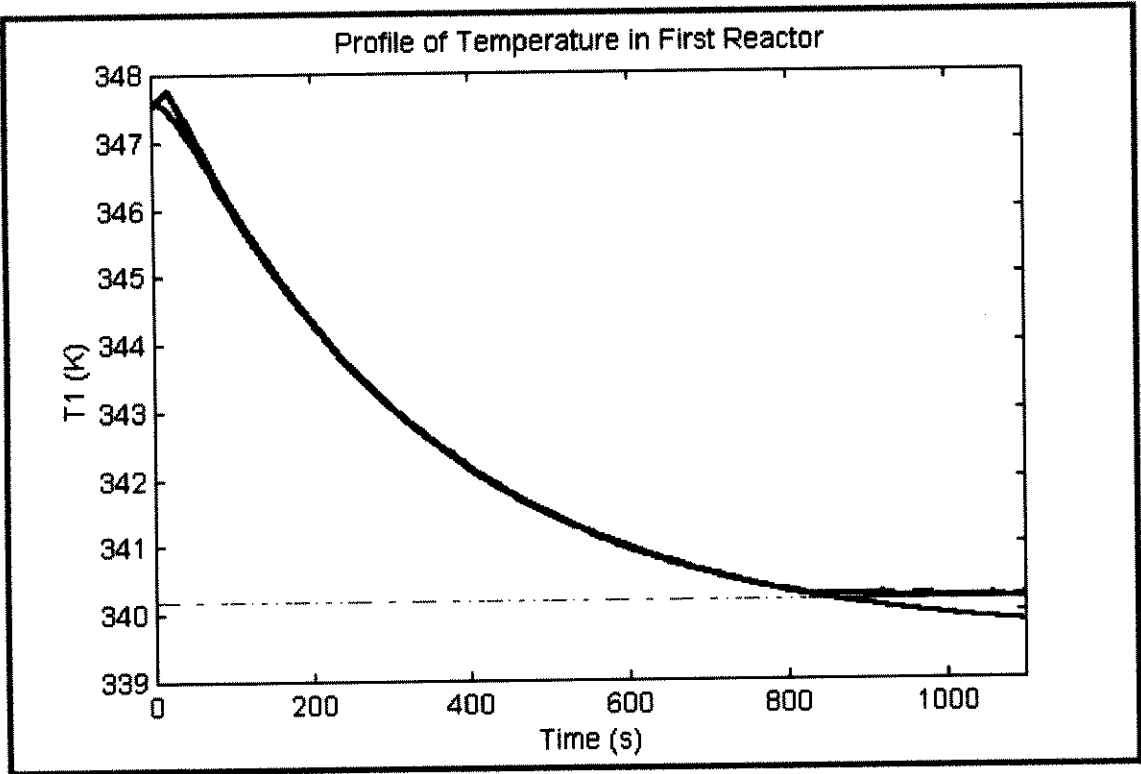


Figure 5.9a Temperature Response in First CSTR (Controlled Variable)

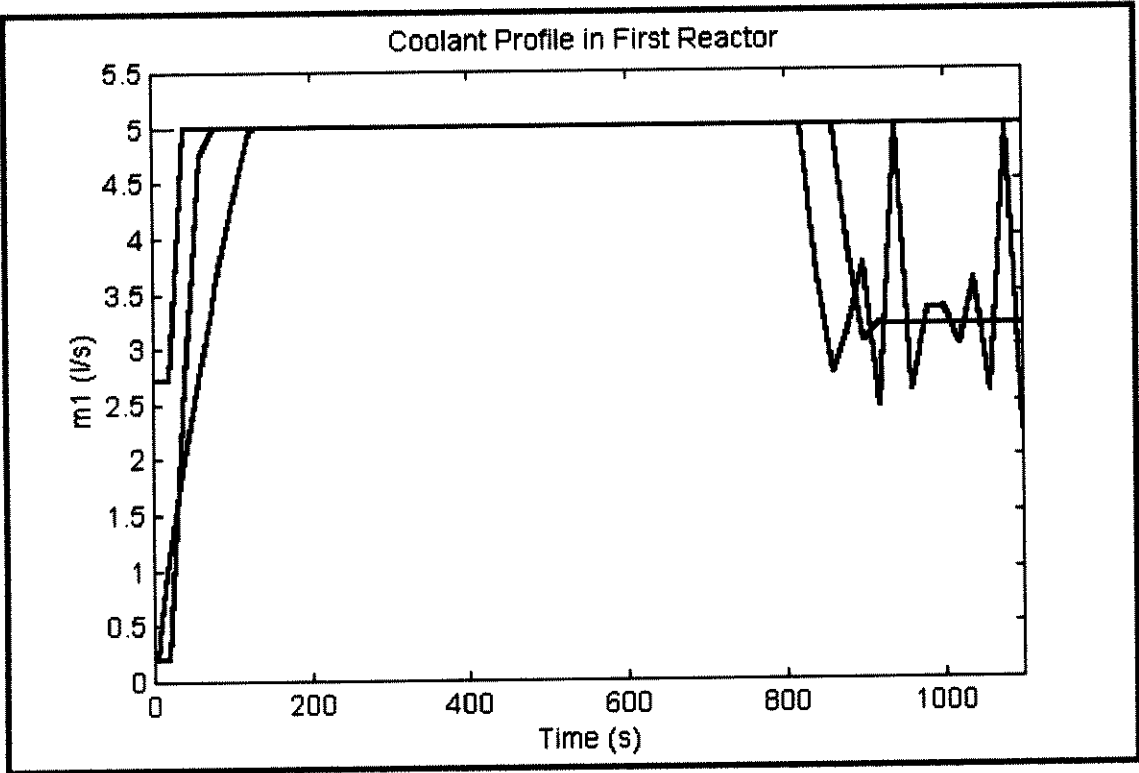


Figure 5.9b Coolant Profile in First CSTR (Manipulated Variable)
(Green: DMC response, Red: NLPC response, Blue: solution of NLP problem)

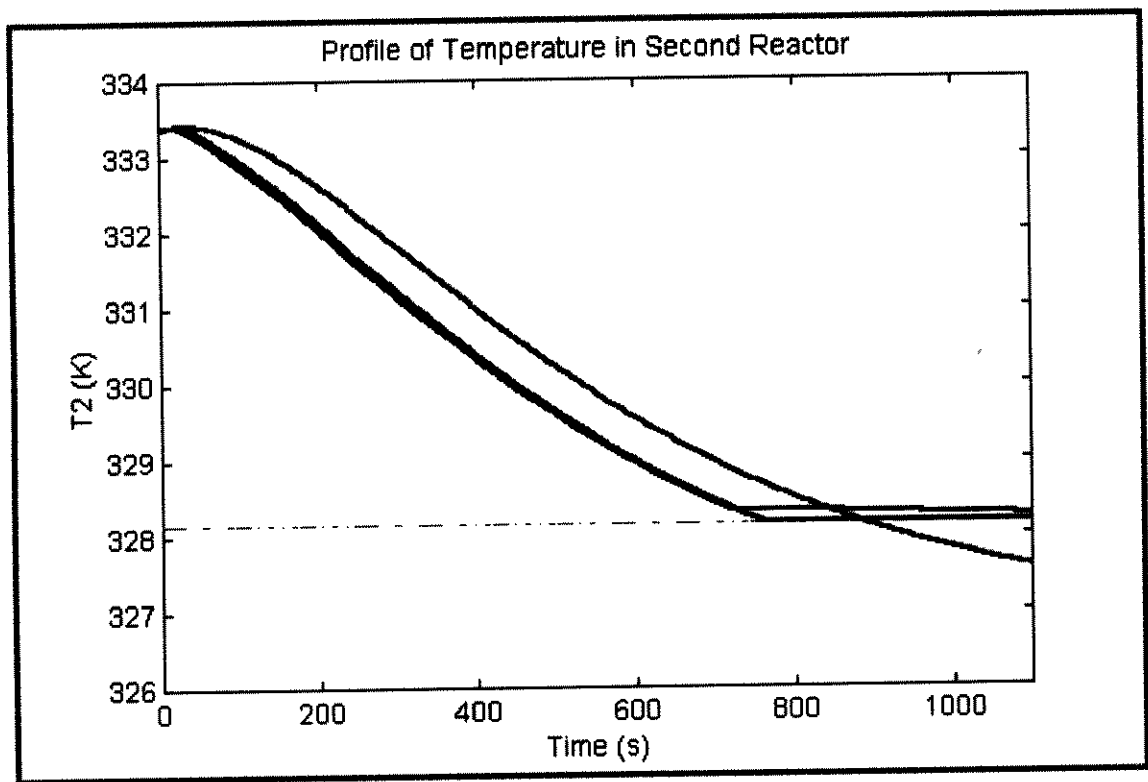


Figure 5.10a Temperature Response in Second CSTR (Controlled Variable)

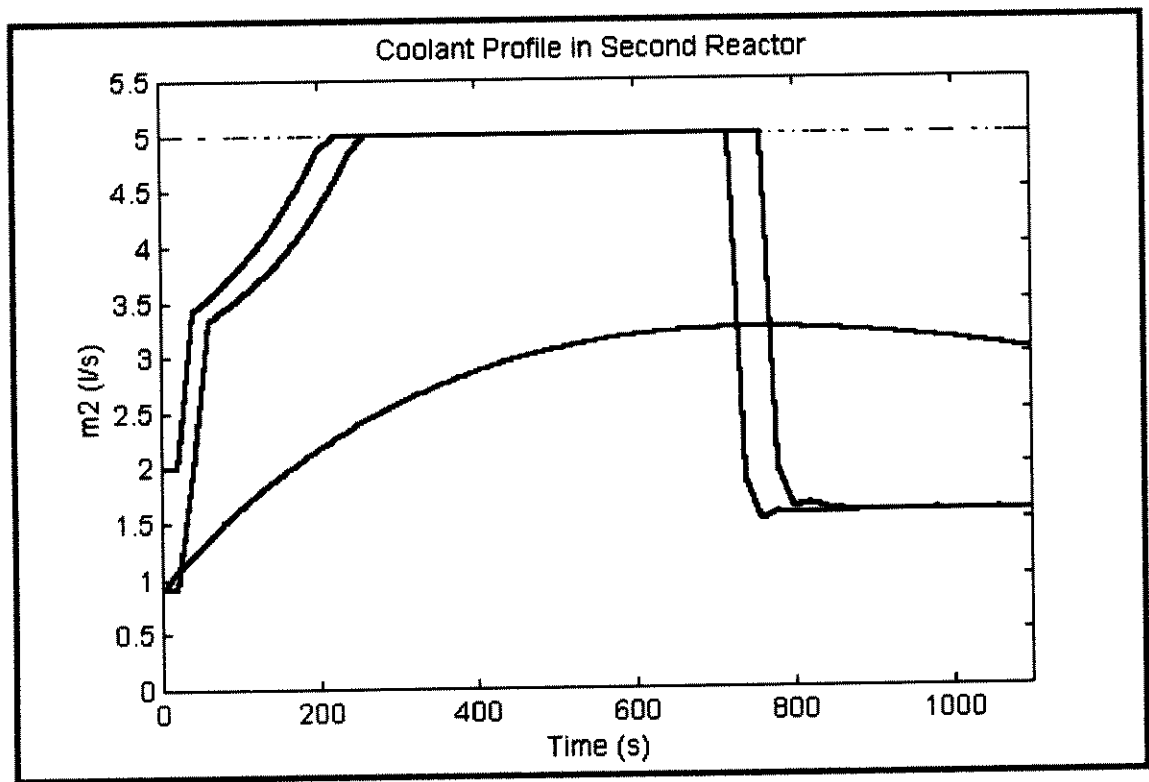


Figure 5.10b Coolant Profile in Second CSTR (Manipulated Variable)
(Green: DMC response, Red: NLPC response, Blue: Solution of NLP problem)

7. Nomenclature

c_i	: Set of equality constraints
cc	: Cost of cooling, $\$.(l.K)^{-1}$
C	: Concentration, $mol.l^{-1}$
$cool$	: Removal heat from the reactor to the cooling jacket, $l.Ks^{-1}$
cp	: Vector of controller parameters
C_{pc}	: Coolant heat capacity, $kJ.(kg.K)^{-1}$
d	: Vector of disturbances or uncertain parameters
F	: Objective function or flexibility index
g_j	: Set of inequality constraints
p	: Vector of process constants
pv	: Product price, $\$.mol^{-1}$
Q	: Flowrate, $l.s^{-1}$
qq	: Adjustable parameter (≥ 0), weighting the adjustments of the manipulated variable (move suppression factor)
t	: Integration variable
T	: Temperature, K
u	: Vector of control (independent) variables
U	: Control horizon
U_a	: Overall heat transfer coefficient/ $(\rho_r C_{pr})$, $l.s^{-1}$
V	: Volume, l
V	: Prediction horizon
x	: Vector of state (dependent) variables
w	: Weighting function
ww	: Adjustable parameter (≥ 0), weighting the controlled variable deviation from set point
y	: Output

Greek Letters

Δt	: Sampling period
Δu	: Change in input

Superscripts and subscripts

1	: First CSTR
2	: Second CSTR

8. References

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Brooke, A. D. Kendrick and A. Meeraus, 1992, *GAMS User's Guide, Release 2.25*, The Scientific Press, San Francisco, CA.

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Appendix 5A: ASPEN Input File

A sample of ASPEN input file illustrates how the final step of the open loop back-off calculation works.

PUR6.INP

```
;INPUT FILE REVISED BY LINH VU SEP 18, 98
;
TITLE 'PURIFICATION COLUMN'
;
IN-UNITS SI MASS-FLOW='KG/HR' MOLE-FLOW='KMOL/HR' &
  VOLUME-FLOW='CUM/HR' ENTHALPY-FLO=KW &
  MOLE-HEAT-CA='KJ/KMOL-K' POWER=KW PRESSURE=KPA &
  TEMPERATURE=C VISCOSITY='MN-SEC/SQM' &
  MOLE-ENTHALP='KJ/KMOL' MASS-ENTHALP='KJ/KG' &
  MOLE-ENTROPY='KJ/KMOL-K' MASS-ENTROPY='KJ/KG-K' &
  ELEC-POWER=KW MASS-HEAT-CA='KJ/KG-K' &
  WORK=KJ HEAT=KJ PDROP=KPA
;
DEF-STREAMS CONVEN ALL
;
RUN-CONTROL MAX-TIME=50000
;
DATABANKS PURECOMP / AQUEOUS / SOLIDS / INORGANIC / &
  NOASPENPCD
;
PROP-SOURCES PURECOMP / AQUEOUS / SOLIDS / INORGANIC
;
COMPONENTS
  EO / EA / MA
;
FLOWSHEET
  BLOCK HID503 IN=HIFEED OUT=HITOP HIBOT HIPROD
  BLOCK NOD503 IN=NOFEED OUT=NOTOP NOBOT NOPROD
  BLOCK LOD503 IN=LOFEED OUT=LOTOP LOBOT LOPROD
  BLOCK PROMIX IN=HIPROD NOPROD LOPROD OUT=MIXED
;
PROPERTIES RK-SOAVE
  PROPERTIES PURI

PROP-REPLACE PURI RK-SOAVE

PROP-SET TXPORT RHOMX MUMX SIGMAMX UNITS='KG/CUM' 'CP' 'N/M' &
  SUBSTREAM=MIXED PHASE=V L
```

```

;
STREAM HIFEED
  SUBSTREAM MIXED TEMP=59 PRES=480 MASS-FLOW=4809 NPHASE=1
  PHASE=L
  MASS-FRAC EO 0.99995 / EA 45E-6 / MA 20E-6
;
STREAM NOFEED
  SUBSTREAM MIXED TEMP=59 PRES=480 MASS-FLOW=4580 NPHASE=1
  PHASE=L
  MASS-FRAC EO 0.99995 / EA 30E-6 / MA 15E-6
;
STREAM LOFEED
  SUBSTREAM MIXED TEMP=59 PRES=480 MASS-FLOW=4351 NPHASE=1
  PHASE=L
  MASS-FRAC EO 0.99995 / EA 45E-6 / MA 20E-6
;
BLOCK PROMIX MIXER
  PARAM PRES=330

BLOCK HID503 RADFRAC
  DESCRIPTION "PURIFICATION COLUMN"
  PARAM NSTAGE=87
  FEEDS HIFEED 70
  PRODUCTS HIPROD 11 L MASS-FLOW=4100 / HITOP 1 L / HIBOT 87 L
  P-SPEC 1 371
  COL-SPECS QN=1750 DP-COL=59 MASS-RDV=0 MASS-D=400.0
  TRAY-RATE 1 2 86 FLEXI TRAY-SPACE=305 <MM> DIAM=1067 <MM> &
    WEIR-HT-A=2 <IN> DC-CLEAR-SID=1 <IN> DC-WTOP-SIDE=6.5 <IN> &
    DC-WBOT-SIDE=6.5 <IN> NVALVES=83 P-UPDATE=NO FLOOD-
METH=GLITSCH
;
BLOCK NOD503 RADFRAC
  DESCRIPTION "PURIFICATION COLUMN"
  PARAM NSTAGE=87
  FEEDS NOFEED 70
  PRODUCTS NOPROD 11 L MASS-FLOW=3900 / NOTOP 1 L / NOBOT 87 L
  P-SPEC 1 371
  COL-SPECS QN=1660 DP-COL=59 MASS-RDV=0 MASS-D=400.0
  TRAY-RATE 1 2 86 FLEXI TRAY-SPACE=305 <MM> DIAM=1067 <MM> &
    WEIR-HT-A=2 <IN> DC-CLEAR-SID=1 <IN> DC-WTOP-SIDE=6.5 <IN> &
    DC-WBOT-SIDE=6.5 <IN> NVALVES=83 P-UPDATE=NO FLOOD-
METH=GLITSCH
;
BLOCK LOD503 RADFRAC
  DESCRIPTION "PURIFICATION COLUMN"
  PARAM NSTAGE=87
  FEEDS LOFEED 70
  PRODUCTS LOPROD 11 L MASS-FLOW=3700 / LOTOP 1 L / LOBOT 87 L
  P-SPEC 1 371
  COL-SPECS QN=1750 DP-COL=59 MASS-RDV=0 MASS-D=400.0
  TRAY-RATE 1 2 86 FLEXI TRAY-SPACE=305 <MM> DIAM=1067 <MM> &
    WEIR-HT-A=2 <IN> DC-CLEAR-SID=1 <IN> DC-WTOP-SIDE=6.5 <IN> &

```

```

DC-WBOT-SIDE=6.5  <IN>  NVALVES=83  P-UPDATE=NO  FLOOD-
METH=GLITSCH
;
CONSTRAINT EQU D1
  DEFINE  HID  BLOCK-VAR  BLOCK=HID503  SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  DEFINE  NOD  BLOCK-VAR  BLOCK=NOD503  SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  SPEC 'HID-NOD' EQ 0.0
  TOL-SPEC 1.0
CONSTRAINT EQU D2
  DEFINE  LOD  BLOCK-VAR  BLOCK=LOD503  SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  DEFINE  NOD  BLOCK-VAR  BLOCK=NOD503  SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  SPEC 'LOD-NOD' EQ 0.0
  TOL-SPEC 1.0
CONSTRAINT EQU B1
  DEFINE LOB STREAM-VAR STREAM=LOBOT VARIABLE=MASS-FLOW
  DEFINE NOB STREAM-VAR STREAM=NOBOT VARIABLE=MASS-FLOW
  SPEC 'LOB-NOB' EQ 0.0
  TOL-SPEC 0.5
CONSTRAINT EQU B2
  DEFINE HIB STREAM-VAR STREAM=HIBOT VARIABLE=MASS-FLOW
  DEFINE NOB STREAM-VAR STREAM=NOBOT VARIABLE=MASS-FLOW
  SPEC 'HIB-NOB' EQ 0.0
  TOL-SPEC 0.5
CONSTRAINT DISFOR
  DEFINE XDF MASS-FRAC STREAM=HITOP COMP=MA
  SPEC XDF LE 1.9E-4
  TOL-SPEC 1E-6
CONSTRAINT PRODA
  DEFINE XPA MASS-FRAC STREAM=MIXED COMP=EA
  DEFINE XPF MASS-FRAC STREAM=MIXED COMP=MA
F      XA=XPA+XPF
  SPEC XA LE 40E-6
  TOL-SPEC 5E-7
CONSTRAINT BOTFL1
  DEFINE BFLOW1 STREAM-VAR STREAM=HIBOT VARIABLE=MASS-FLOW
  SPEC BFLOW1 GE 100
  TOL-SPEC 1
CONSTRAINT BOTFL2
  DEFINE BFLOW2 STREAM-VAR STREAM=NOBOT VARIABLE=MASS-FLOW
  SPEC BFLOW2 GE 100
  TOL-SPEC 1
CONSTRAINT BOTFL3
  DEFINE BFLOW3 STREAM-VAR STREAM=LOBOT VARIABLE=MASS-FLOW
  SPEC BFLOW3 GE 100
  TOL-SPEC 1
CONSTRAINT BOT TMA
  DEFINE XBA MASS-FRAC STREAM=LOBOT COMP=EA
  SPEC XBA LE 2.0E-3

```

```

TOL-SPEC 1E-5
OPTIMIZATION MIXPRO
  DEFINE MPROD STREAM-VAR STREAM=MIXED VARIABLE=MASS-FLOW
  MAXIMIZE MPROD
  CONSTRAINTS
  PRODA/BOTFL1/BOTFL2/BOTFL3/DISFOR/EQUD1/EQUD2/BOTTMA/ &
    EQUB1/EQUB2
  VARY    BLOCK-VAR    BLOCK=HID503    SENTENCE=PRODUCTS
  VARIABLE=MASS-FLOW &
    ID1=HIPROD
  LIMITS 3900 4400
  VARY    BLOCK-VAR    BLOCK=NOD503    SENTENCE=PRODUCTS
  VARIABLE=MASS-FLOW &
    ID1=NOPROD
  LIMITS 3700 4200
  VARY    BLOCK-VAR    BLOCK=LOD503    SENTENCE=PRODUCTS
  VARIABLE=MASS-FLOW &
    ID1=LOPROD
  LIMITS 3600 4000
  VARY    BLOCK-VAR    BLOCK=HID503    SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  LIMITS 350 500
  VARY    BLOCK-VAR    BLOCK=NOD503    SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  LIMITS 350 500
  VARY    BLOCK-VAR    BLOCK=LOD503    SENTENCE=COL-SPECS
  VARIABLE=MASS-D
  LIMITS 350 500
;
CONV-OPTIONS
  PARAM TOL=0.001 COMPS=CONVERG TRACE=0.0005
  SQP MAXIT=500 MAXPASS=1000 QMIN=-15 QMAX=1

STREAM-REPORT MOLEFRAC MASSFLOW MASSFRAC
;

```

Chapter 6

Switchability and Operability of Real Processes

1	Introduction.....	6.1
2	Application 1: Two CSTRs in series.....	6.2
2.1	Plant description and modeling.....	6.2
2.2	Result and discussion.....	6.5
2.3	Improvement of current design.....	6.14
3	Application 2: Binary distillation column.....	6.14
3.1	Plant description and modeling.....	6.14
3.2	Steady state ASPEN model.....	6.20
3.3	Optimal feed location using GAMS model.....	6.22
3.4	Steady state open loop back-off using SPEEDUP.....	6.24
3.5	Switching problem using sequential technique.....	6.26
4	Application 3: Multicomponent distillation column.....	6.42
4.1	Plant description.....	6.42
4.2	Steady State ASPEN model.....	6.44
4.3	Steady State open loop back-off using ASPEN model.....	6.45
4.4	Dynamic problems using compartmental in SPEEDUP....	6.49
5	Conclusion.....	6.57
6	Nomenclature.....	6.57
7	References.....	6.58

The simultaneous formulation for switchability and operability proposed in Chapter 2 and Chapter 3 is applied to improve the performance of some real chemical processes. The applications start from a simple pilot plant including two CSTRs in series to a complex distillation unit. The optimal operating conditions are found first, and the optimal trajectories for switching operations are then considered for each application. Simulation results are compared with data collected from real plants. A possible improvement of the plant design is finally proposed.

1. Introduction

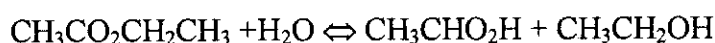
Theories on open loop, dynamic closed-loop back-off, switching calculations and their use in flexibility, switchability and controllability analysis were built up in previous chapters. These theories can only be turned into profit, if their applications are successful in real processes. To achieve this goal, a good model is the essential key in the prediction of process behaviors, and an appropriate control strategy should be applied to the process. Some special systems, however, face the problem of large dead time and inverse response. In these situations, the conventional controllers P, PI and PID cannot provide satisfactory control performances. Advanced control techniques must be employed instead. Chemical processes using physical and thermodynamic properties such as distillation processes require special treatments. The model equations, which describe the process must include the calculations of these properties or can extract them from some internal and external sources. Using mixed integer and nonlinear programming method (MINLP), the optimum feed and side product locations can be determined. For large size industrial columns, shortcut models usually replace rigorous models due to the size limitation of the software packages and the solvers. This would result in significant errors, if the columns make high purity products. Furthermore, some properties of these chemical processes in real time cannot be measured fast enough so that control actions can be calculated, based on their measurements (Marlin 1995). An inferential controller is applied to solve the problem. In distillation processes, the temperature at a special tray is a common variable to refer the compositions of the liquid coming from that tray. However, in some distillation columns, the temperature variation due to composition changes is within the measurement accuracy of the sensor (Marlin). In this case, tray temperature inference cannot replace on-line analyzers. All these problems will be considered next through three real plant applications.

2. Application 1: Two CSTRs in Series

2.1. Plant Description and Modeling

The plant has just been built in the Department of Chemical Engineering for research work. The flowsheet consists of two Continuous Stirred Tank Reactors (CSTRs) in series and an intermediate mixer, which is used to join streams before these enter the second reactor (see Figure 6.1).

The reverse of the esterification referred to as the hydrolysis of ethyl acetate produces ethanol and acetic acid from a two-percent solution of ethyl acetate over catalyst.



It is assumed that the reaction is irreversible, first order and temperature dependent. The rate constant and activation energy of the hydrolysis reaction was determined in off-line experiments. The heat of reaction is given in literature. Since the heat of this exothermic reaction is very small, extra heat is provided by the hot water, which flows through the jacket surrounding the reactors. The plant has two level control loops and a share temperature control loop. Manipulating the outflow controls the level in each reactor. Water is heated by steam through a heat exchanger before entering the heating jacket. Adjusting the amount of steam will vary the temperature of water and hence can indirectly control the temperature in the reactor. The setup of this control loop results in very slow response. Since two reactors share the same steam line and the same heating water line, only one temperature in the reactors can be controlled.

With the assumptions that the density and heat capacity of the mixtures are constant and independent of temperature and concentration of the solutions, the equality constraints describing the model (based on Ethyl Acetate (EA)) are:

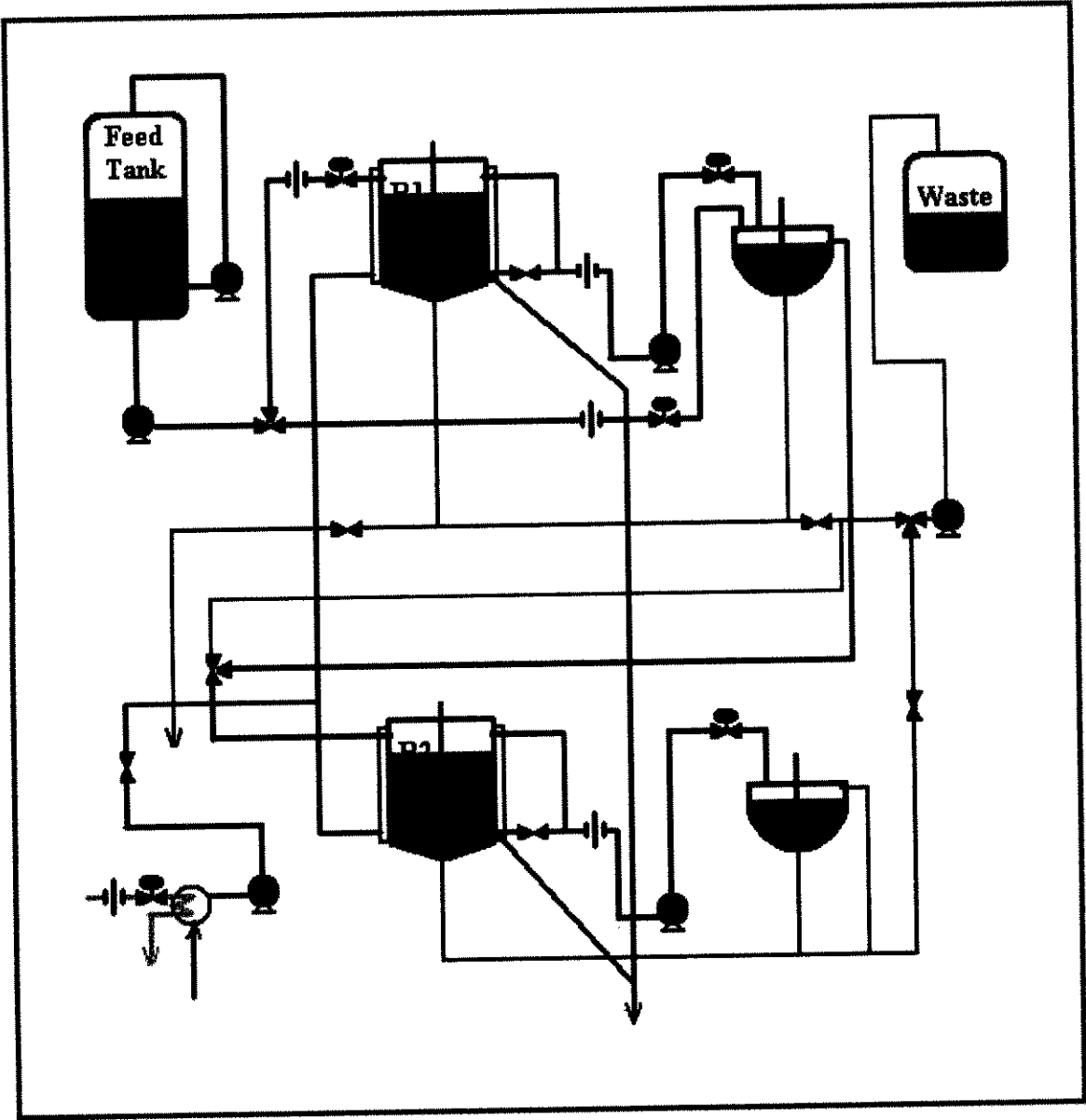


Figure 6.1: Plant 1: Two CSTRs in Series

Rate of consuming EA	$\text{Rate} = -k_0 e^{(-E/RaT)} VC$	(6.1)
Mass balance for EA	$\{d(VC)/dt\} = \text{Rate} + Q_{in}C_{in} - Q_oC_o$	(6.2)
Rate of heat provided	$\text{Heat} = Ua(T_{co} - T) = \{m_c C_{pc}/(\rho_r C_p)\}(T_{ci} - T_{co})$	(6.3)
Energy balance	$\{d(VT)/dt\} = DH * \text{Rate} + Q_{in}T_{in} - Q_oT_o + \text{Heat}$	(6.4)
where	$DH = -\{\Delta H_r/(\rho_r C_p)\}$	(6.5)
Perfect mixing	$C = C_o; T = T_o$	(6.6)
Overall mass balance	$V_{max}(dH/dt) = Q_{in} - Q_o$	(6.7)
	$V = V_{max}H$	(6.8)
Temperature control	$m = \text{Gain}_t[\text{Stp}_t - T + (Int_t/Rst_t)] + m_{ss}$	(6.9)
	$\{d(Int_t)/dt\} = \text{Stp}_t - T$	(6.10)
Level control	$Q_o = Q_{max}\text{Gain}_h[\text{Stp}_h - H + (Int_h/Rst_h)] + Q_{ss}$	(6.11)
	$\{d(Int_h)/dt\} = \text{Stp}_h - H$	(6.12)

The above equations are applied for both reactors. If the by-pass stream is on, the equations required for the intermediate mixer are:

$$\text{Overall mass balance} \quad Q^2_{in} = Q^1_o + Q^2 \quad (6.13)$$

$$\text{Mass balance for EA} \quad C^2_{in} Q^2_{in} = C_1 Q^1_o + C_f Q^2 \quad (6.14)$$

$$\text{Energy balance} \quad T^2_{in} Q^2_{in} = T_1 Q^1_o + T_f Q^2 \quad (6.15)$$

The inequality constraints on the systems are:

Safety restriction	$303 \leq T_1, T_2 \leq 353 \text{ (K)}$	Constraint 1
Process limitation	$5.0 \leq V_1, V_2 \leq 8.5 \text{ (l)}$	Constraint 2
Maximum, minimum Throughput	$0.5 \leq Q_f \leq 3.0 \text{ (l.min}^{-1}\text{)}$	Constraint 3
	$0.05 \leq Q^1_{in}, Q^1_o, Q^2_o \leq 2.5 \text{ (l.min}^{-1}\text{)}$	Constraint 4

The system of equality and inequality equations describes the whole plant. However, with the current design, hot water running through the jacket cannot provide enough heat to keep the hydrolysis reaction at the upper limit temperature. The plant is now operating under these following conditions: the by-pass stream has to be off and the steam valve is fully open. The temperature control loop is removed as well.

Maximizing the production of the plant, subject to constraints from 1 to 4, defines the nominal optimal operating condition.

$$\text{Production} = \text{Throughput} \cdot (C_{in} - C_o) \quad (6.16)$$

The optimization problem is solved for the feed flowrate Q_{in} . Under the current design, hot water flowing through the jacket cannot provide enough heat for the hydrolysis reaction. The first tank is actually served to preheat the fluid, since the rate of reaction is not significant in the first reactor. The optimum feed flowrate is also the minimum throughput at 0.75 l.min^{-1} , which brings the conversion up to 36%.

The plant is started up at the minimum throughput and is operated at the feed rate of 1.8 l.min^{-1} . Since the mixers do not have level controllers, if the level of any mixer exceeds 85% of its volume, the alarm system will automatically close the feed valve. The flow from the mixer to the second tank is by gravity force. To maintain a continuous flow, the switchability problem is solved for the optimal trajectory connecting the startup and operating flowrates subject to constraints 2 and 4. The objective function for the switchability problem is:

$$F = \int_{t_0}^{t_f} \{w_p (Q_{in} - Q_{sf})^2 + w_c (C - C_{sf})^2 + w_t (T - T_{sf})^2\} dt \quad (6.17)$$

2.2. Result and Discussion

The sets of equality and inequality equations describing the plant is tested first by matching simulation results with data collected from the plant. The level control loops in the real plant are cascade loops. To describe these loops using a nonlinear model, it is essential to include time delays in the model equations. Equations (6.11) and (6.12) related to level controllers are written for two reactors including time delays.

$$H_1(t) = \text{lev}_1(t + \text{lag}_1) \quad (6.18)$$

$$Q_o^1 = Q_{\max} \text{Gain}_{h1} [\text{Stp}_{h1} - \text{lev}_1 + (\text{Int}_{h1}/\text{Rst}_{h1})] + Q_{ss1} \quad (6.19)$$

$$\{d(\text{Int}_{h1})/dt\} = \text{Stp}_{h1} - \text{lev}_1 \quad (6.20)$$

$$H_2(t) = \text{lev}_2(t + \text{lag}_2) \quad (6.21)$$

$$Q_o^2 = Q_{\max} \text{Gain}_{h2} [\text{Stp}_{h2} - \text{lev}_2 + (\text{Int}_{h2}/\text{Rst}_{h2})] + Q_{ss2} \quad (6.22)$$

$$\{d(\text{Int}_{h2})/dt\} = \text{Stp}_{h2} - \text{lev}_2 \quad (6.23)$$

“lag₁” and “lag₂” denote level time delays in the first and second reactors, respectively. The second loop has a smaller time delay than the first loop because any small change in the first will greatly affect the second one. Figure 6.2 compares responses of the manipulated variables in two CSTRs. Green curves represent results from simulations and red curves are for experimental data. The outflow profiles and the level profiles (see Figures 6.2 and 6.3) show very good matching. As discussed in Chapter 5, time delay is an important element in mathematical modeling of chemical processes and controller design. A large time delay means the system is closer to the verge of instability, which creates more oscillation in the responses similar to real plant responses. However, there is a three-degree difference and lag effect in temperature responses (Figure 6.4). If the design was changed so that steam ran directly through the coils inside the tanks, rather than hot water through the surrounding jackets, the temperature control loop would be closed, then the above problem could be fixed.

A step change in flowrate will violate constraints 2 and 4 as shown in Figure 6.2. Figure 6.5 shows the optimal feed policy (red curve) to avoid constraint violations. This profile is solved using the sequential optimization technique with time steps fixed for twenty seconds. The upper bound posed on the outflow from the second tank is set at 2.1 l.min⁻¹. The policy found is fed back to the plant as the set point. The green curve in the same figure represents the real process feed value. Figure 6.6 shows the corresponding outflow responses.

Figure 6.7 compares results from two different software packages, using the sequential optimization technique with time steps fixed for thirty seconds. Green curves plot data points from MATLAB and red curves from SPEEDUP plus OPT. The results are quite different because the weighting W_t and W_c (see Equation 6.17) used in MATLAB and SPEEDUP are different.

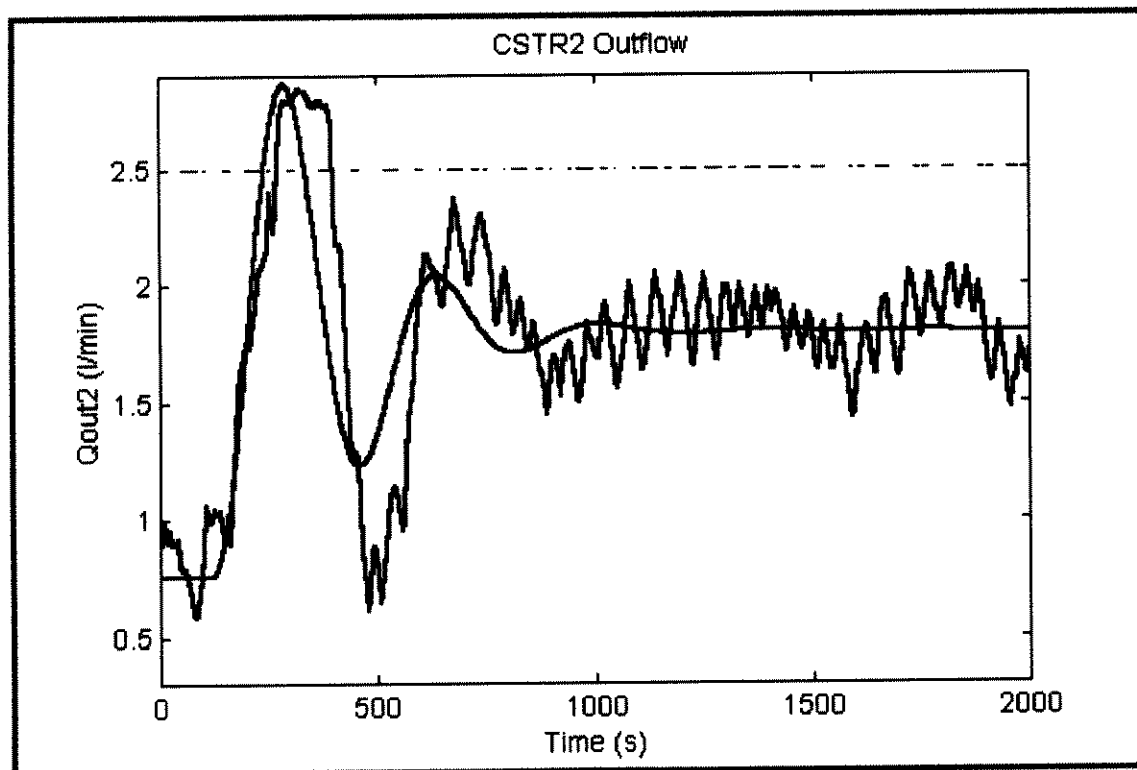
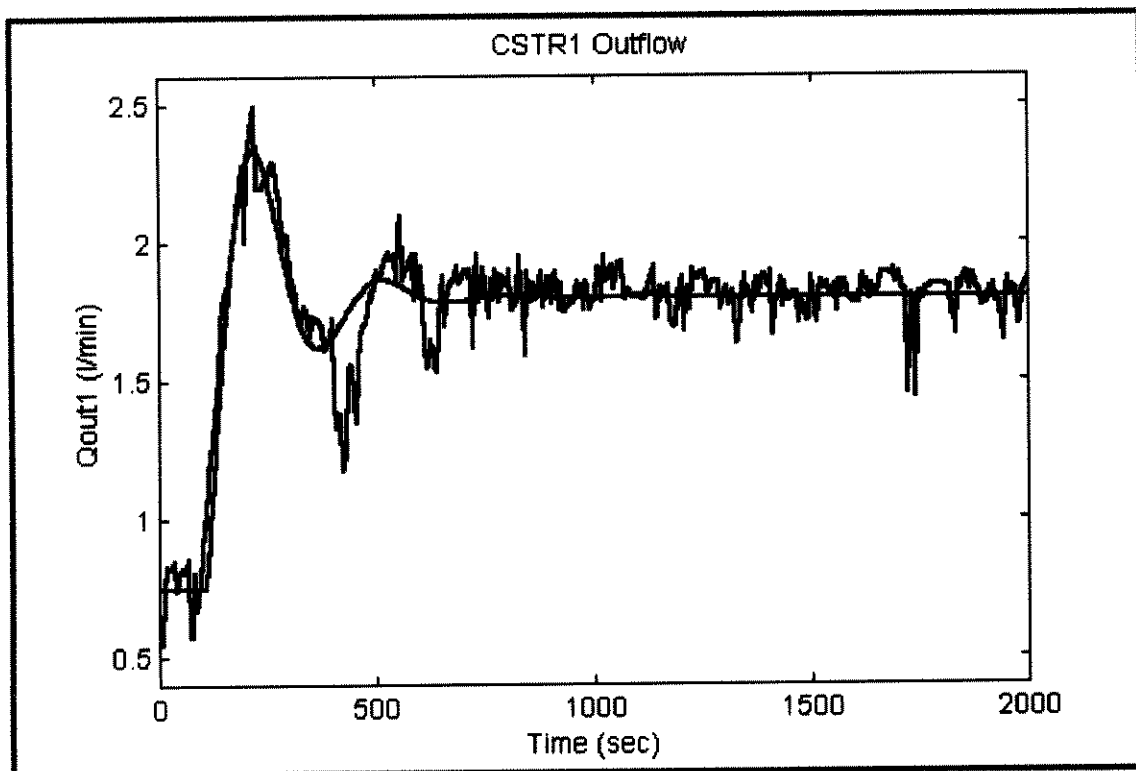


Figure 6.2a, b: Outflow Profiles in First and Second Reactors

(Green curve: Simulation result)

(Red curve: Experimental result)

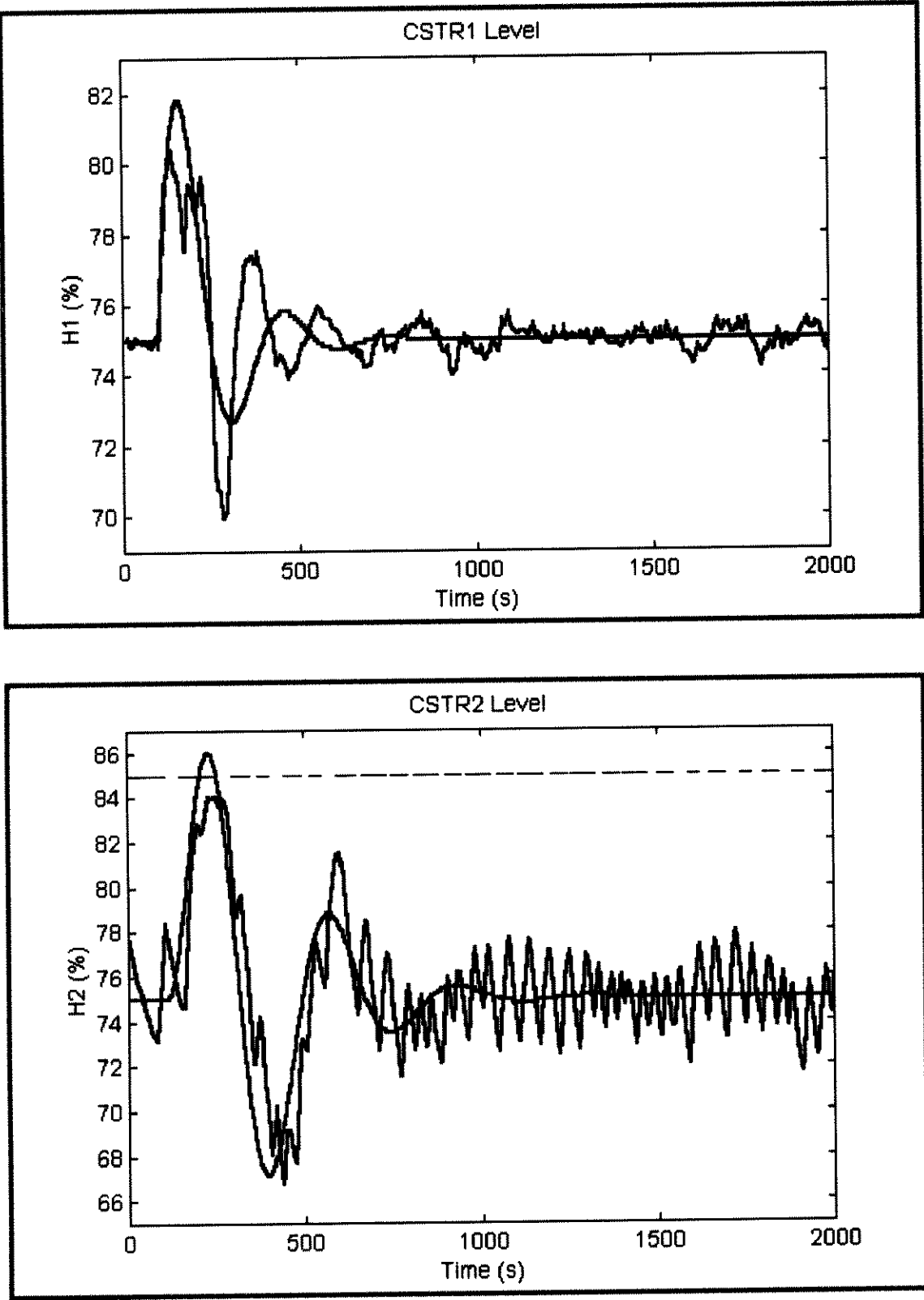


Figure 6.3a, b: Level Profiles in First and Second Reactors

(Green curve: Simulation result)

(Red curve: Experimental result)

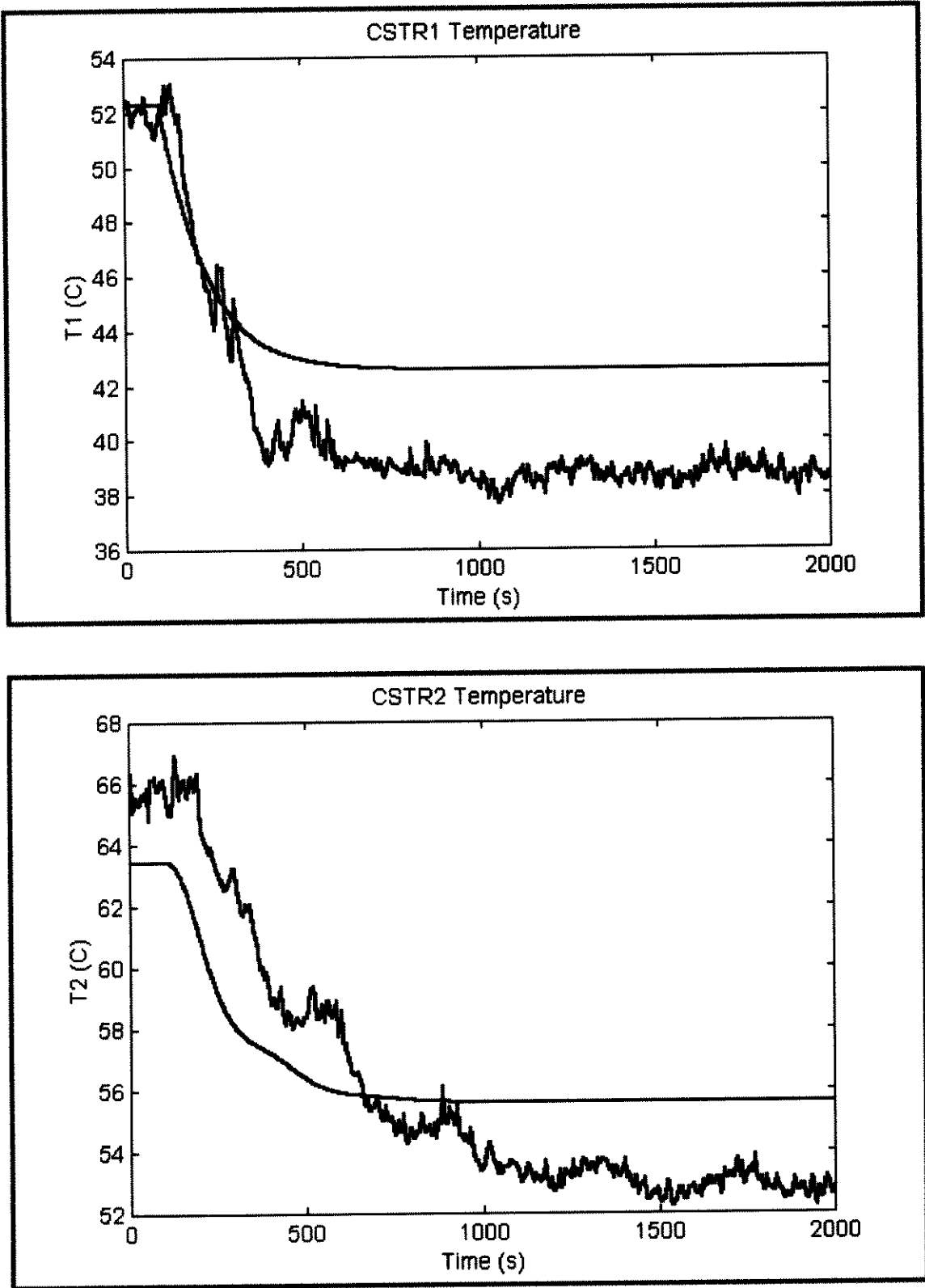


Figure 6.4a, b: Temperature Profiles in First and Second Reactors

(Green curve: Simulation result)

(Red curve: Experimental result)

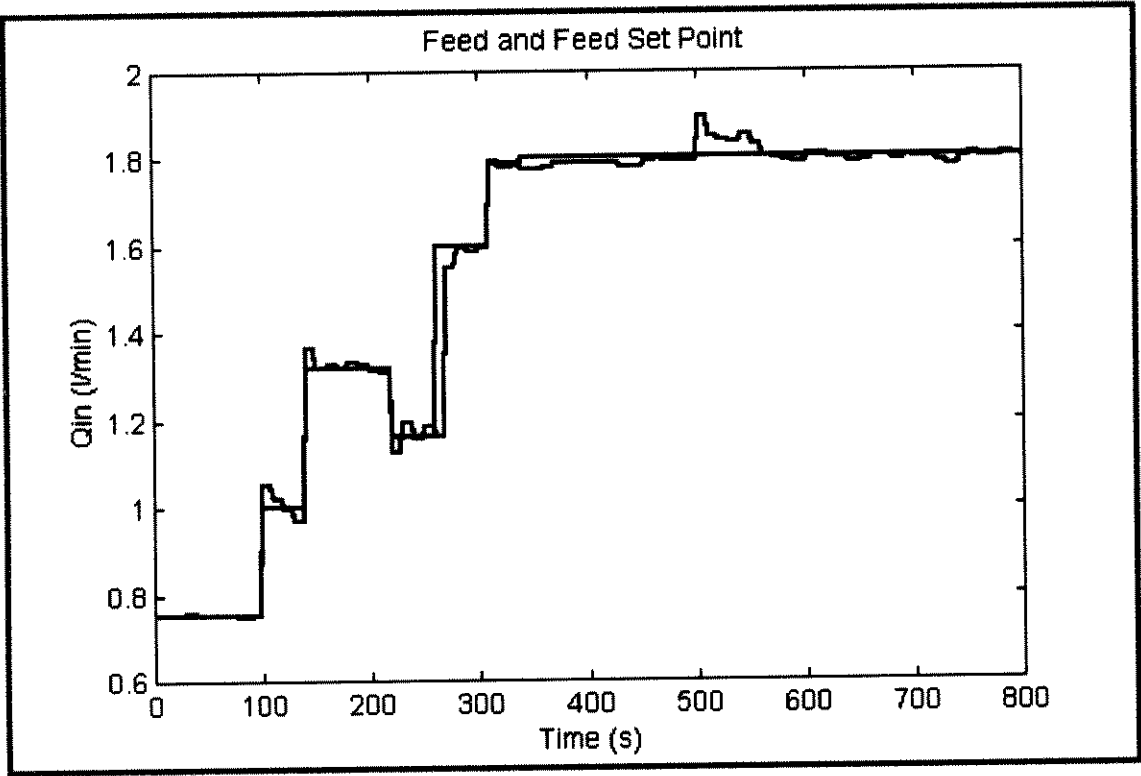


Figure 6.5: Feed Policy

(Green curve: Feed process value; Red curve: Feed set point)

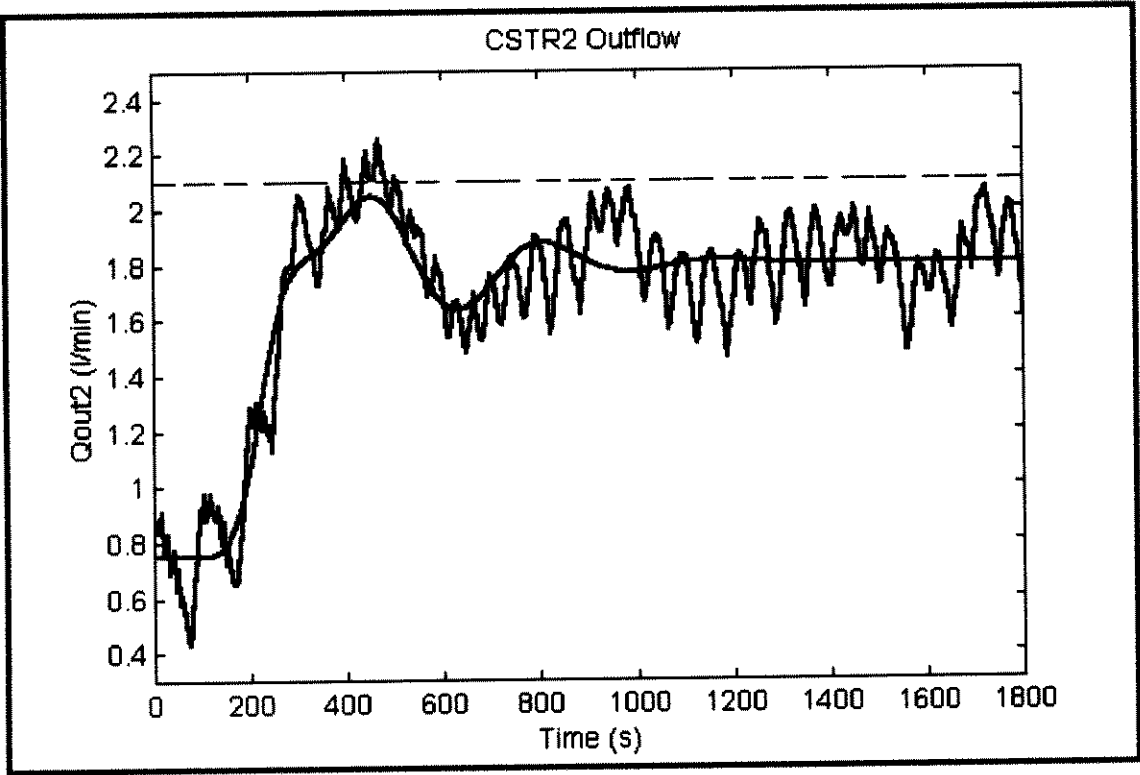


Figure 6.6: Outflow Response in Second Reactor

(Green curve: From simulation; Red curve: From real plant)

As MATLAB includes the optimization toolbox in its package, it is easier to sum up concentration and temperature deviations, and more terms can be included in the summation without increasing the computational time. SPEEDUP, however, cannot perform optimization within the dynamic simulation environment. Since it must interface to an external optimizer, fewer deviation terms are used in the summation due to the complexity of the interfacing. If the feed policies found from these two packages are fed back to perform dynamic simulations, the outputs are quite similar. Figures 6.8 and 6.9 show the outputs from MATLAB and SPEEDUP dynamic simulations, respectively. The feed policy from MATLAB results in constraint violations (green curves), when it is fed back in SPEEDUP simulations (Figures 6.9a, b). The error caused by different package usage is within an acceptable limit under the engineering application viewpoint.

The same problem is solved using the simultaneous integration and optimization technique. The optimal feed profile is smoother compared to the step curve from the previous technique (red curve compared to green curve in Figure 6.10a). The sequential method gives the step profile because it uses a few larger time steps to reach convergence and reduce the computational time. The simultaneous technique requires many smaller time steps to solve the stiff problem so the profile is rather a curve than a series of steps. If the time steps used in the second technique are large, the problem is converged with difficulty. Figure 6.10b also shows the effect of constraints posed on the sensitivity of the inlet valve. These constraints help to avoid a sudden change in the feed that may upset downstream units. As shown in this figure, the blue and yellow curves represent the effect of constraints on feed valves but the yellow one uses larger time steps. The red curve is without constraints on the feed valve. Generally, the simultaneous technique gives more reliable optimal solutions in shorter computational time. However, these solutions are used more as references than in real applications. Solutions given by the sequential method are more practical under the application viewpoint, because these series of steps can be easily fed back to the DCS or even manually set as feed set points.

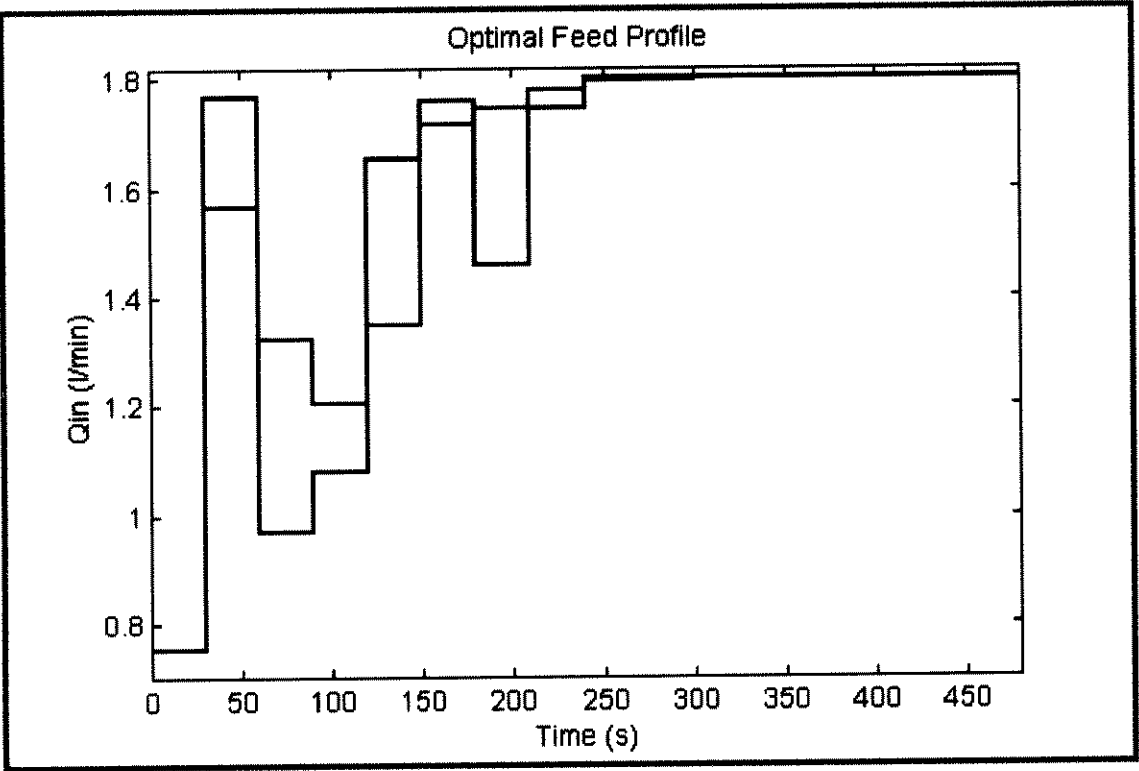


Figure 6.7 Optimal Feed Policy

(Green curve: From MATLAB; Red curve: From SPEEDUP)

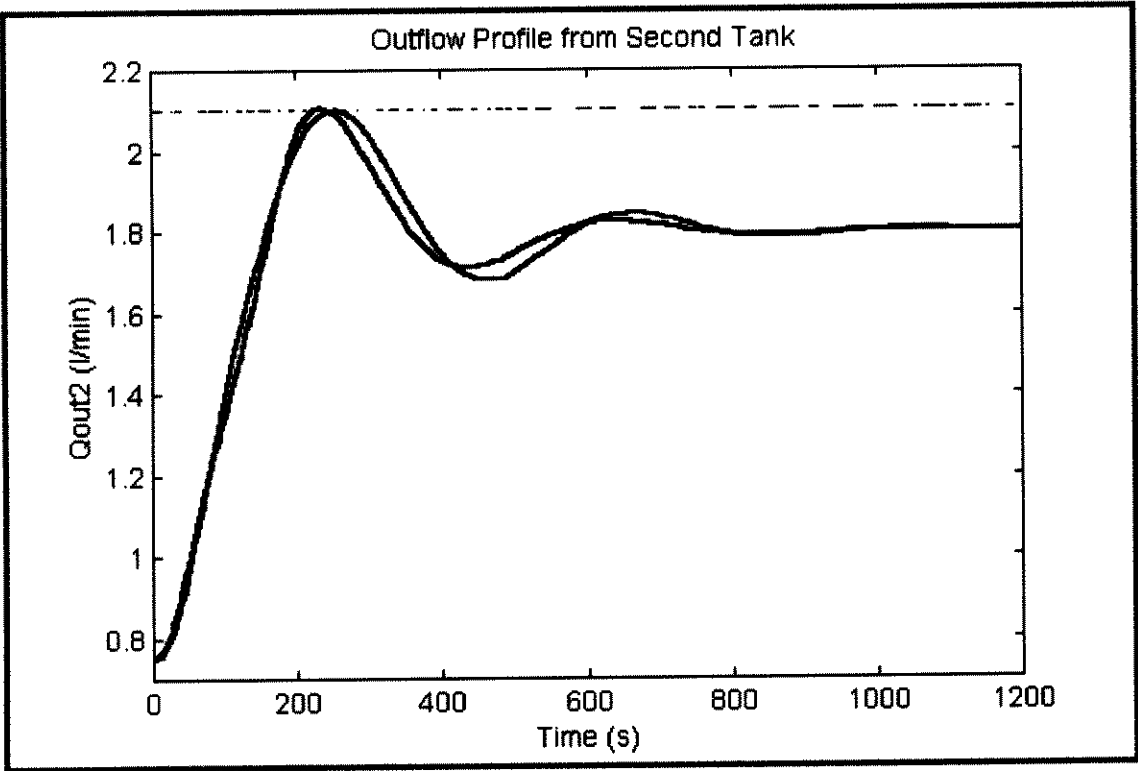


Figure 6.8 Responses from MATLAB Dynamic Simulations

(Green curve: Optimal feed policy obtained from MATLAB)

(Red curve: Optimal feed policy obtained from SPEEDUP)

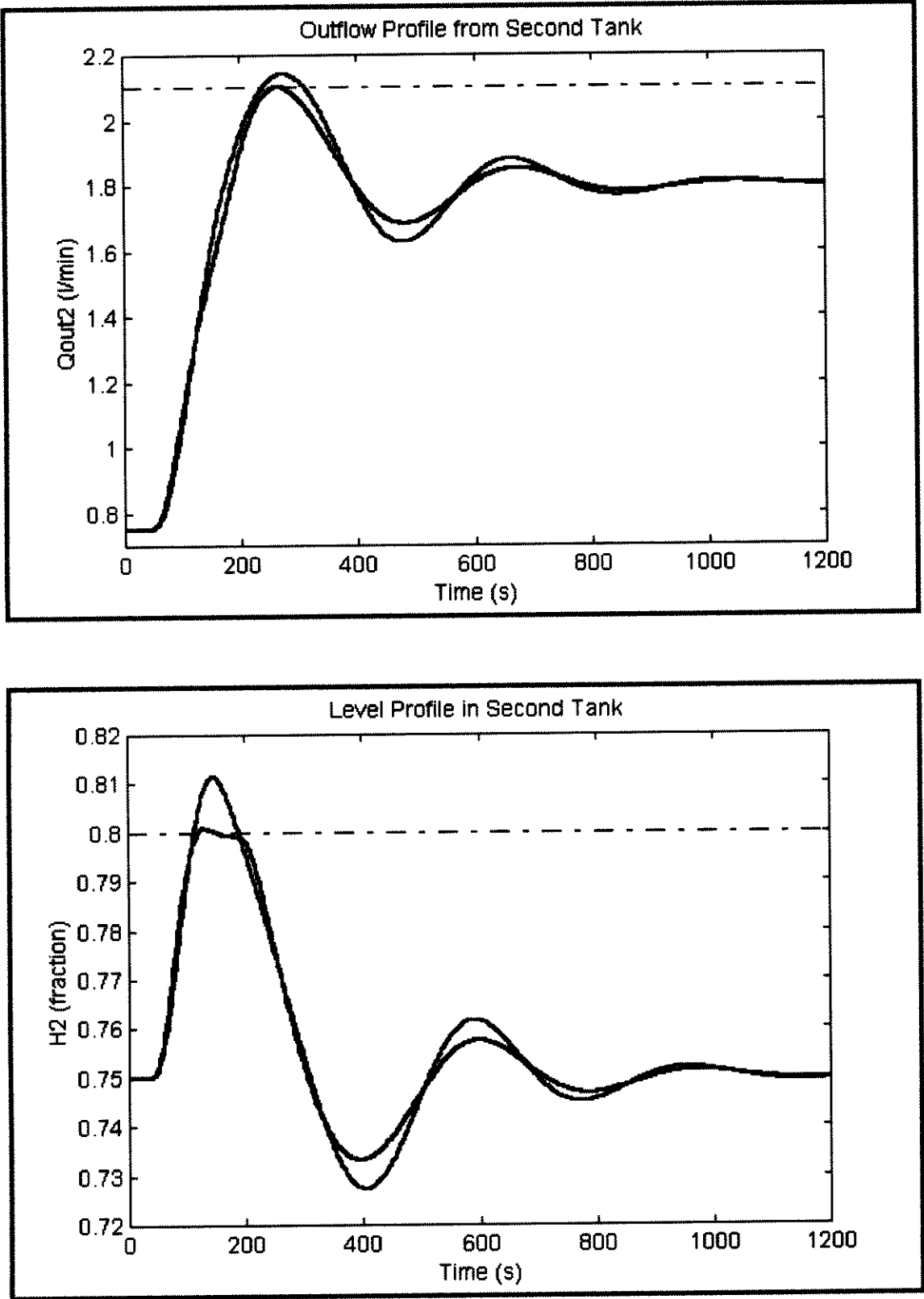


Figure 6.9a, b Responses from SPEEDUP Dynamic Simulations
(Green curve: Optimal feed policy obtained from MATLAB)
(Red curve: Optimal feed policy obtained from SPEEDUP)

2.3. Improvement of Current Design

With the current design as mentioned before, hot water running through the jacket cannot provide enough heat to keep the hydrolysis reaction at the upper limit temperature. The setup of the temperature control loop produces very slow responses as well. Therefore, the temperature controller is removed and the steam valve is set fully open. This results in temperature lag and low conversion, when the plant is operated at a higher feed rate. If the design is changed so that steam runs directly through the coils inside the tanks, rather than hot water through the surrounding jackets, the temperature control loop will be closed. The optimal feed flowrate in this case is 2.3 l.min^{-1} with 39% conversion. The startup problem will be a very interesting case, because the first reactor will be started at the minimum feed rate (0.75 l.min^{-1}), while the second reactor at a higher feed rate (1.5 l.min^{-1} , approximately), using the bypass line. The total operating feed rate is 2.3 l.min^{-1} . Two thirds of this rate goes to the first reactor, and the rest enters the bypass line. With this arrangement the conversion is maintained above 40 %, and the level in the second reactor is less than 0.8 during the transition, as shown in Figure 6.11.

3. *Application 2: Binary Distillation Column*

3.1. Plant Description and Modeling

For teaching and research work, the Department of Chemical Engineering is using a pilot binary distillation column, which separates ethanol from water. The column includes twelve 9-inch-sieve trays numbered from the top tray. The feed may enter at one of three feed positions: 7th, 9th and 11th trays (including the condenser and the reboiler as 1st and 14th trays, respectively). The vapor holdup in the column is neglected. Current geometrical data of the column, the condenser, the reflux drum and the reboiler are used for liquid holdup calculations. The liquid holdup in each tray is assumed to be constant.

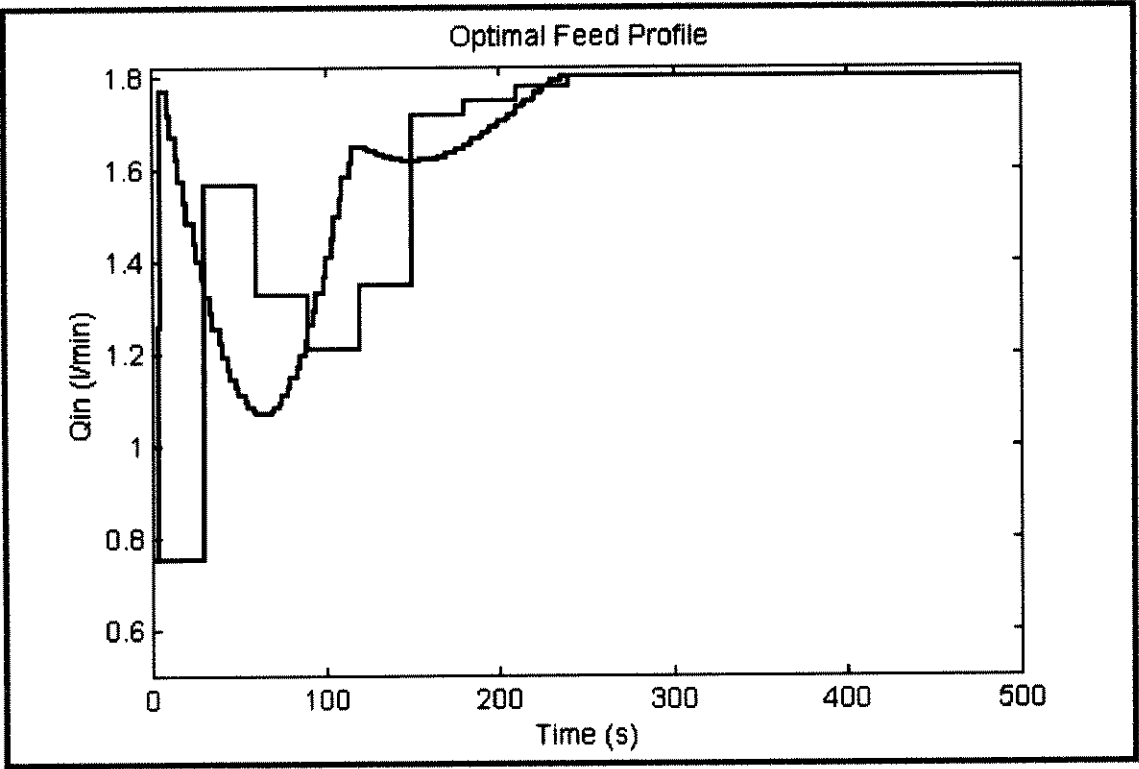


Figure 6.10a: Feed Profiles from Different Solving Techniques
(Green curve: Sequential with MATLAB; Red curve: Simultaneous with GAMS)

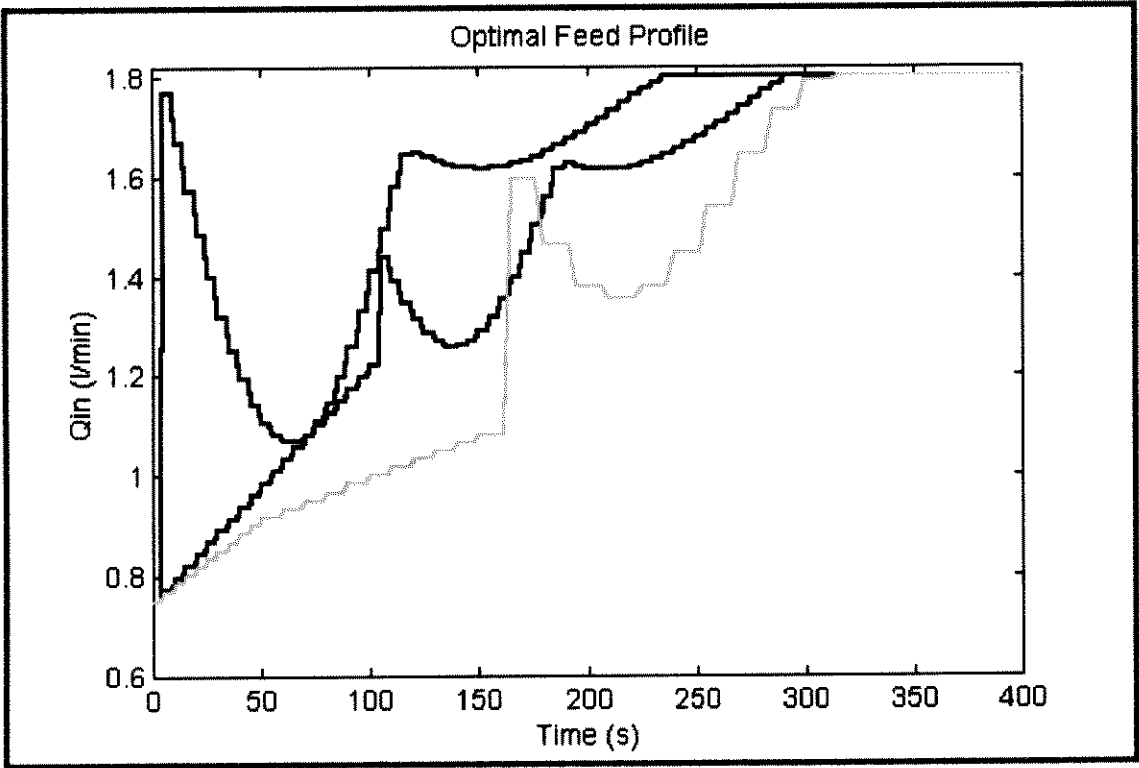


Figure 6.10b: Feed Profiles from Simultaneous Technique with GAMS
(Red: No constraint on inlet valve; Blue: Constraint on inlet valve)
(Yellow: Constraint on inlet valve, large time steps)

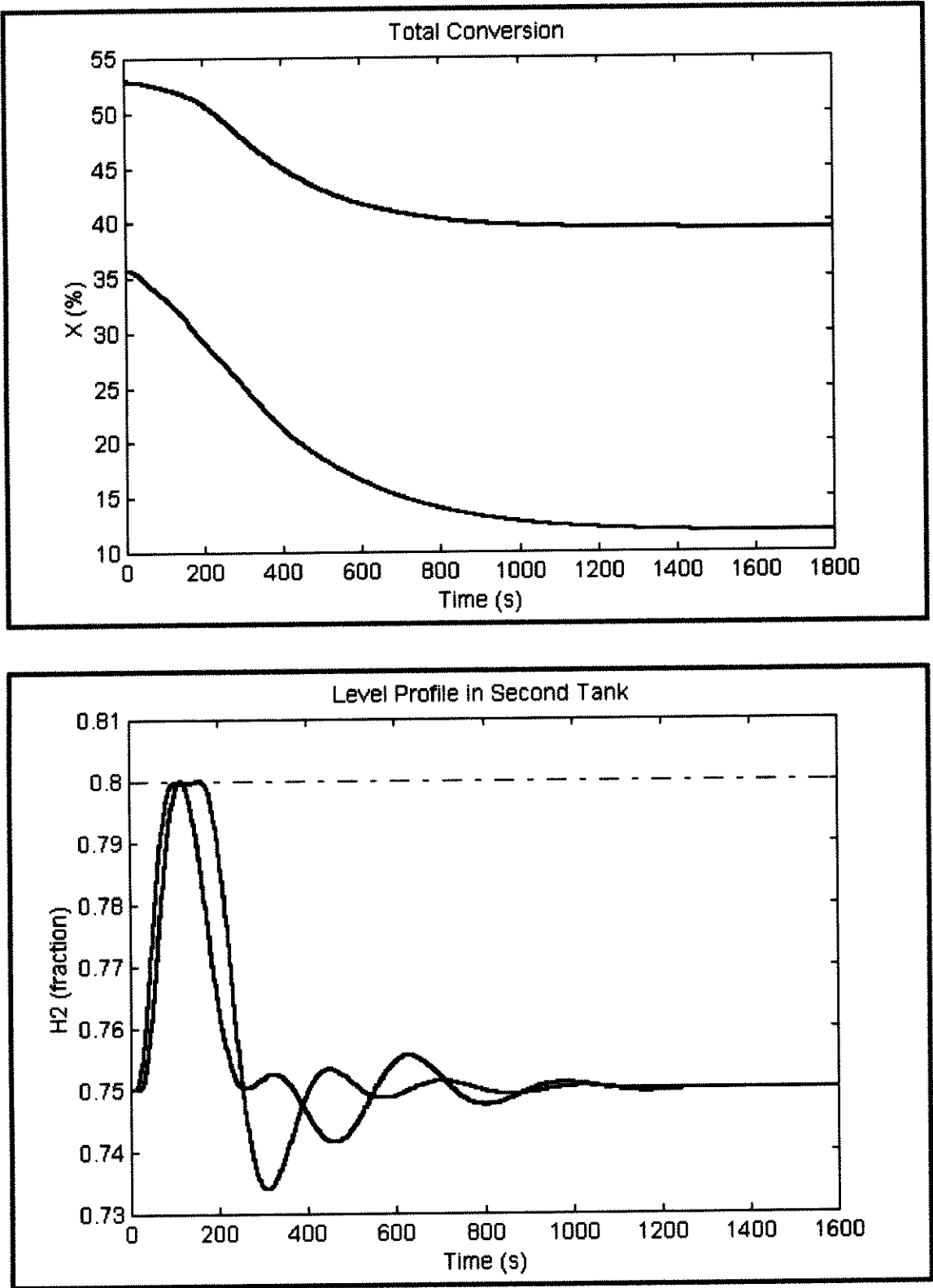


Figure 6.11a, b Total Conversion and Level Profile in Second Reactor
(Green curves: Current design; Red curves: Improved design)

Figure 6.12 is the flowsheet of the binary distillation column. Possible control loops for the column includes:

1. Adjusting the base product (B) controls the level of the reboiler (H_{reb}).
2. Adjusting the distillate (D) controls the level of the condenser (H_{con}).
3. Adjusting simultaneously the distillate and reflux (L) controls the reflux ratio (RR) and indirectly the level of the condenser.
4. Adjusting the reflux (L) controls the temperature (T_2) of the 2nd tray, to infer the composition of ethanol (x_D) in the distillate.
5. Adjusting the steam rate controls the temperature (T_{13}) of the 13th tray to infer the composition of ethanol (x_B) in the base product.

Different control strategies will be discussed in this section. Basically the levels of the reboiler and the condenser are controlled so loops 1 and 3 are closed. Then either the composition of the distillate or the base product is controlled so loop 4 or loop 5 is closed. Four models of the column are used in different problems. Thermodynamic properties required for the binary distillation are extracted from steady state simulations using ASPEN models. Optimal operating conditions are solved using GAMS models. SPEEDUP and MATLAB models are used for dynamic simulations and switching calculations. The conventional control technique with time delay effect is applied to the column, using SPEEDUP. The application of DMC technique is performed in MATLAB, since this package can properly handle matrix operations. For the rigorous steady-state model, each tray except the 1st, 14th and feed is described by three equations: total mass, energy and component balances. Different sets of equations are required for the feed, the condenser with condenser duty and the reboiler with reboiler duty. For the dynamic model all equations, which describe the component balance are changed. If the level control loops are closed, the mass balances for the condenser and the reboiler are also changed.

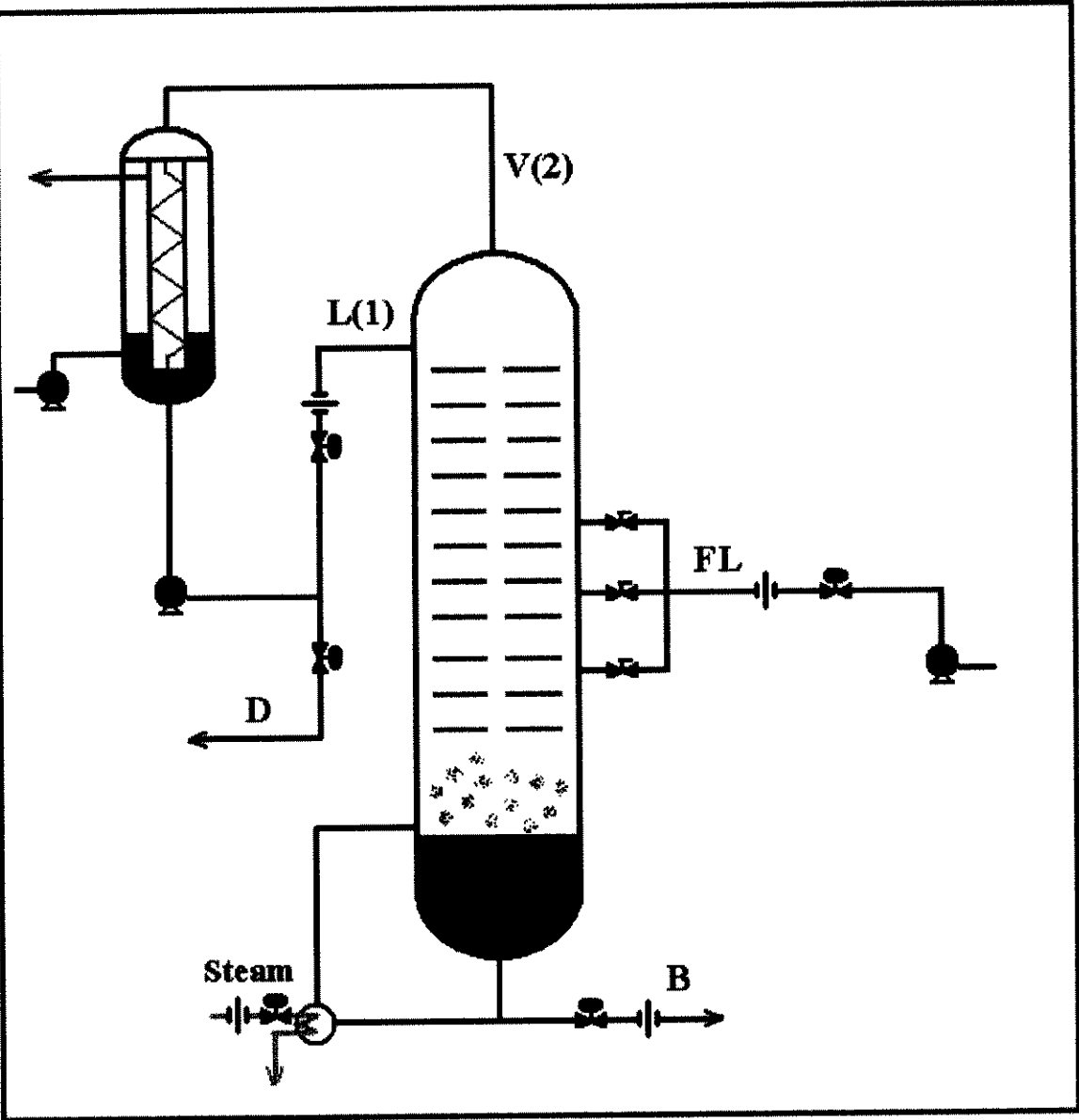


Figure 6.12: Plant 2: Binary Distillation Column

For $k = 1, 2, \dots, 12$ and $k \neq 6$ (or 8, or 10)

$$\text{Total mass balance} \quad L(k) + V(k+2) - L(k+1) - V(k+1) = 0 \quad (6.24)$$

$$\text{Energy balance} \quad H_L(k)L(k) + H_V(k+2)V(k+2) - H_L(k+1)L(k+1) - H_V(k+1)V(k+1) = 0 \quad (6.25)$$

$$\text{Component balance} \quad x(k)L(k) + y(k+2)V(k+2) - x(k+1)L(k+1) - y(k+1)V(k+1) = 0 \quad (6.26)$$

For the condenser, reboiler and feed tray

$$\text{Mass balance} \quad L(1) + D - V(2) = 0 \quad (6.27)$$

$$L(13) - B - V(14) = 0 \quad (6.28)$$

$$FL + L(10) + V(12) - L(11) - V(11) = 0 \quad (6.29)$$

$$\text{Energy balance} \quad Q_{CD} + H_{LD}(L(1) + D) - H_V(2)V(2) = 0 \quad (6.30)$$

$$Q_{RE} + H_L(13)L(13) - H_L(14)B - H_V(14)V(14) = 0 \quad (6.31)$$

$$H_{LF}FL + H_L(10)L(10) + H_V(12)V(12) - H_L(11)L(11) - H_V(11)V(11) = 0 \quad (6.32)$$

$$\text{Component balance} \quad x_D(L(1) + D) - y(2)V(2) = 0 \quad (6.33)$$

$$x(13)L(13) - x_B B - y(14)V(14) = 0 \quad (6.34)$$

$$x_F FL + x(10)L(10) + y(12)V(12) - x(11)L(11) - y(11)V(11) = 0 \quad (6.35)$$

For $k = 1, 2, \dots, 14$

$$\text{Phase equilibrium} \quad y_s(k)\{1 + x(k)(\alpha(k) - 1)\} - x(k)\alpha(k) = 0 \quad (6.36)$$

$$\text{Murphree efficiency} \quad y(k) - y(k+1) - \text{meff}(k)(y_s(k) - y_s(k+1)) \quad (6.37)$$

Differences in the dynamic model with two level controllers include:

For $k = 1, 2, \dots, 12$ and $k \neq 6$ (or 8, or 10)

$$\text{Component balance} \quad M(k+1)\{dx(k+1)/dt\} = x(k)L(k) + y(k+2)V(k+2) - x(k+1)L(k+1) - y(k+1)V(k+1) \quad (6.38)$$

For the condenser, reboiler and feed tray

$$\text{Component balance} \quad M(1)\{dx(1)/dt\} = V(2)\{y(2) - x_D\} \quad (6.39)$$

$$M(14)\{dx(14)/dt\} = L(13)\{x(13) - x(14)\} + V(14)\{x(14) - y(14)\} \quad (6.40)$$

$$M(11)\{dx(11)/dt\} = x_F FL + x(10)L(10) + y(12)V(12) - x(11)L(11) - y(11)V(11) \quad (6.41)$$

Mass balance

For the condenser and reboiler

$$M(1)\{dH_1/dt\} = H_1\{L(1) + D - V(2)\} \quad (6.42)$$

$$M(14)\{dH_2/dt\} = H_2\{L(13) - B - V(14)\} \quad (6.43)$$

3.2. Steady State ASPEN Model

The distillation process requires thermodynamic properties, which can be extracted from ASPEN simulations. Some specifications for the model development include:

- ❖ The methods and models to calculate physical properties are defined by the NRTL system option. This option set uses Renon activity coefficient model for the liquid phase and ideal gas equation ($PV = RT$) for the vapor phase.
- ❖ The column operates under atmospheric pressure. The pressure drop of the column is 0.35 atm. The condenser produces subcooled reflux and distillate. Murphree stage efficiency is 0.3 for all trays except the 1st, 13th and 14th.

Figure 6.13 compares temperatures and compositions of ethanol predicted by the model and experimental data. Temperatures of the 4th and 8th trays are well predicted. Good matching is also found in ethanol compositions of the distillate and the stream coming from the 3rd tray. Experimental points are selected from many runs with various feeds, distillate rates and reflux ratios under the condition that the ethanol composition of the distillate is greater than 0.69 (mole fraction).

During a normal operation, the reflux ratio and the rate of steam, which supplies heat to the reboiler, are fixed. Distillate, reflux and base product rates are measured. However, due to the uncertainty in the conversion of steam rate to energy, the reflux ratio and the distillate rate are specified in the model instead of the reboiler duty. This results in temperature discrepancy at the trays below the feed tray. Increasing the predicted reboiler duty by 10% would reduce this discrepancy less than one degree. Temperatures of the 4th and 13th trays will be selected for the inferential control.

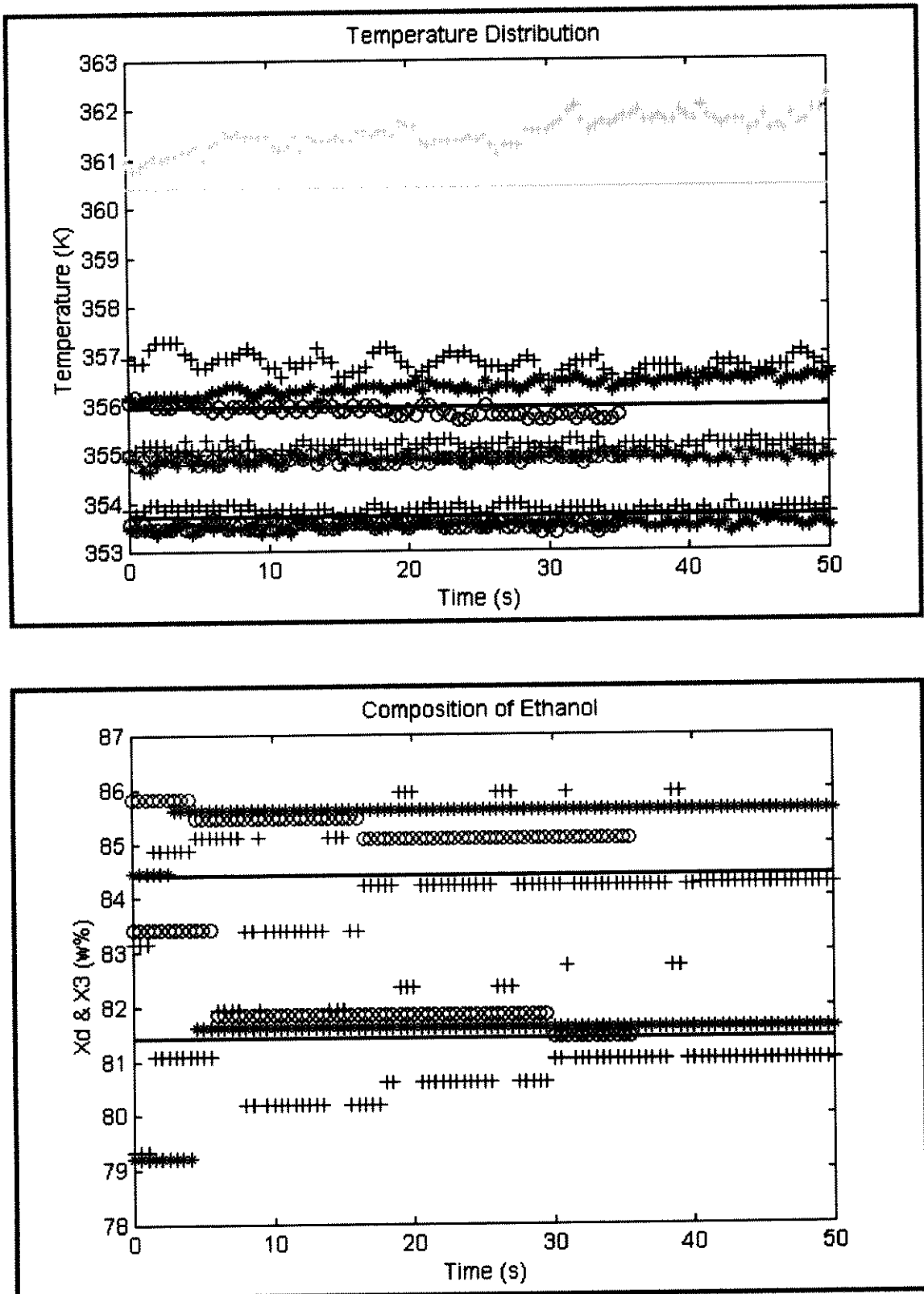


Figure 6.13 Temperature and Composition Distributions
 (Green: Tray 2; Red: Tray 4; Blue: Tray 8; Yellow: Tray 10)
 (Straight line: Result predicted by ASPEN model)

Liquid densities are measured to infer compositions but this simple technique cannot provide reliable information of low ethanol samples. Therefore, compositions of the samples extracted below the feed tray cannot be matched with those given by the model.

With thermodynamic properties from ASPEN simulations, other models in GAMS, MATLAB and SPEEDUP can be derived. Optimization problems using these models will be discussed after identifying the constraints posed on the column. They might be:

<i>Product purity</i>	$0.69 \leq x_D \leq 0.75$	Constraint 1
	$0.01 \leq x_B \leq 0.028$	Constraint 2
<i>Process limitation</i>	$30 \leq Q_{reb} \leq 180 \text{ (MJ.hr}^{-1}\text{)}$	Constraint 3
<i>Maximum, minimum</i>		
<i>Throughput</i>	$1 \leq VFL \leq 3 \text{ (l.min}^{-1}\text{)}$	Constraint 4
<i>Reflux rate</i>	$0.7 \leq VL \leq 1.3 \text{ (l.min}^{-1}\text{)}$	Constraint 5
<i>Distillate rate</i>	$0.19 \leq VD \leq 0.7 \text{ (l.min}^{-1}\text{)}$	Constraint 6
<i>Reflux ratio</i>	$0.8 \leq RR \leq 4$	Constraint 7

The ranges of operating conditions set by these above inequality constraints guarantee a stable performance. Maximizing the profit objective function (Nooraii, 1995) will define the optimal operating conditions.

$$\text{Profit} = cd_1 * D * x_D + cd_2 * x_D - cf * FL * x_F - cq * Q_{reb} - cc * Q_{con} \quad (6.44)$$

In equation (6.44) cd_1 and cd_2 indicate selling prices of pure ethanol; cf , cq and cc denote cost of feed, steam and water, respectively. A $\pm 2\%$ disturbance on the feed composition is significant for the pilot plant.

3.3. Optimal Feed Location Using GAMS Model

The optimization problem, which finds the nominal optimal operating condition, can be modified to identify the optimal feed location as well. Each tray except the

condenser and the reboiler is considered as a possible feed tray, being described by three equations.

For $k = 2, 3, \dots, 12$

$$\text{Mass balance} \quad f(k)FL + L(k) + V(k+2) - L(k+1) - V(k+1) = 0 \quad (6.45)$$

$$\text{Energy balance} \quad f(k)H_{LF}FL + H_L(k)L(k) + H_V(k+2)V(k+2) - H_L(k+1)L(k+1) - H_V(k+1)V(k+1) = 0 \quad (6.46)$$

$$\text{Component balance} \quad f(k)x_FFL + x(k)L(k) + y(k+2)V(k+2) - x(k+1)L(k+1) - y(k+1)V(k+1) = 0 \quad (6.47)$$

$$\text{where} \quad Y_f(k)FL - f(k) = 0 \quad (6.48)$$

$$\sum Y_f(k) = 1 \quad (6.49)$$

$Y_f(k)$ are binary variables, which take the value of one or zero. Since nonlinear terms cannot be used with binary variables, equations (6.48) and (6.49) help to avoid this situation. As a result, MINLP technique must be used instead of NLP method to solve the optimization problem. The nominal optimal solutions are shown in Table 6.1 for two different feed rates.

	First Steady State	Second Steady State
<u>Input</u>		
Feed Rate ($l.min^{-1}$)	1.0	2.0
Feed Composition (w% Ethanol)	18	20

In Table 6.1, the highlighted specifications are set, when operating the column. Others are outputs from the operation. The same problem can be actually solved using NLP technique, if $Y_f(k)$ is treated as non-integer variables. In both cases tray 12 is the optimal feed location. This feed location is dependent on the efficiency but not on the throughput of the column. The column has three feed positions: 7th, 9th and 11th trays. The last position is then selected as the feed tray in the following optimization problems.

	First Steady State	Second Steady State
<u>Optimal Solution</u>		
Objective Value (\$)	52.09	48.58
Optimal Feed Composition	Tray 12	Tray 12
Reflux Ratio	3.69	3.71
Distillate Rate (l.min ⁻¹)	0.190*	0.393
Reboiler Duty (kW)	62.3	69.1
Reflux Rate (l.min ⁻¹)	0.700*	0.700*
Distillate Composition (w% Ethanol)	86.2	85.3
B-Product Composition (w% Ethanol)	4.9	6.9*
Active Constraints (*)	(5) & (6)	(2) & (5)

Table 6.1 Nominal Optimal Operating Conditions

3.4. Steady State Open Loop Back-Off Calculation Using SPEEDUP Model

The solution found in Table 6.1 is tested with possible values of the feed composition. The nominal solutions cause constraint violations when they are tested with the uncertain vector $[x_{mf}]$. SPEEDUP model is selected to solve the back-off problem because it must deal with three identical units. Each unit is subject to an element of the uncertain vector.

$$x_{mf} = \begin{bmatrix} 0.18 \\ 0.20 \\ 0.22 \end{bmatrix}$$

The feasible solution of the second case is located at the intersection of two active constraints 1 and 2, which is shown in Figure 6.14. Table 6.2 presents the back-off operating conditions.

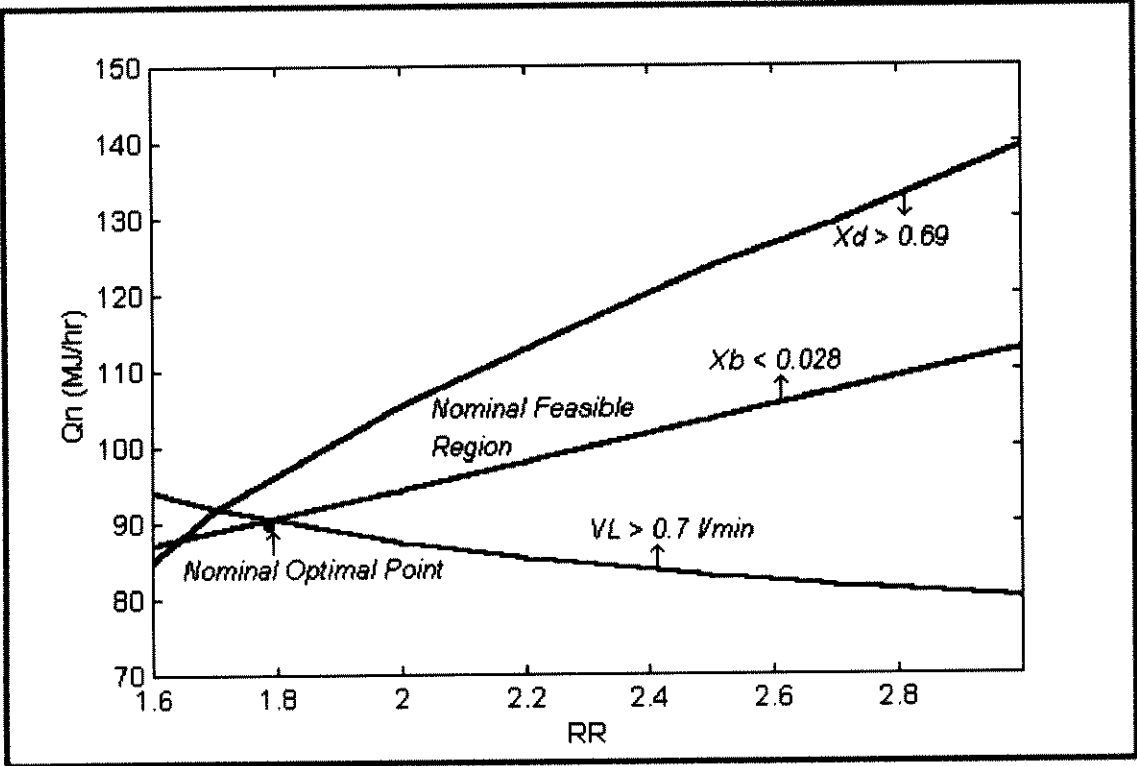


Figure 6.14a Second Case: Nominal Feasible Region and Optimal Point

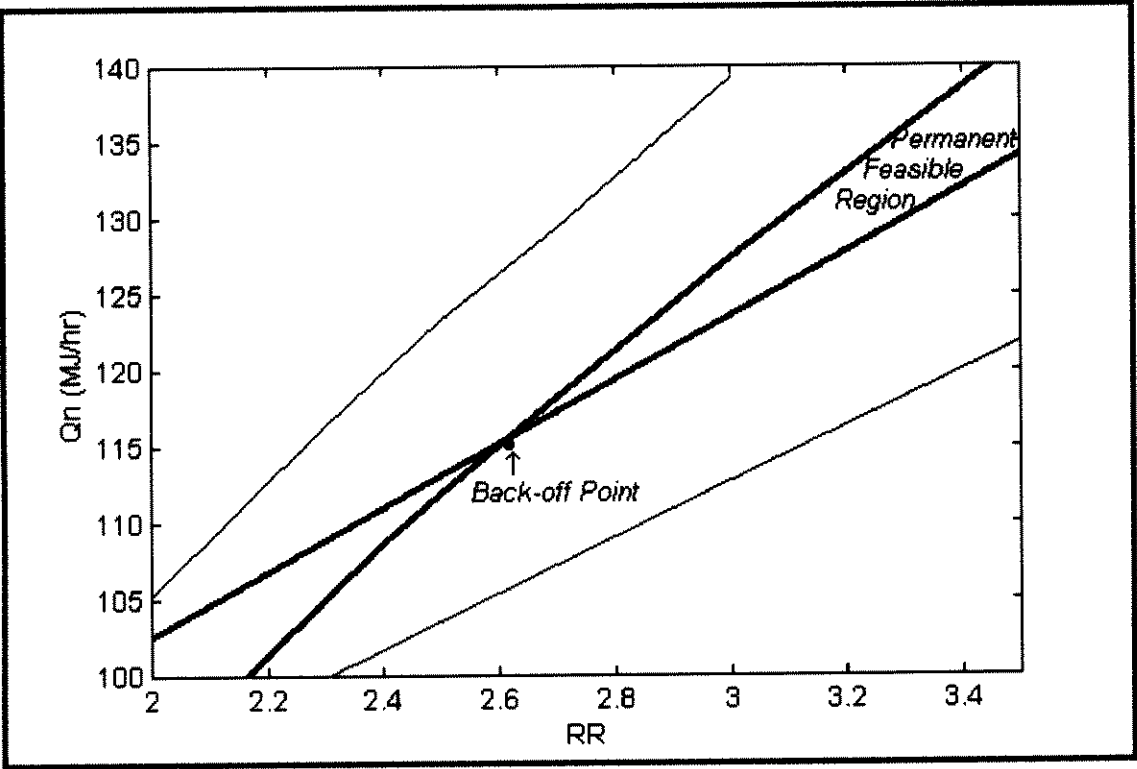


Figure 6.14b Second Case: Permanent Feasible Region and Back-Off Point

	First Steady State	Second Steady State
Reflux Ratio	3.68	2.6
Reboiler Duty(MJ.hr ⁻¹)	64	115

Table 6.2 Back-Off Conditions

The above conditions are used for the column start-up problem, in which the feed flowrate increases from 1 to 2 l.min⁻¹ and ethanol composition in the feed changes from 18 to 20 (w%).

3.5. Switching Problem Using Sequential Optimization Technique

The column is operated with the following control strategy:

- Adjusting the base product (VB) controls the level of the reboiler (H_{reb}).
- Adjusting simultaneously the distillate (VD) and reflux (VL) controls the reflux ratio (RR) and indirectly the level of the condenser.

The start-up problem searches for three optimal trajectories of the feed to the column, the reflux ratio, and the reboiler duty. The feed flowrate increases from 1 to 2 l.min⁻¹, the reflux ratio goes down from 3.7 to 2.6 and the reboiler duty goes up from 64 to 110 MJ.hr⁻¹. The objective function for the start-up problem is:

$$F = \int_{t_i}^{t_f} \{w_f (VFL_{in} - VFL_{sf})^2 + w_d (VD_{in} - VD_{sf})^2 + w_l (VL_{in} - VL_{sf})^2\} dt \quad (6.50)$$

The switching policy aims to keep the composition of ethanol in the distillate above 0.69 (mole fraction or 85 w%) and in the base product under 0.028 (mole fraction or 6.9 w%). It is much more complicated to solve the distillation than the reactor problem. If a series of steps is used to approximate the optimal trajectories, additional constraints are posed to avoid the discontinuity of the integration and help the convergence of the highly nonlinear problem (Vu et al., 1998). For instance, the

following constraint indicates the size of a step change can be made for the feed flowrate.

$$FL(k+1) - FL(k) \leq 0.3 \text{ (in molar flowrate)}$$

$$FL(k) - FL(k+1) \leq 0.05$$

Constraint 8

This constraint does not really represent the limitation of the feed valve but it is required for the solver in SPEEDUP and the optimizer, while iterating within bounds. However, a series of ramps replacing fine steps can avoid the problem of discontinuity during the integration. Column responses, as a result, are smooth and continuous curves. Solving for three start-up policies simultaneously is a time consuming task, especially using the sequential optimization technique. Profiles of reflux ratio and reboiler duty are thus assumed to be sets of equally increased steps. The problem is solved first for the feed policy. The feed profile is approximated by a series of ramps. The value at the end of each ramp is a decision variable selected by the solver. The feed profile found is then applied to the problem; the reboiler duty policy is solved next, and finally the reflux ratio policy. Since the transition time is quite fast and values of the gaps between two ends are small, there is not much difference between profiles obtained from solving the problem simultaneously or sequentially. However, the column responses are very much different, if ramp profiles are used instead of step profiles. Since the DCS system used can not automatically change the set point, to test the feasibility of the solution found, the policies found are manually fed back to the DCS as set points.

In the following figures, the green color represents the case, in which the feed policy is a ramp profile, while other two profiles are approximated by sets of steps. The red color is used when both feed and reboiler duty policies are ramp profiles. The blue color is used when feed, reboiler duty and reflux policies are all approximated by series of ramps. Yellow asterisks show data points collected from the plant. Figure 6.15 presents feed and reboiler duty policies. The reflux ratio policy is not shown because it linearly decreases. The biggest discrepancy between simulation and experimental results is due to the uncertainty in the conversion of steam rate to energy. The ABB MOD 300 DCS records data at 30-second intervals. Values of steam rates provided from the DCS are converted to energy ($\text{MJ}\cdot\text{hr}^{-1}$) by a factor of 96. These are shown as

yellow asterisks in Figure 6.15b. Distillate and reflux profiles are found in Figure 6.16. As discussed above, ramp policies avoid the discontinuity problem during the integration (smooth and continuous blue responses compared to red and green responses). Ethanol compositions in the distillate, base product, feed and in some trays are recorded but the analyzer can take only one sample at a time. Hence, it takes more than 10 minutes to update composition information, and any change during that period can not be recognized. Temperature profiles at the 4th and 13th trays are shown instead of composition profiles in Figure 6.17. Temperatures of the 4th tray are very well predicted so they will be used to infer compositions later. A larger discrepancy between plant data and simulation results is found in temperatures of the 13th tray. Temperatures of the last tray of the column are very sensitive to reboiler duties. A small error in the conversion of steam rate to energy might create a large error in the temperature prediction.

It is assumed that the transition is fast and the switchability problem is solved for the case $x_{mf} = 18$ (w% ethanol). However, if the feed composition increases from 18 to 20 (w% ethanol) during the transition, the policies found will violate constraint 2. Under the mathematical viewpoint, the problem should be solved again for two identical columns. One column is fed with 18 (w% ethanol); the other has the feed composition increasing from 18 to 20 (w% ethanol) during the transition. Under the engineering application viewpoint, this violation is acceptable because it is smaller than the accuracy of the sensor. Figure 6.18 shows composition violation of the base product, if the feed composition changes.

In addition to the fixed reflux ratio and controlled reboiler level, the temperature of tray 13 is also controlled to infer the composition of ethanol in the base product. This control loop is selected for investigation because the steam rate will be automatically adjusted to satisfy the condition of the base product without upsetting the column too much. This can avoid the task of matching the steam rate used in the plant with the value given by the simulation. This might also avoid the task of solving the dynamic open loop back-off problem for the column as discussed in the previous paragraph. The feed policy in this case is shorter, and the switching time is faster. However, with two active control loops the response of the reboiler level is more aggressive. Figure 6.19 shows the feed and reboiler level profiles of two cases, in which x_B is not controlled (green curves) or controlled (red curves).

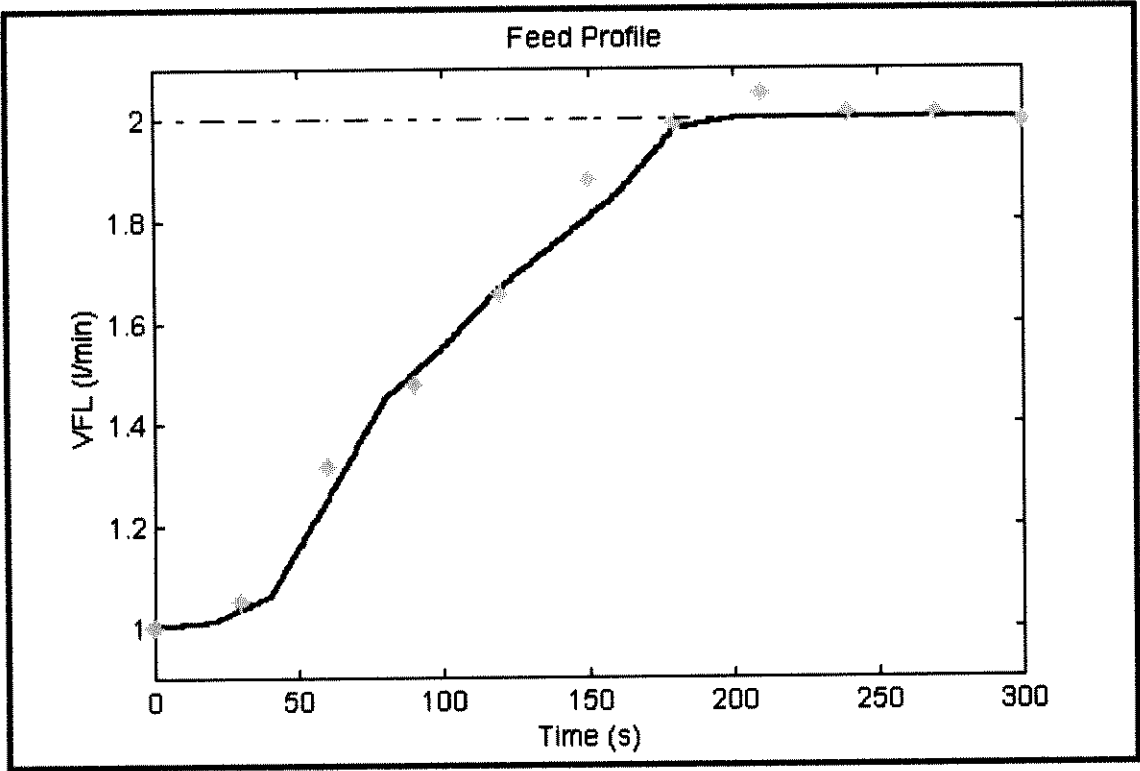


Figure 6.15a Optimal Feed Profile

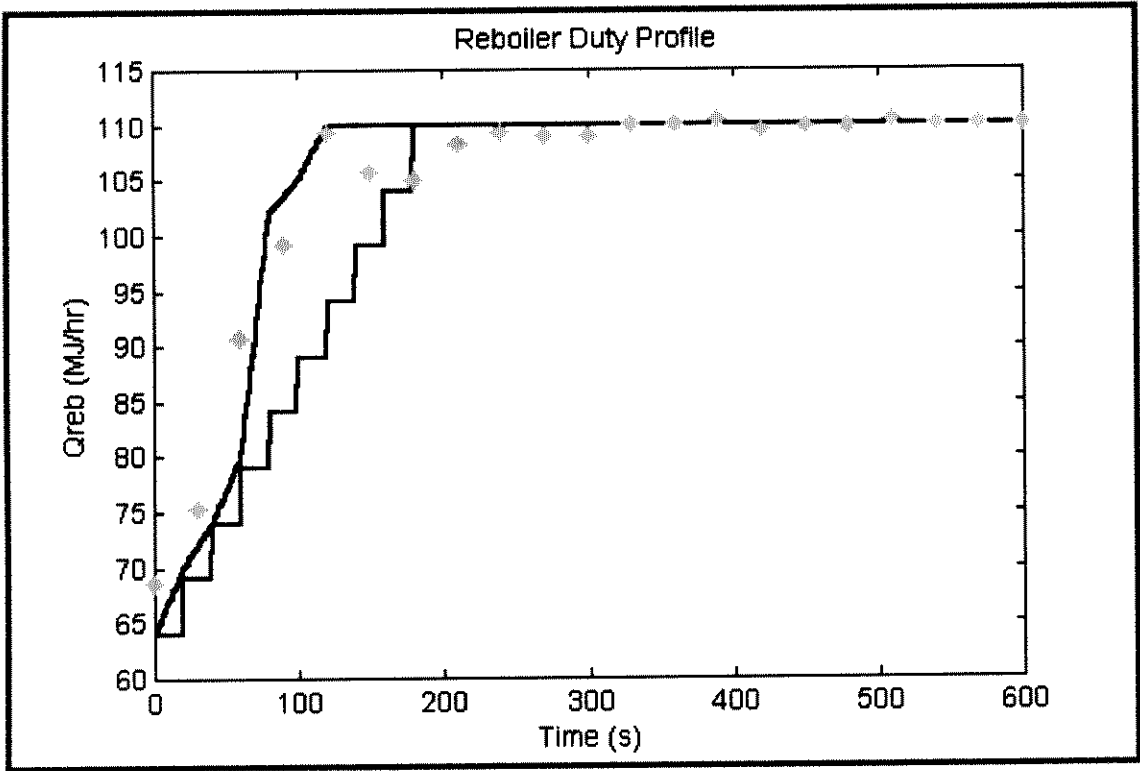


Figure 6.15b Reboiler Duty Profile

(Blue: Ramp policy; Green: Step policy)
(Yellow: Plant data)

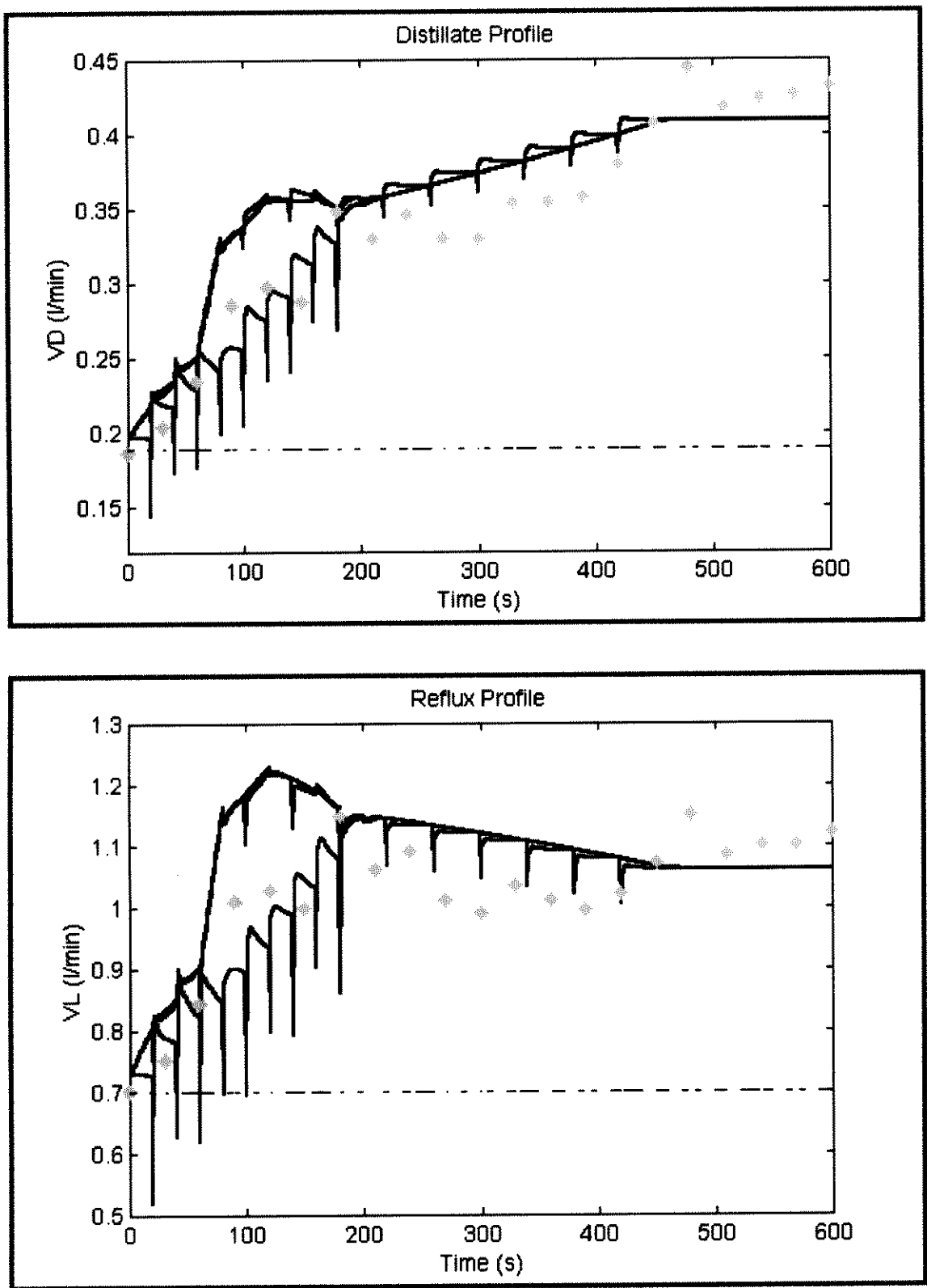


Figure 6.16 Distillate and Reflux Profiles

(Green: Response to feed ramp policy, reboiler duty and reflux ratio step policies)

(Red: Response to feed and reboiler duty ramp policies, and reflux ratio step policy)

(Blue: Response to feed, reboiler duty and reflux ratio ramp policies)

(Yellow: Plant data)

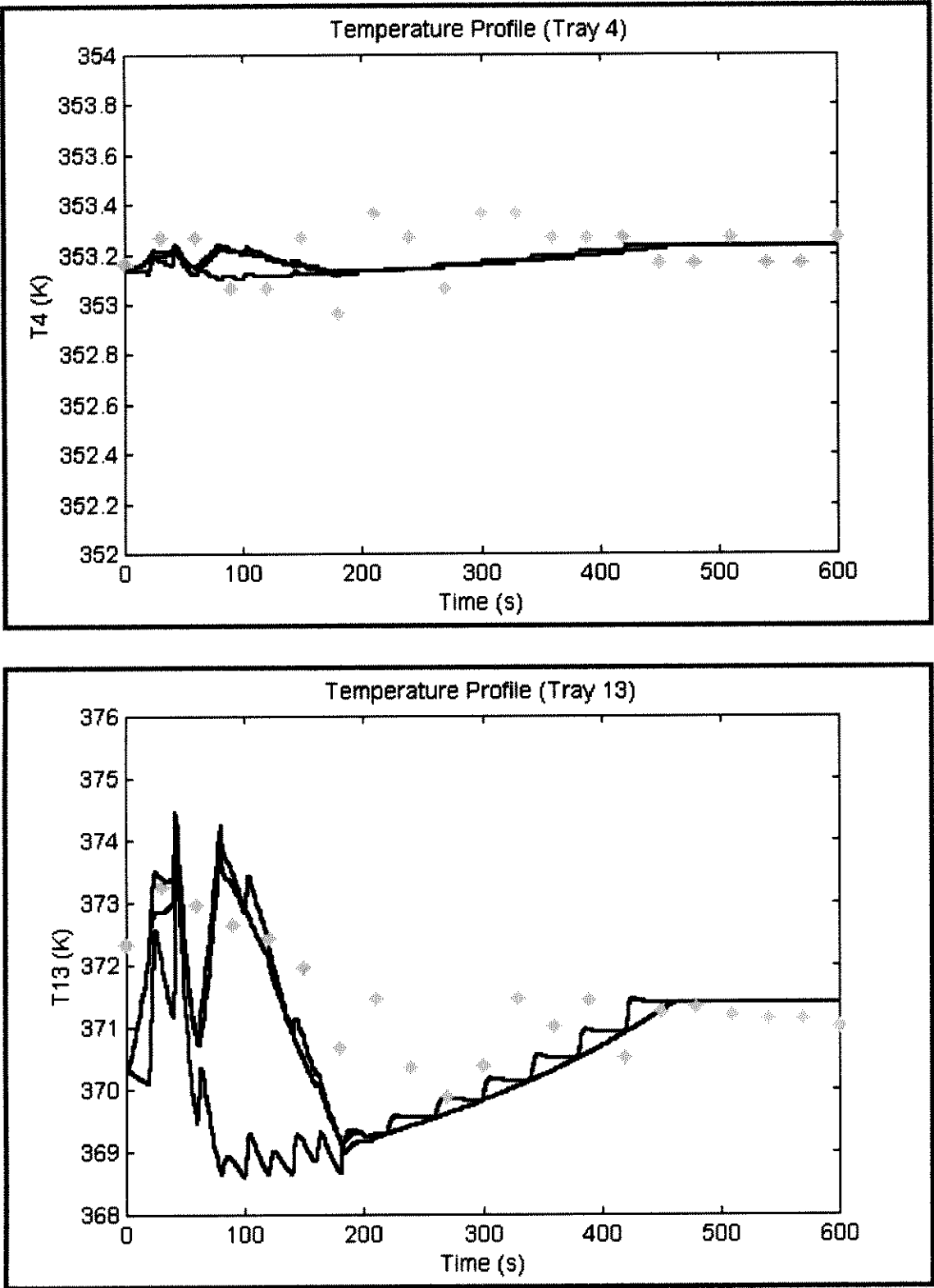


Figure 6.17 Profiles of Temperatures at Tray 4 and Tray 13

- (Green: Response to feed ramp policy, reboiler duty and reflux ratio step policies)
- (Red: Response to feed and reboiler duty ramp policies, and reflux ratio step policy)
- (Blue: Response to feed, reboiler duty and reflux ratio ramp policies)
- (Yellow: Plant data)

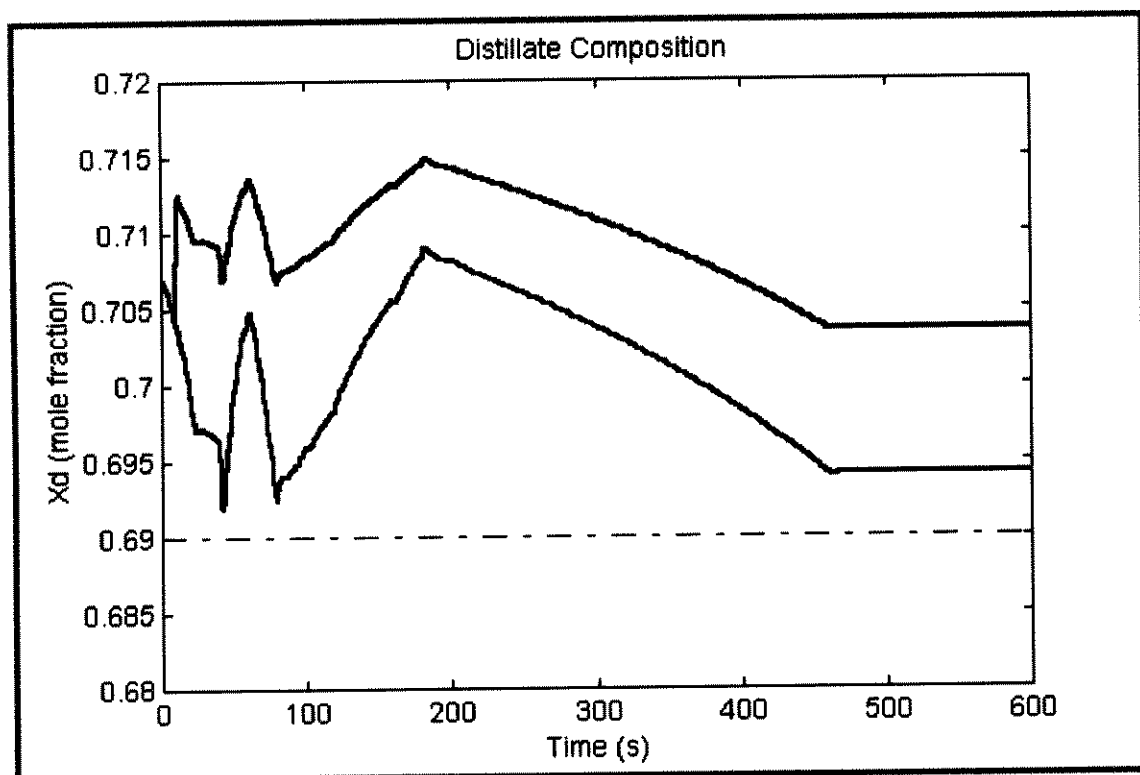


Figure 6.18a Composition Profile of Ethanol in Distillate

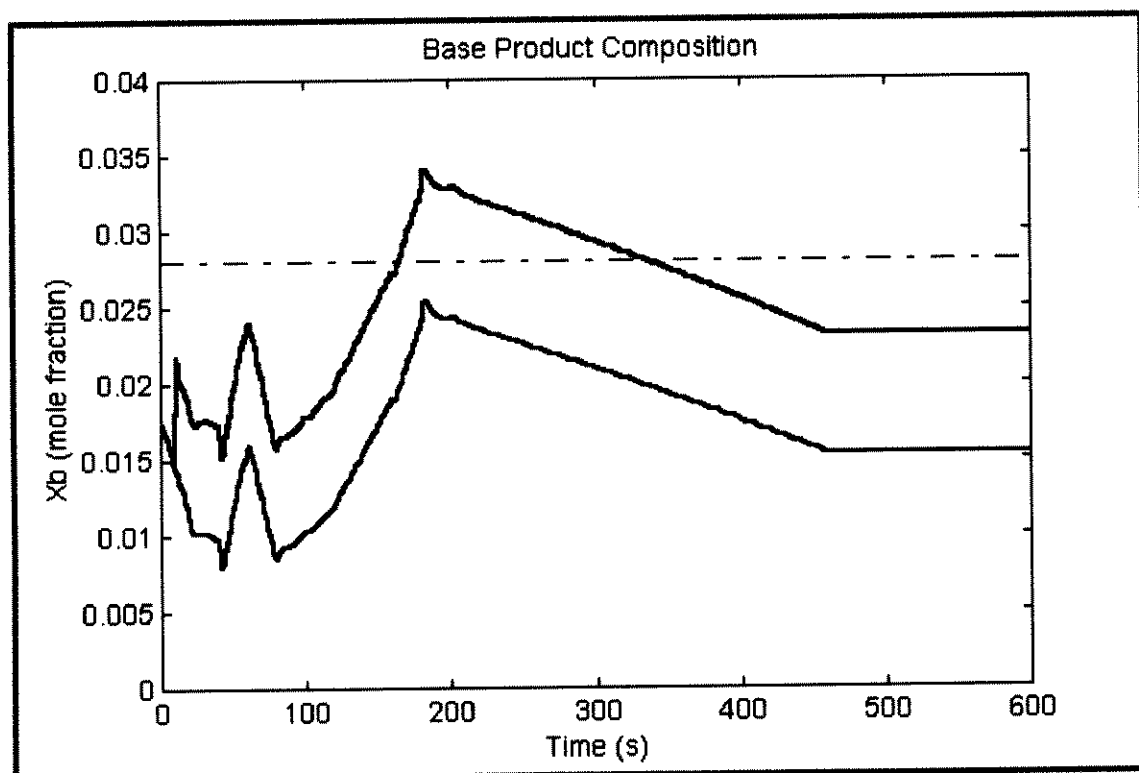


Figure 6.18b Composition Profile of Ethanol in Base Product

(Green: $x_{mf} = 18$ w%)

(Red: $x_{mf} = 18 \rightarrow 20$ w%)

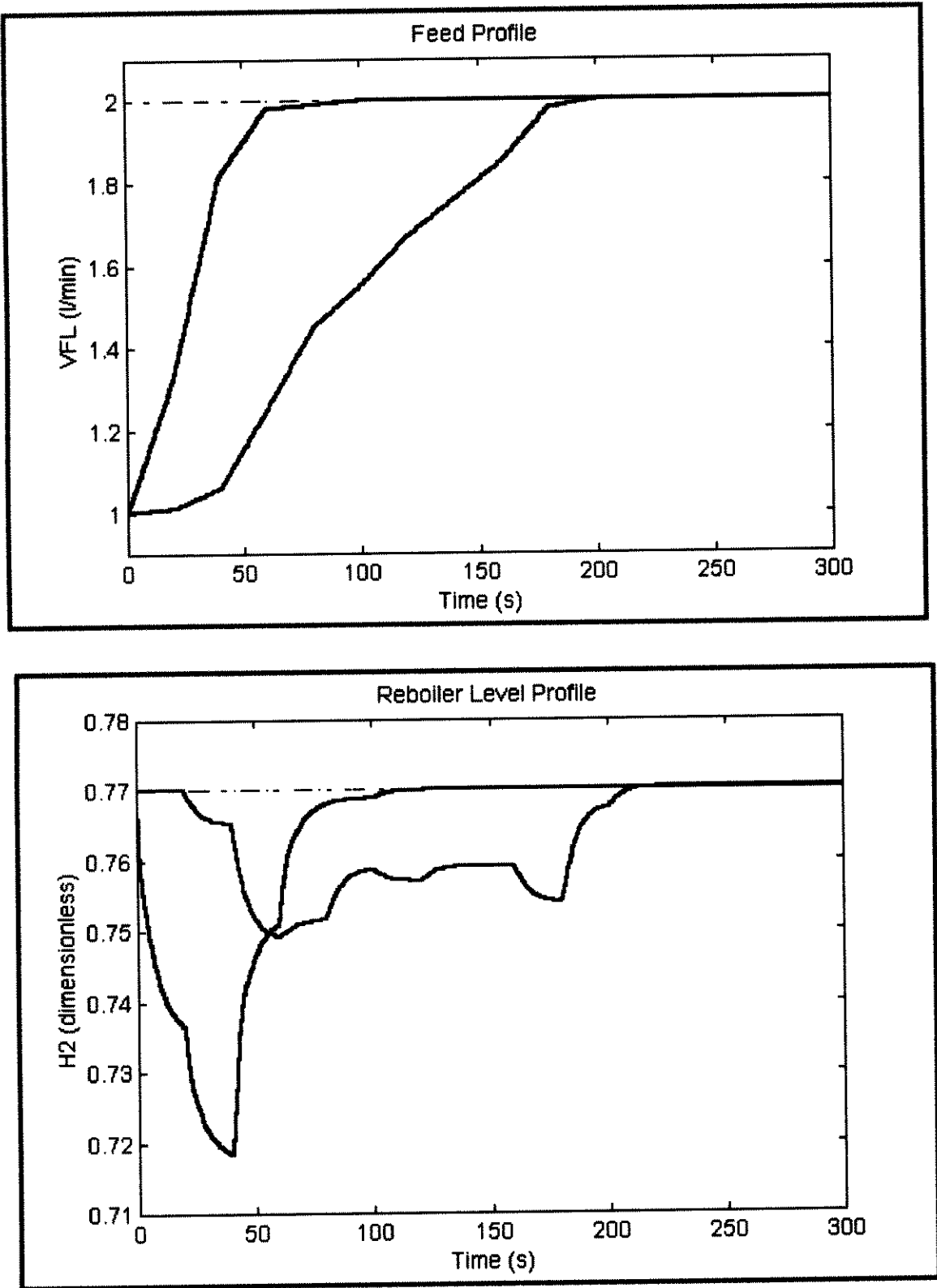


Figure 6.19 Feed and Reboiler Level Profiles

(Green: X_B is not controlled)

(Red: X_B is controlled)

Finally, the temperature of the 4th tray (T_4) is controlled to infer the composition of ethanol in the distillate. The reflux ratio is used instead of the reflux rate as the manipulated variable. T_4 is selected as the controlled variable, since it is more stable and predictable than T_2 . Figures 6.20 and 6.21 present compositions and corresponding controlled temperatures for three cases:

1. Green curves show $x_F = 18\%$.
2. Red curves show $x_F = 18\% \rightarrow 20\%$.
3. Blue curves show $x_F = 18\% \rightarrow 16\%$.

These curves are simulation results. In the real plant, the control scheme with three control loops is not realizable due to the problem of interaction and large time delay. Since the temperature controllers are cascade loops, the effect of lagging on plant responses is a very important element. Introducing a small time delay can create more oscillation in the outputs. An example of this feature is shown in Figure 6.22. The graph plots temperature responses of the 13th tray with time delay (red) and without dead time (green). Responses of the corresponding manipulated variables are plotted in the same figure.

The control performance and stability of the column are strongly influenced by interaction. The manipulated variables, which are reboiler duty and reflux ratio, affect both compositions of ethanol in the distillate and base product. The control strategy with the base level and both temperature-loops being closed is not successful, because too much oscillation in responses of manipulated variables damage the stability of the column.

In conclusion, the graphs on pages 6.39, 6.40 give a general view of controllability and switchability analysis of the column. Data points are collected from the plant for 150 minutes. The feed rate increases from 1 to 2 l.min⁻¹. Two control loops are active. The base level is kept at 68% of the total volume of the reboiler. The set point temperature of tray 13th is 99 °C. Figure 6.23 on page 6.39 plots feed and distillate rates. Figure 6.24 shows the controlled temperature of the 13th tray and the steam rate (manipulated variable).

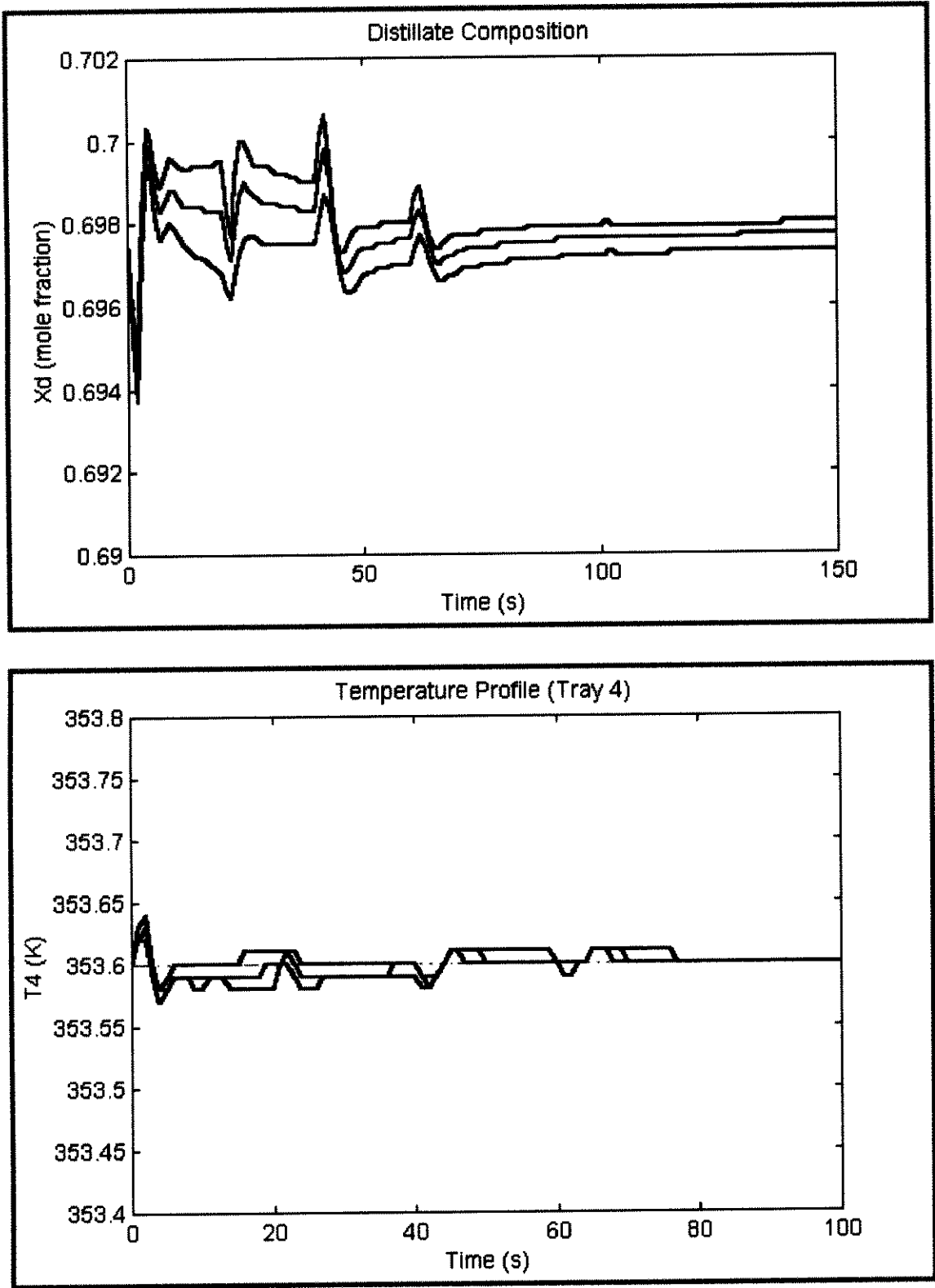


Figure 6.20 Ethanol Composition and Inferential Variable Profiles (Tray 4)

(Green curves: $x_F = 18\%$)
(Red curves: $x_F = 18\% \rightarrow 20\%$)
(Blue curves: $x_F = 18\% \rightarrow 16\%$)

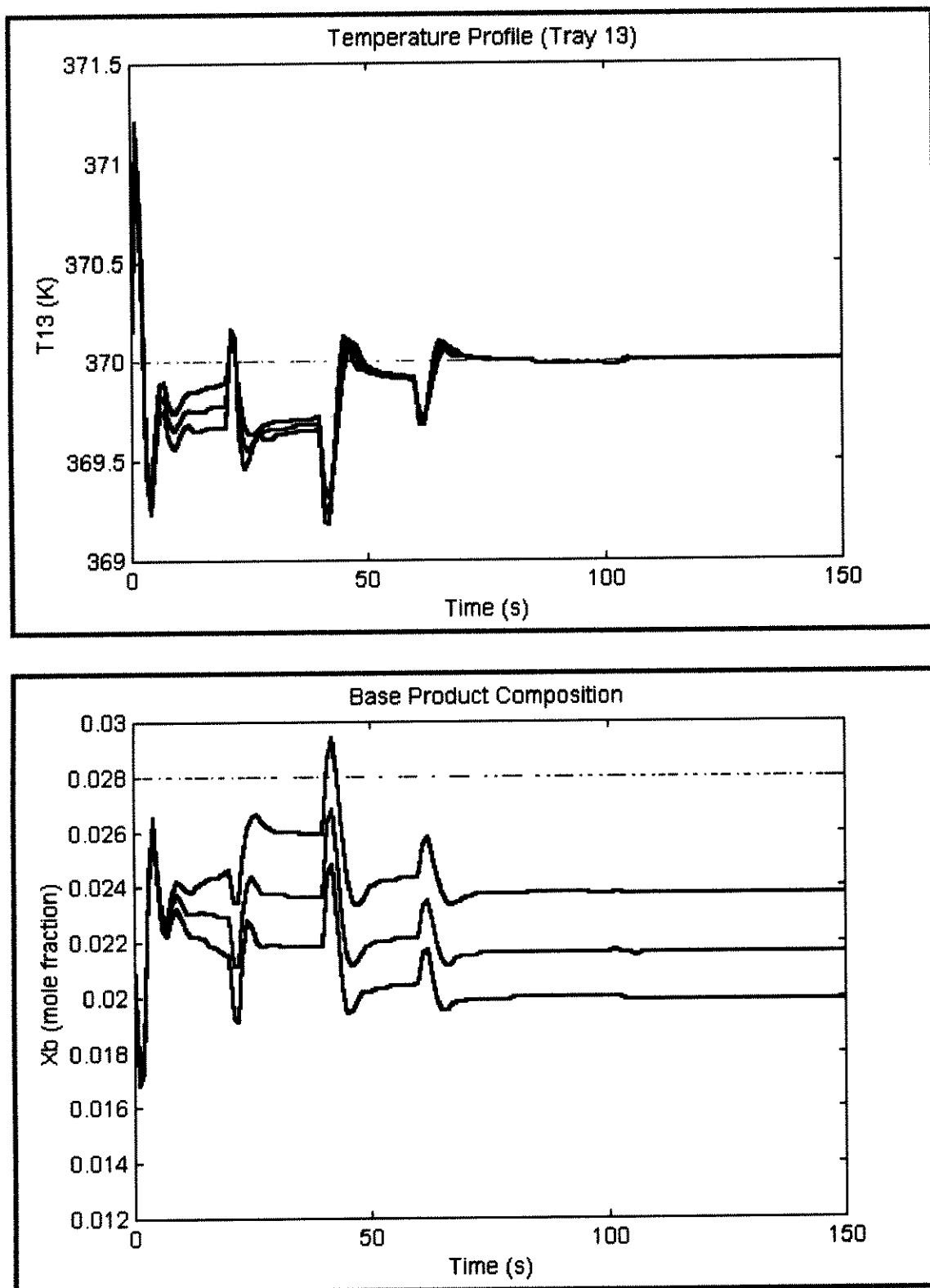


Figure 6.21 Ethanol Composition and Inferential Variable Profiles (Tray 13)

(Green curves: $x_F = 18\%$)

(Red curves: $x_F = 18\% \rightarrow 20\%$)

(Blue curves: $x_F = 18\% \rightarrow 16\%$)

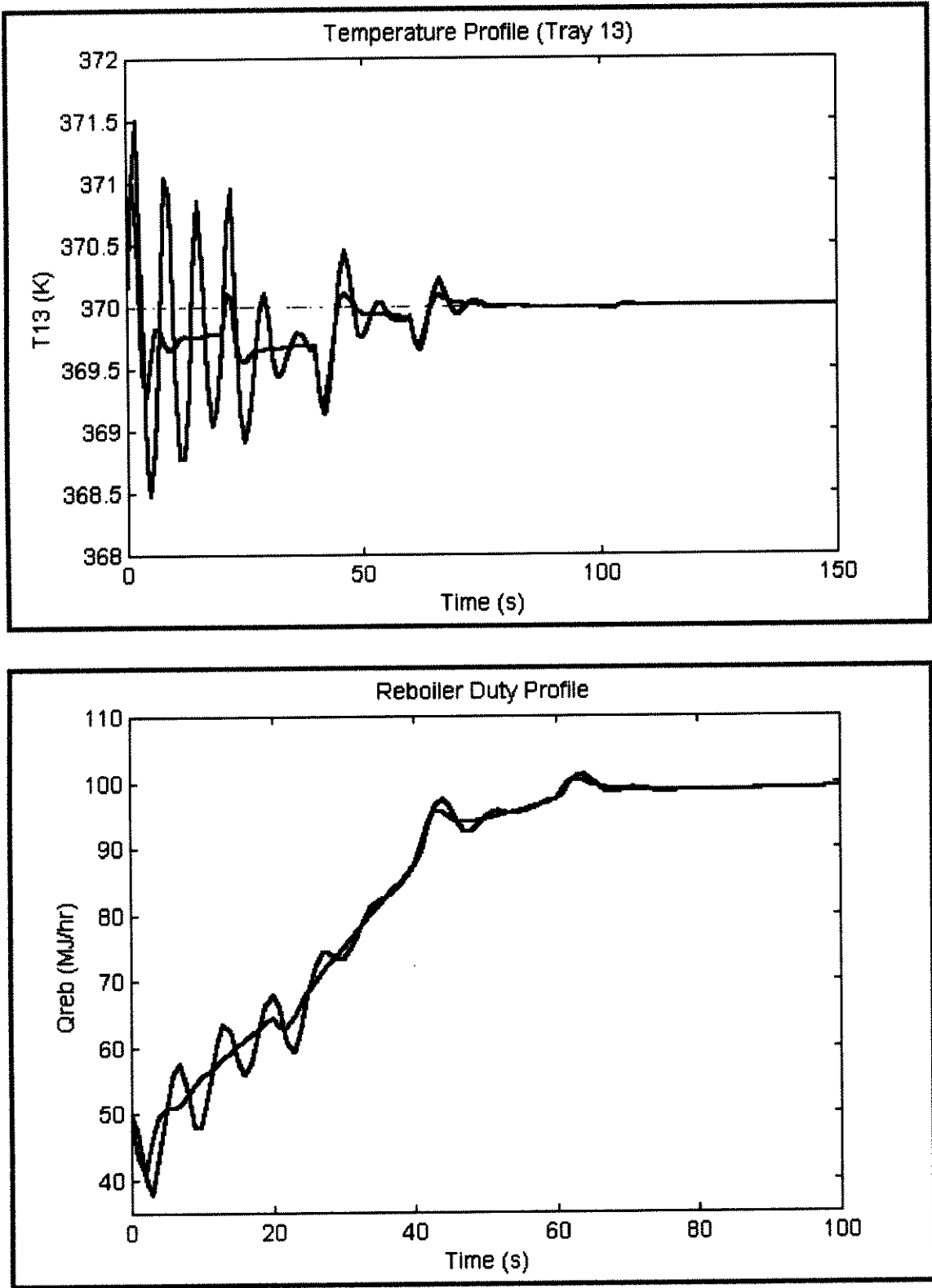


Figure 6.22 Profiles of Temperature (Tray 13) and Reboiler Duty
(Green curves: Without time delay)
(Red curves: With time delay)

Figures 6.23 and 6.24 show that the column is more stable, when operating at the feed rate of 2 l.min^{-1} than at the lower feed rate (1 l.min^{-1}). In other words, the ranges of oscillation of all variables (temperature, distillate, steam, etc) are smaller at the higher feed rate. These figures also prove the necessity of including time delays in operating and controlling the column. The effect of dead time sometimes is so large that the conventional controller (P, PI and PID) cannot handle. The possibility of using DMC instead of PID to control the temperature of the 13th tray is under investigation. At the design stage, as on-line measurements are not available, the model is assumed to be perfect. Responses of controlled and manipulated variables are obtained from simulations. Figures 6.25 plot temperature of the 13th tray (T_{13}) and reboiler duty (Qreb) for three cases:

1. Green curves plot responses of the PI controller without time delay.
2. Red curves plot responses of the PI controller with time delay.
3. Blue curves plot responses of DMC.

As discussed in Chapter 4, DMC does not offer a significant advantage over a well-tune PI in SISO control problems. However, under the effect of dead time, especially in this case the time delay is a result of the cascade loop, DMC gives a better control performance. A step change in the steam rate is introduced to the column. The step response of temperature at the 13th tray is measured. The dynamic coefficient matrix (A) is then constructed, based on the response curve. Matrix A is not constant, since the switching problem deals with feed rate change. It is not necessary to update A during the transition, if it is constructed at the feed rate of 2 l.min^{-1} , due to the short switching time. The selection of adjustable parameters such as prediction horizon V, control horizon U, weighting factor qq and ww can improve the DMC performance. DMC can also replace PID in controlling the temperature of the 4th tray. These tasks are left for the project "DMC implementation in UNAC system", which will be carried out in the department soon.

The last application is the distillation column dealing with multicomponent separation at the back end of the olefin plant. The column capacity, production rate, feed impurity and component names are changed as requested by Orica to protect confidential information.

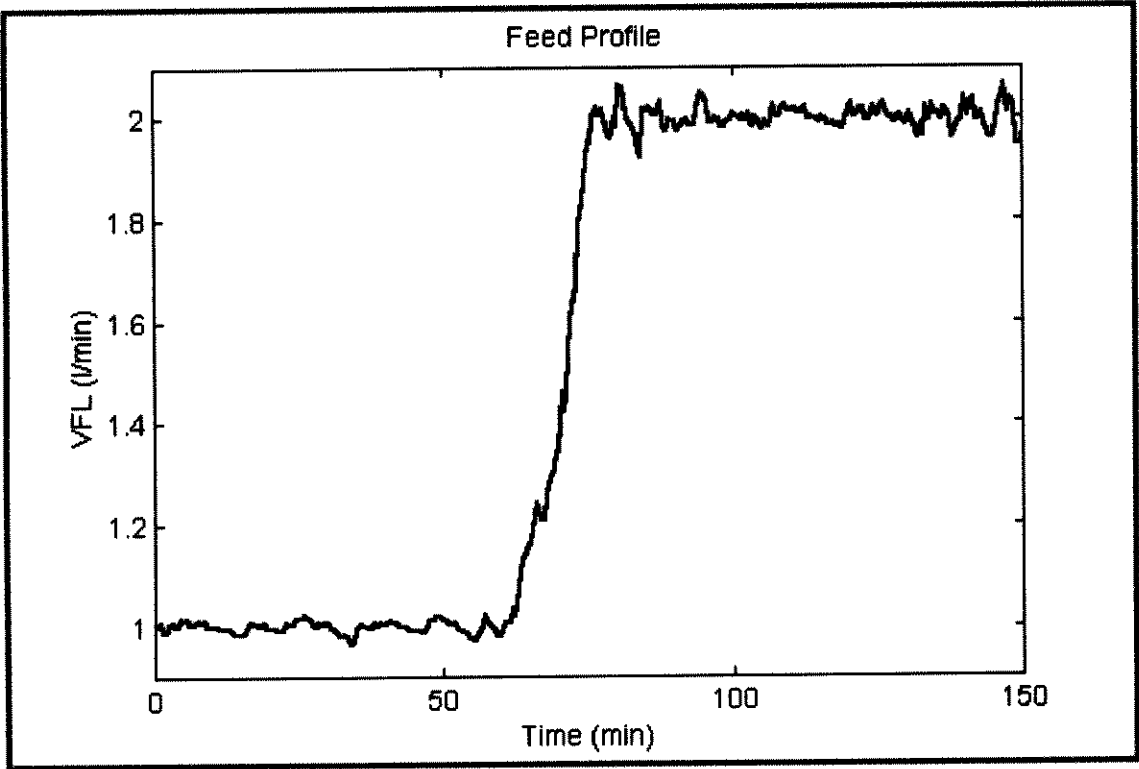


Figure 6.23a **Feed Profile** (Data collected from the plant)

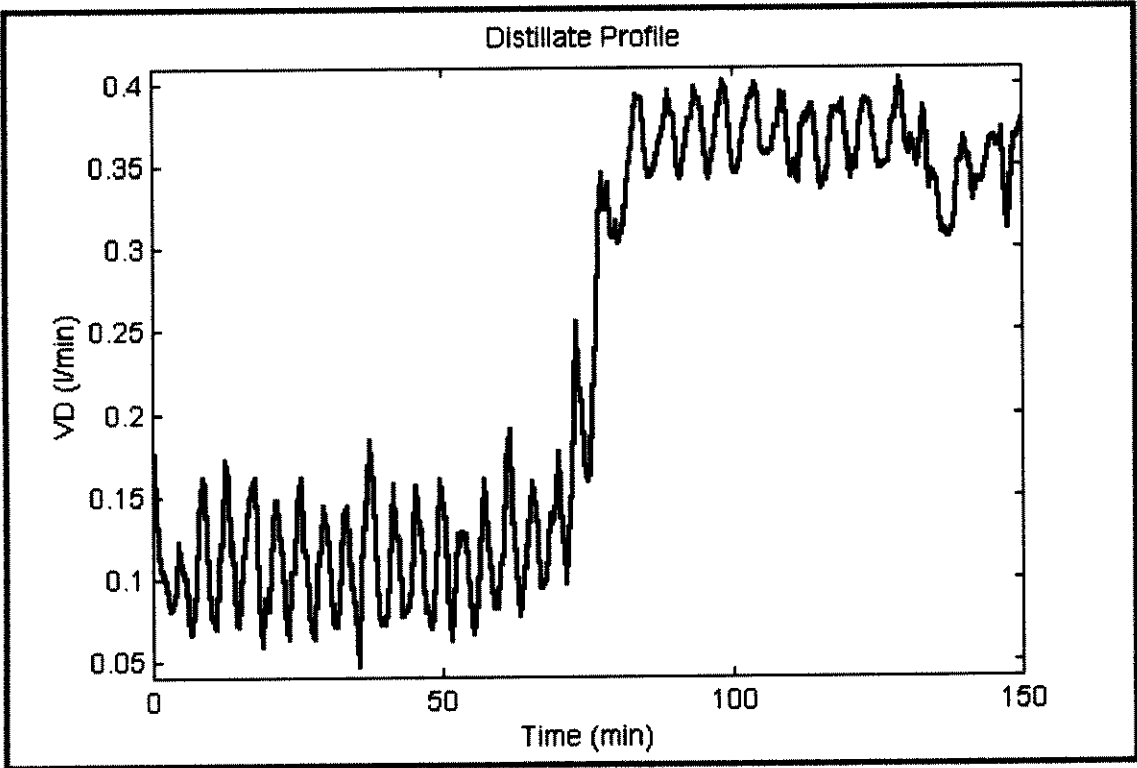


Figure 6.23b **Distillate Profile** (Data collected from the plant)

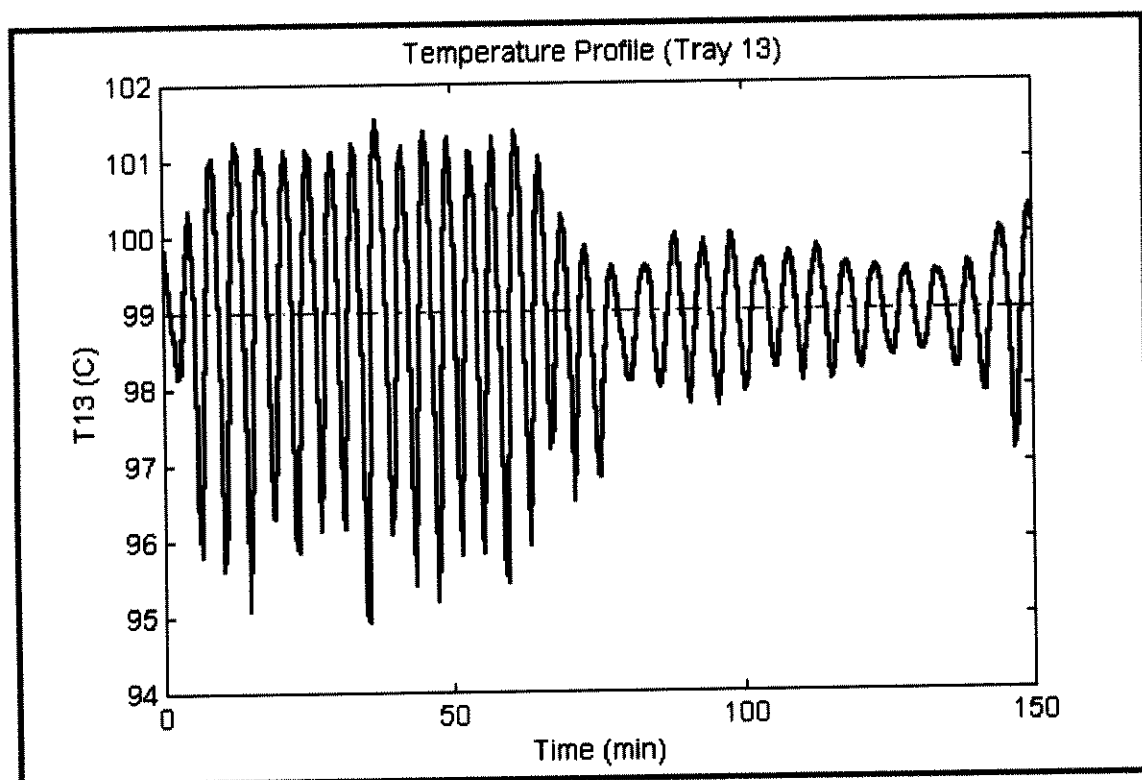


Figure 6.24a Controlled Temperature (T_{13}) Profile (Data collected from the plant)

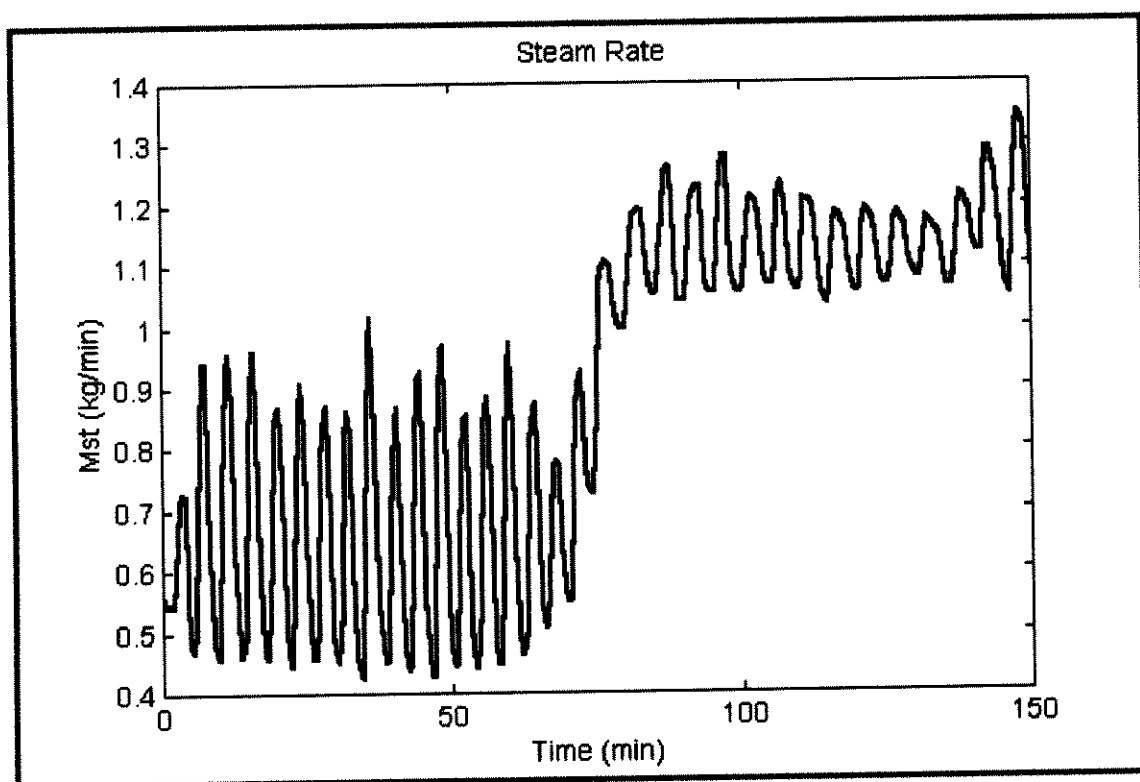


Figure 6.24b Steam Rate Profile (Data collected from the plant)

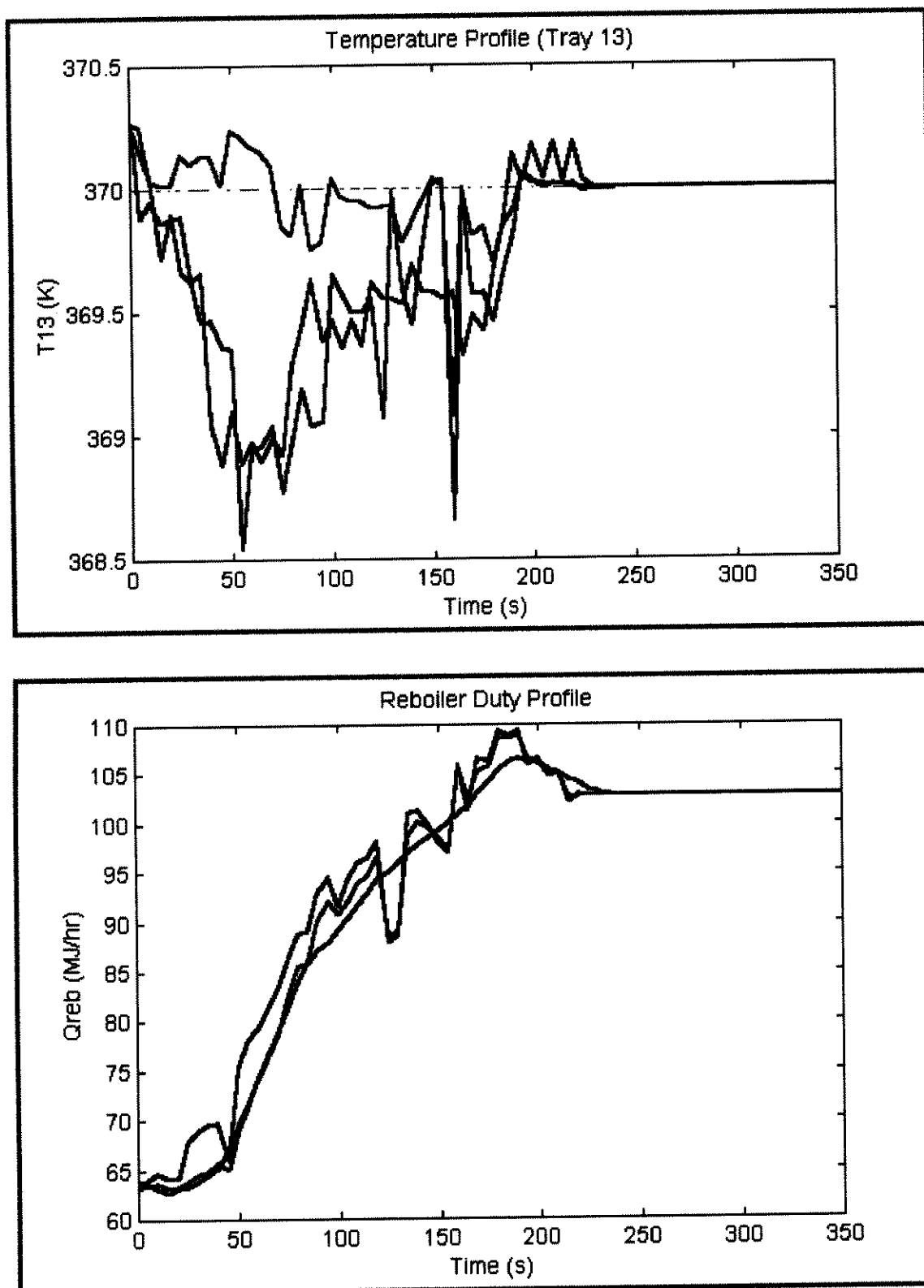


Figure 6.25 Profiles of Temperature (Tray 13) and Reboiler Duty
 (Green curves: PI controller without time delay)
 (Red curves: PI controller with time delay)
 (Blue curves: DMC)

4. Application 3: Multicomponent Distillation Column

4.1. Plant Description

Orica (Australia) has identified the energy consumed by distillation columns in the plant as a major cost. This application investigates the operation of the purification column at the back-end of the plant. The aim is to achieve the best performance of the distillation unit that is maximizing the high-grade product olefin oxide (HO) with the minimum energy required.

The purification column separates olefin oxide (EO) from aldehyde E (EA) and aldehyde M (MA) to produce the high-grade olefin oxide (HO) from the upper side stream. Manipulating the distillate bleeding rate controls the concentration of MA in this stream, to prevent the formation of solid para-aldehyde, which might result in tray obstructions and line and instrument blockages. The removal of the base product has a lower limit to ensure the pump working with an adequate flow. The normal grade olefin oxide (NO) from the distillate and the base streams is used in the manufacture of glycols and glycol ethers.

Since the aldehyde species are present only in trace quantities, pressure drops and temperature differences between trays are very small. The column pressure is controlled by throttling the cooling water flow.

The column has 85 trays with the upper liquid side stream off tray 10, and the feed entering the column at tray 69. Current geometrical data of the column, two total condensers, the reflux drum and two reboilers are used for liquid holdup calculations. The vapor holdup in the column is neglected. The liquid holdup in other compartments, except the reboilers and the reflux drum is assumed to be constant.

The column has two liquid level control loops. Manipulating the reflux rate controls the level of the reflux drum. Adjusting the upper side stream rate controls the base level.

Figure 6.26 shows the diagram of the purification column.

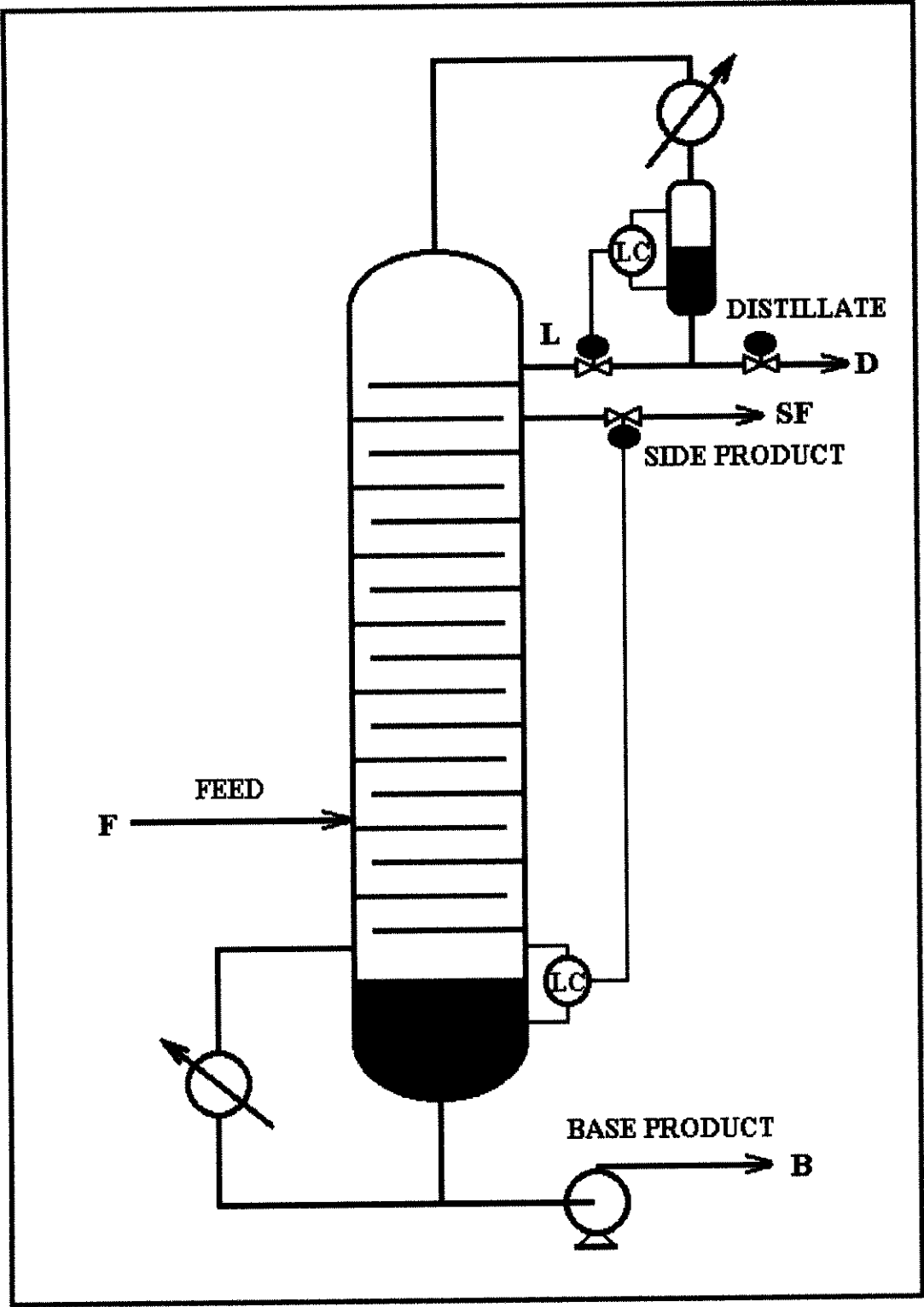


Figure 6.26 Plant 3: Purification Column

4.2. Steady State ASPEN Model

The rigorous model for this industrial column distillation was developed in ASPEN. Some specifications for the model development include:

- ❖ The methods and models to calculate physical properties are defined by the RK-SOAVE system option. This option set uses Redlich-Kwong-Soave cubic equation of state for all thermodynamic properties except the liquid molar volume.
- ❖ The pressure set point at the top of the column is kept at 364 kPa. The pressure drop through the column is 60 kPa.

The following table compares results collected from the plant and laboratory analysis with results predicted by ASPEN model.

	Measured	Calculated
Temperature at the top (°C)	48.0	47.6
Temperature at the base (°C)	53.0	52.7
Composition		
<u>Stream D</u>		
MA (ppm)	117	113
EA (ppm)	0.30	0.39
<u>Stream SP</u>		
MA (ppm)	2.3	2.0
EA (ppm)	8.2	7.0
<u>Stream Mixed (=B+D)</u>		
MA (ppm)	31	32
EA (ppm)	1291	1330

Table 6.3 Simulation Result Compared to Laboratory Analysis

The above analysis is carried out at the operating condition:

Feed (ton/day): **F = 116**

Distillate Feed (ton/day): **D = 10.8**

Side Product Feed (ton/day): **SP = 78**

Reflux Ratio: **RR = 30**

Feed composition (ppm): **MA = 12, EA = 442**

ASPEN model gives well predicted result compared to the laboratory analysis. Due to the uncertainty in the conversion of steam rate to energy, as in the binary distillation column, the reflux rate is specified in the model instead of the reboiler duty. Meanwhile, in the plant the rate of steam, which supplies heat to the reboiler, is fixed. The reboiler duty predicted by the model is 177 GJ/day, equivalent to 64.7 ton/day of 35-psig steam. The efficiency of steam usage (defined as ratio of real over theory values) is about 87%. More than 10% of consumed energy is waste due to heat lost and uncondensed steam in the heat exchanger.

The purity of the high-grade olefin oxide (HO) is sensitive to the reboiler duty. With the current column specification, ASPEN model predicts that the stream coming from tray 6 contains the least aldehyde. If the predicted reboiler duty is increased by 15%, the highest grade HO can be found in tray 7 or tray 8. In the real plant, the side product is taken from trays 10 or 11.

Since this column deals with high purity products, the rigorous model will be used to find the feasible operating region of the column.

4.3. Steady-State Open Loop Back-Off Calculation Using ASPEN Model

Constraints on the distillation unit are identified before solving the nominal optimal conditions. Four constraints are introduced.

1. To prevent the formation of solid para-aldehyde that might result in tray obstructions and line and instrument blockages, the composition of MA in the distillate must be less than 190 ppm.
2. The product specification requires the total composition of total aldehyde in the side product stream less than 40 ppm.

3. The mixed stream of distillate and base product is the feed of the downstream plant. The feed specification requires the composition of EA in the mixed stream less than 2000 ppm.
4. The removal of the base product has a lower limit to ensure the pump working with an adequate flow.

$$MA_D \leq 190 \text{ ppm}$$

$$MA_{SP} + EA_{SP} \leq 40 \text{ ppm}$$

$$EA_D + EA_B \leq 2000 \text{ or } EA_B \leq 2000 \text{ ppm}$$

$$B \geq 12 \text{ ton/day}$$

Uncertainties at the moment might be found in the feed flowrate and the impurities of the feed.

	Lower Bound	Nominal Value	Upper Bound
<i>Feed (ton/day)</i>	110	116	121
<i>MA_F (ppm)</i>	10	12	20
<i>EA_F (ppm)</i>	400	442	480

The goal is maximizing the production of high-grade olefin oxide (HO) by adjusting the distillate, the upper side stream and the reboiler duty. The nominal optimal operating conditions are:

Objective Value (1 st decision variable):	SP = 85.6 ton/day
Distillate rate (2 nd decision variable):	D = 6.3 ton/day
Reboiler duty (3 rd decision variable):	Q_{reb} = 157 GJ/day

Constraints 1, 2 and 3 are active. The nominal operating point is located at the intersection of three surfaces representing three active constraints. Due to uncertainties, the original optimum will cause constraint violations, when the feed flow rate and the impurities tend upwards. Therefore, the steady state open loop back-off problem must be solved for the back-off operating conditions. The flowsheet and results of the final iteration is shown in Chapter 5 (on page 5.9). In that example, distillate and side product rates are decision variables, and the reboiler duty is one of the uncertain parameters. The same problem is solved in this section but the reboiler duty is included

as the third decision variable. Thus the nominal problem is fully constrained, as the number of active constraints is equal to the number of decision variables. The feasible solution found in the second iteration, which involves three identical columns. Each column is subject to a different row of the uncertainty matrix.

$$d^n = \begin{vmatrix} F(\text{ton/day}) & MA(\text{ppm}) & EA(\text{ppm}) \\ 116 & 12 & 442 \\ 122 & 20 & 480 \\ 110 & 10 & 400 \end{vmatrix}$$

As mentioned before, this exercise should be performed using ASPEN model, since the aldehydes are present in trace quantities. Actually, the first two identical columns, which are subject to the first two rows of matrix d^n , guarantee the feasible solution. The third column is just included in the problem to calculate the side product rate, when the feed rate tends downwards. In the plant, the rate of side product (SP) varies because it is adjusted to control the level in the condenser. In the simulation, SP also varies between the upper and lower limits, and the average value of these limits is reported. Table 6.4 shows the differences between nominal and back-off operating conditions. Figure 6.27 presents the flowsheet of the final iteration. The operating regions are plotted in Figures 6.28 and 6.29. Some values used in the plots and reported in the tables are scaled up, as requested by Orica.

Decision Variables	Nominal Optimum	Back-Off	Current Operating
Side Product <i>SP</i> (ton/day)	85.6	77.0 (71.0 – 83.0)	78.0
Distillate <i>D</i> (ton/day)	6.3	11	11
Reboiler Duty <i>Q_{reb}</i> (GJ/day)	157	163	176

Table 6.4 Steady State Open Loop Back-Off Operating Conditions

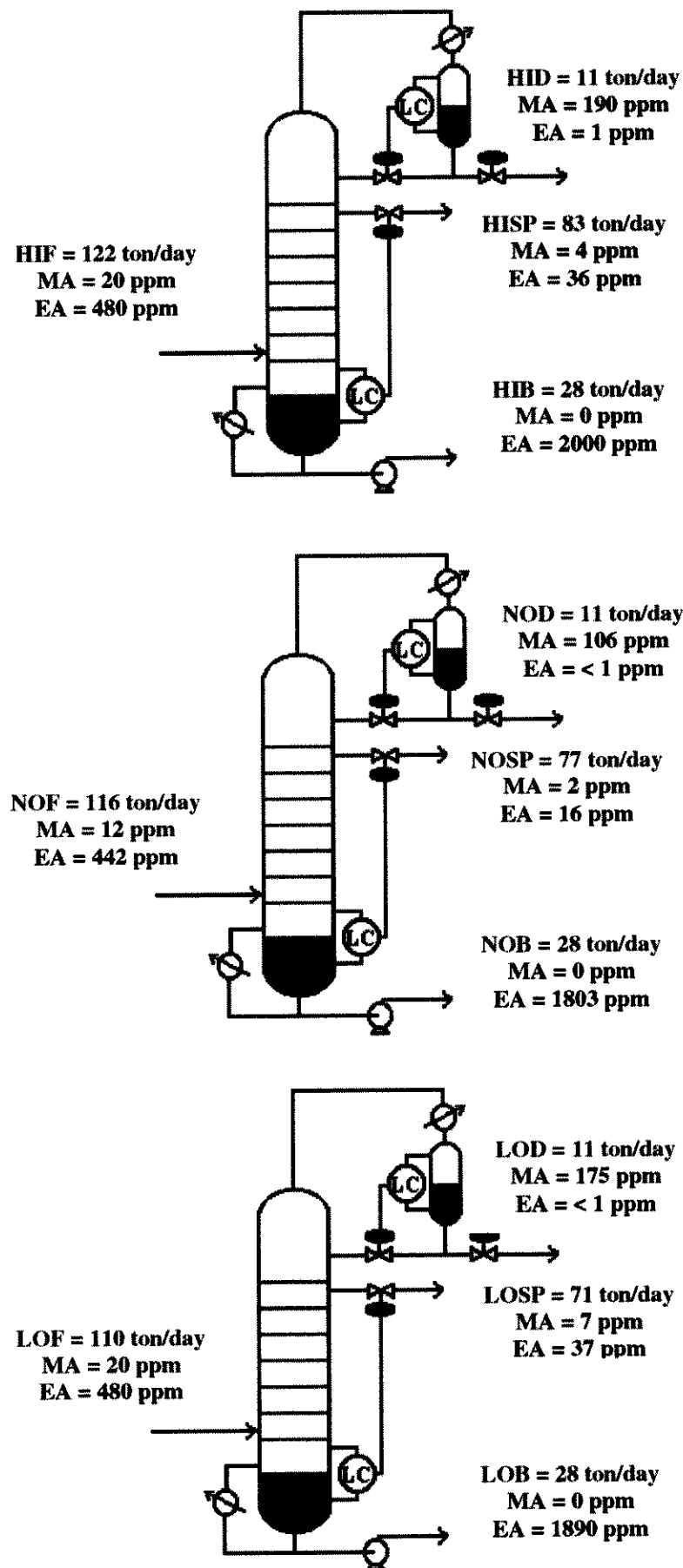


Figure 6.27 The Flowsheet of Purification Column (Last Iteration)

One special characteristic of this separation is that the top tray does not give the highest-grade olefin oxide. The bleeding rate of the top tray controls the composition of MA in the distillate. The higher bleeding rate leads to the purer distillate. The best location (from tray 6 to tray 11), which produces the highest-grade olefin is dependent on the heat supplied to the reboiler. Since the column has only two positions either tray 10 or 11 to withdraw the side product, the heat supplied to the reboiler is 8% higher than predicted (shown in Table 6.4) to maintain the quality of the product within the specification.

Figure 6.28 plots the nominal optimal operating region in decision variable space. The space is bounded by three surfaces representing the active constraints.

- ❖ Green surface plots constraint 1. $MA_D = 190$ ppm.
- ❖ Blue surface plots constraint 2. $MA_{SP} + EA_{SP} = 40$ ppm.
- ❖ Magenta surface plots constraint 3. $EA_B \leq 2000$ ppm.

The intersection point of these surfaces is referred to as the nominal optimum.

If disturbances enter the system, either the feed rate or the impurities in the feed are higher than expected, then the distillate-bleeding rate must be increased. The green surface in Figure 6.28 moves to a new position. The permanent feasible operating space is narrower than the original one. The back-off point shown in the figures moves between two limits. The upper limit is the intersection point of three constraint surfaces.

The rigorous model in ASPEN can predict very well the behavior of the column. Unfortunately, this model cannot be used in the dynamic mode. A compartmental model in SPEEDUP must be used to deal with the dynamic situation.

4.4. Dynamic Problems Using Compartmental Model in SPEEDUP

A rigorous model for distillation columns can be found in SPEEDUP library, but in this case the compartmental model (Lear, 1992) is used to save computational time, if it is necessary to solve the switching problem by sequential technique.

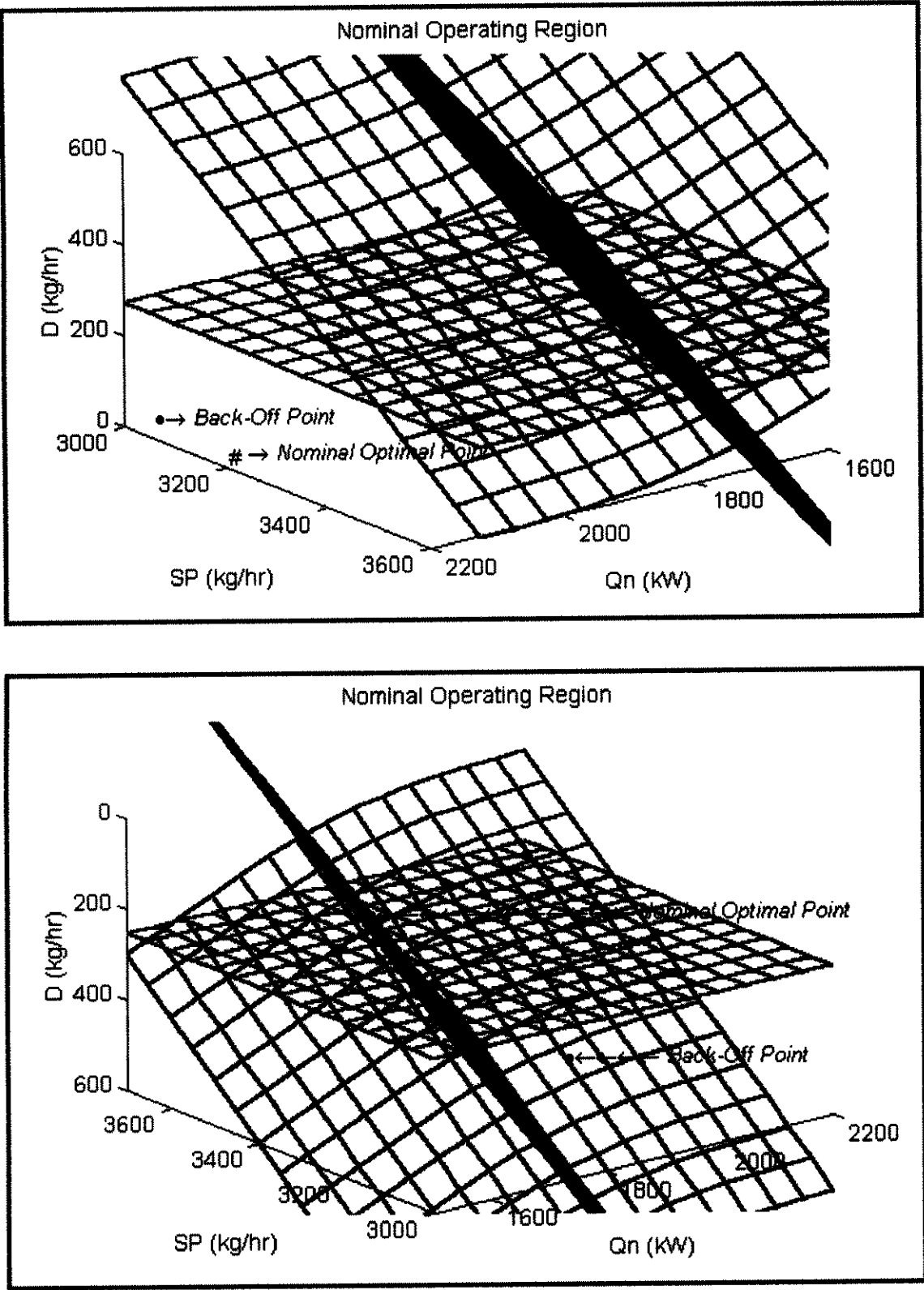


Figure 6.28 Nominal Optimum Operating Regions at Different Angles
(Decision Variable Space)
(Green surface: $MA_D = 190$ ppm)
(Blue surface: $MA_{SP} + EA_{SP} = 40$ ppm)
(Magenta surface: $EA_B \leq 2000$ ppm)

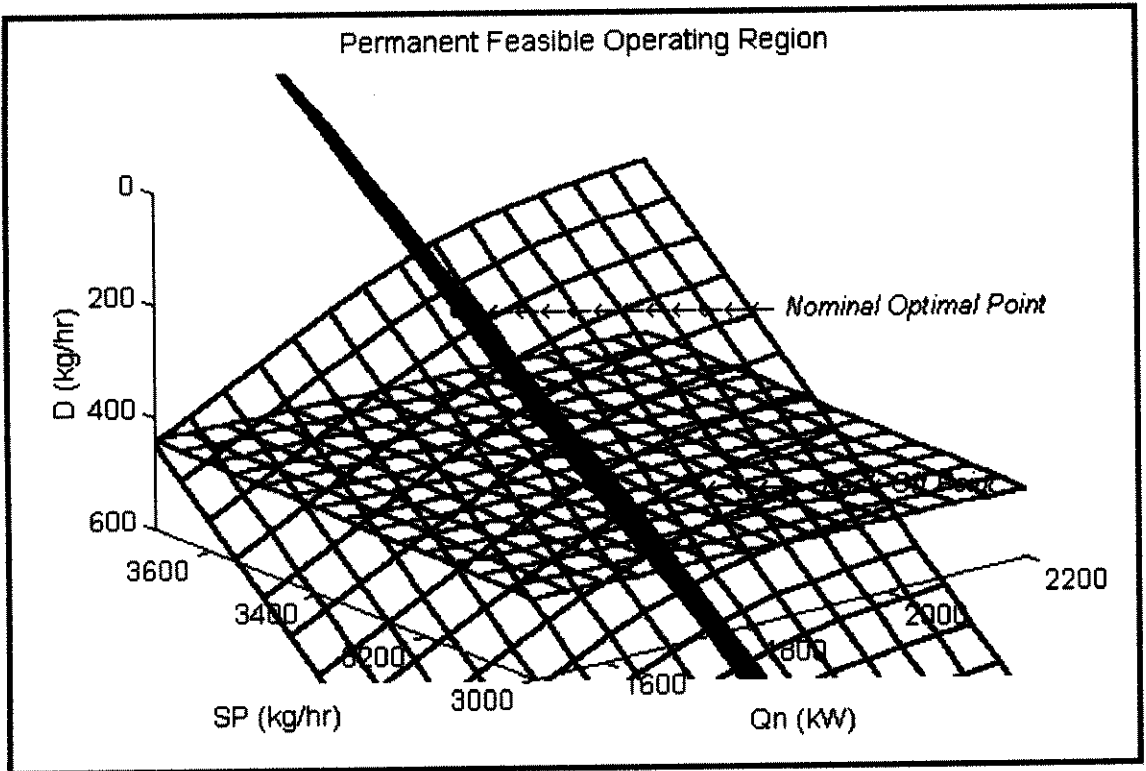
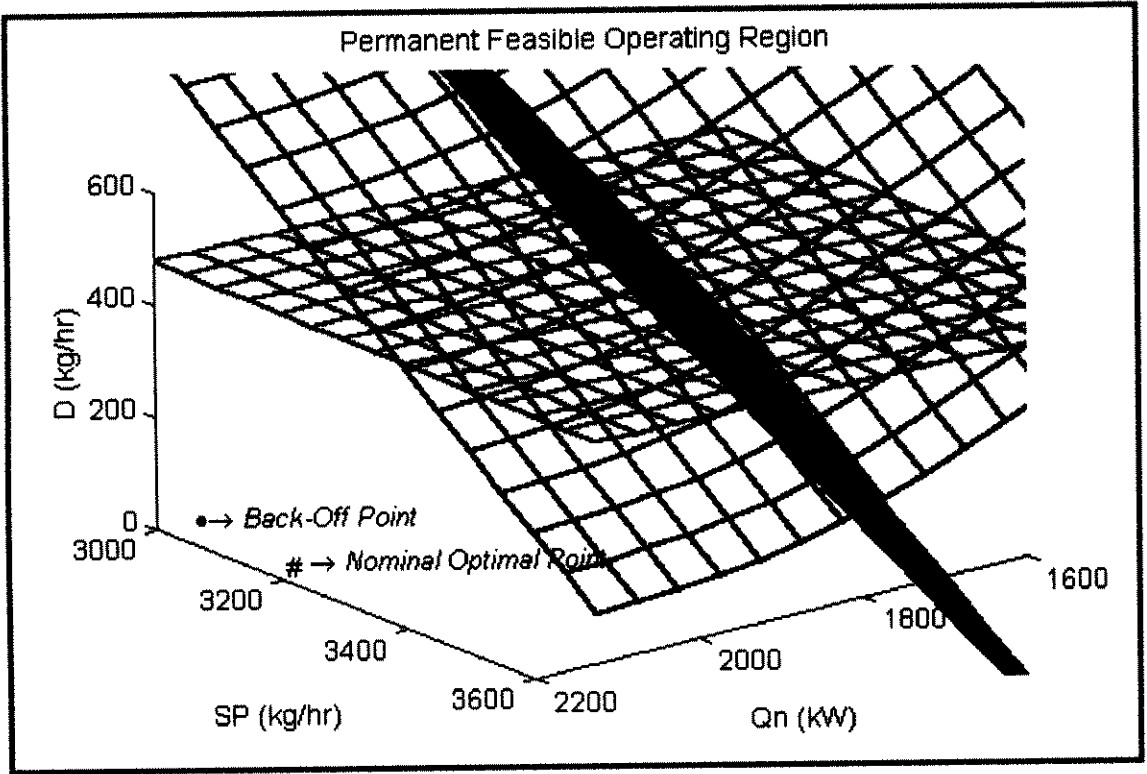


Figure 6.29 Permanent Feasible Operating Regions at Different Angles

(Decision Variable Space)

(Green surface: $MA_D = 190$ ppm)

(Blue surface: $MA_{SP} + EA_{SP} = 40$ ppm)

(Magenta surface: $EA_B \leq 2000$ ppm)

Groups of trays within the column are collected into compartments. One tray within each compartment is selected as the sensitive stage. The composition of this tray is taken to be representative of the other trays. The sensitive stage is usually the lowest tray in the compartment. Thus, the model describing the purification column consists of four compartments. Each has a special tray such as condenser, side product, feed and reboiler. Model equations for the compartments are similar to those written for the binary distillation column on page 6.19. Thermodynamic properties are extracted from ASPEN simulations. Table 6.5 compares results obtained from ASPEN and shortcut models.

	Shortcut Model	ASPEN Model
Temperature at the top (°C)	47.8	47.6
Temperature at the base (°C)	52.9	52.7
Composition		
<u>Stream D</u>		
MA (ppm)	166	161
EA (ppm)	3.7	0.4
<u>Stream SP</u>		
MA (ppm)	4.0	2.0
EA (ppm)	2.4	3.0
<u>Stream B</u>		
MA (ppm)	0	0
EA (ppm)	1701	1707

Table 6.5 Results from ASPEN and Shortcut Models

Since aldehyde species are present only in trace quantities, the shortcut model can also predict well the performance of the column, but the reboiler duty is higher than it is predicted.

The above analysis is carried out at the operating condition:

Feed (ton/day): **F = 111.6**

Distillate Feed (ton/day): **D = 10.8**

Side Product Feed (ton/day): **SP = 72**

Reflux Ratio: **RR = 29**

Feed composition (ppm): **MA = 12, EA = 442**

The dynamic model is tested based on the transition period of the plant. The feed is increased by the rate of 29 ton/day for 30 minutes, then decreased by the same rate. Information collected from the plant and simulation are plotted in Figure 6.30. Blue curves represent feed profiles, and red curves are for side product profiles. Figure 6.31 plots MA composition in the distillate and EA composition in the base product. Green curves show the feed impurities at nominal values, and red curves are for the feed impurities at the upper limit. In all cases the constraints are satisfied. Therefore, the switching problem is not relevant for this application.

Another possible control scheme for the purification column is adjusting the base product stream to control the base level and keeping the side product stream fixed (see Figure 6.32). This scheme maintains the production rate at the highest fixed level 83 ton/day, instead of a varying rate between 71 and 83 ton/day (see Table 6.4, page 6.47). However, it will create much noise in the base product stream due to the effect of bubbling in the reboiler. The current control scheme can avoid oscillation in the base product stream. This condition is more favorable, since the base stream enters the downstream plant as a feed. The steady feed is required to avoid upsetting interconnected plants. Finally, an additional control loop is introduced to control the MA composition in the distillate by manipulating the distillate-bleeding rate (see Figure 6.33). Since the sensitivity of temperature measurement is very low, temperature cannot be used to infer composition. An on-line analyzer such as a gas chromatograph must be installed. The major disadvantage is due to dead time encountered in sampling, transporting and analyzing the sample. Moreover on-line analyzers are expensive and demand proper maintenance. However, as a trade-off, controlling the MA composition in the distillate guarantees product quality and safe operation.

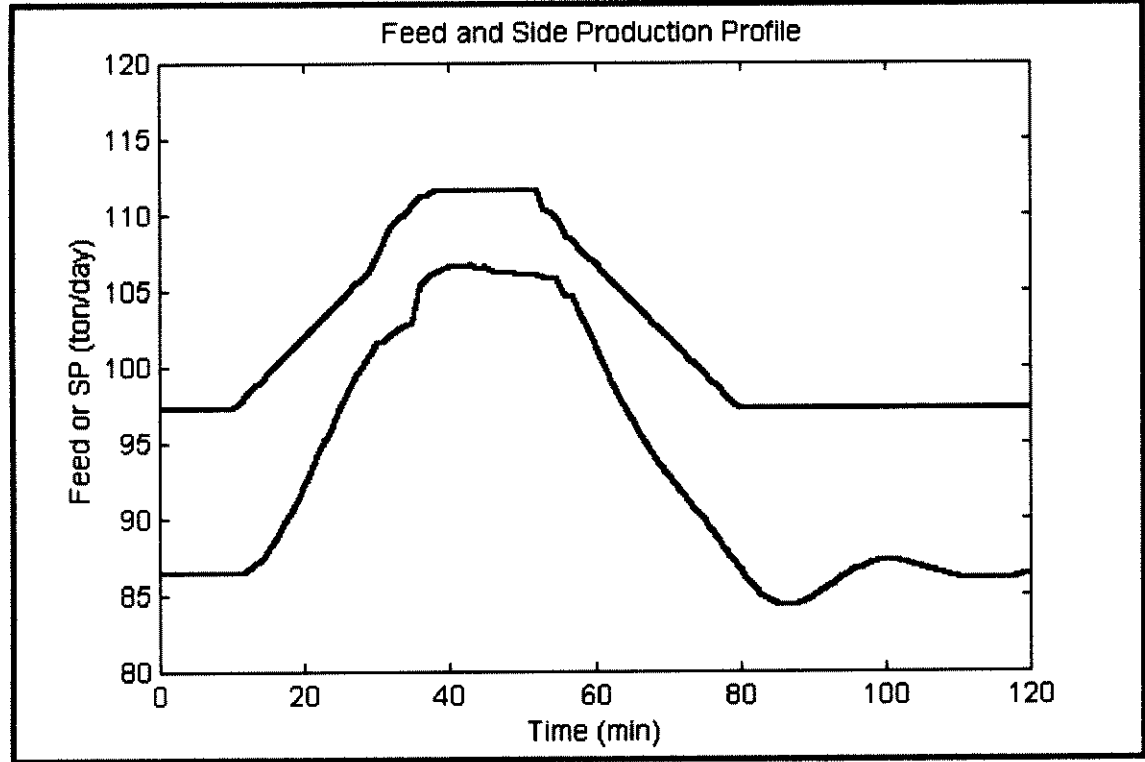
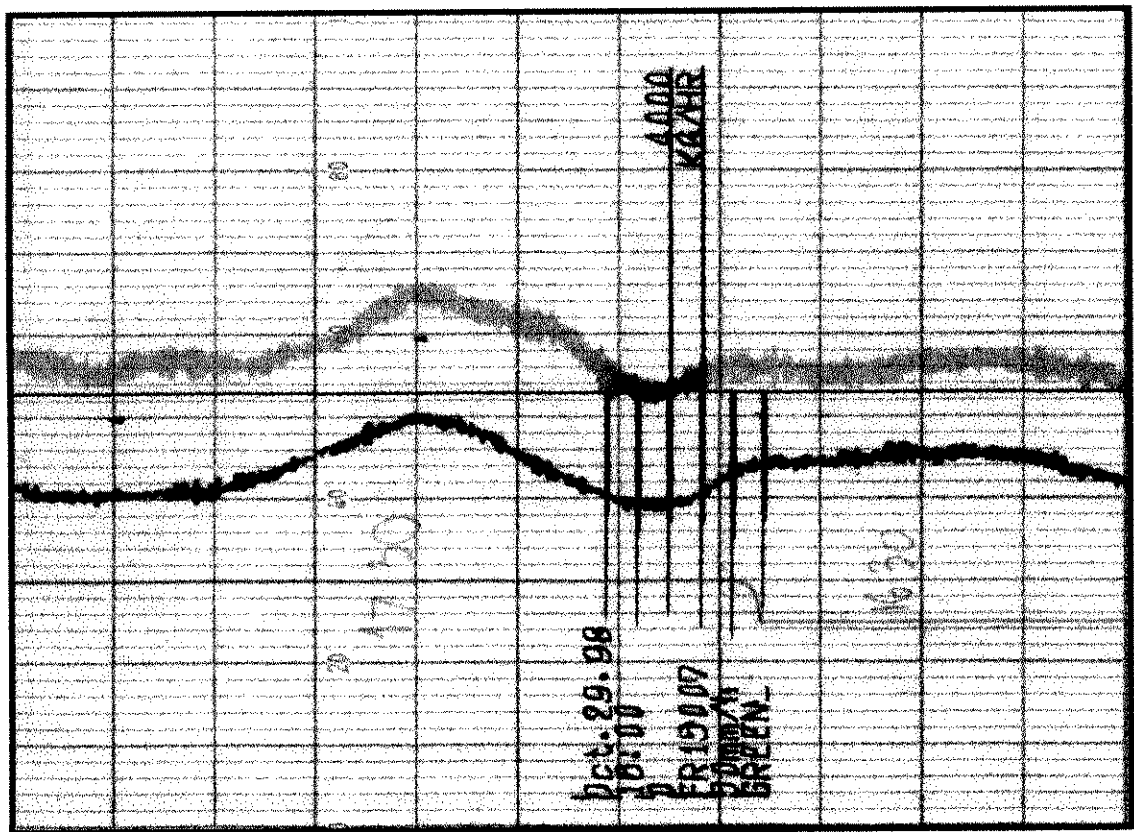


Figure 6.30 Feed and Side Product Profiles
(Blue curves: Feed; Red curves: Side product)

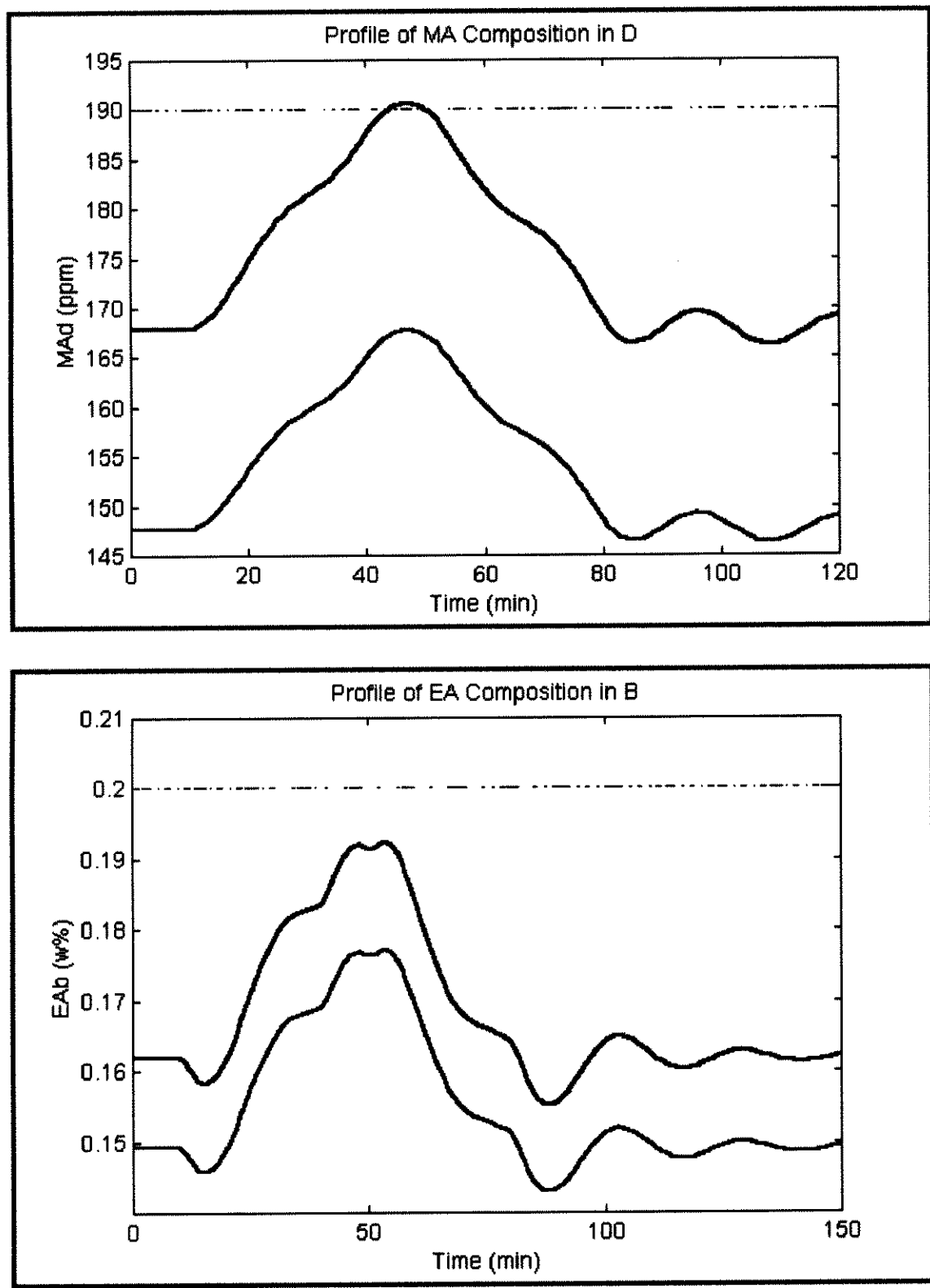


Figure 6.31 MA Composition in D and EA Composition in B

(Green curves: $EA_F = 442$ ppm, $MA_F = 12$ ppm)

(Red curves: $EA_F = 480$ ppm, $MA_F = 20$ ppm)

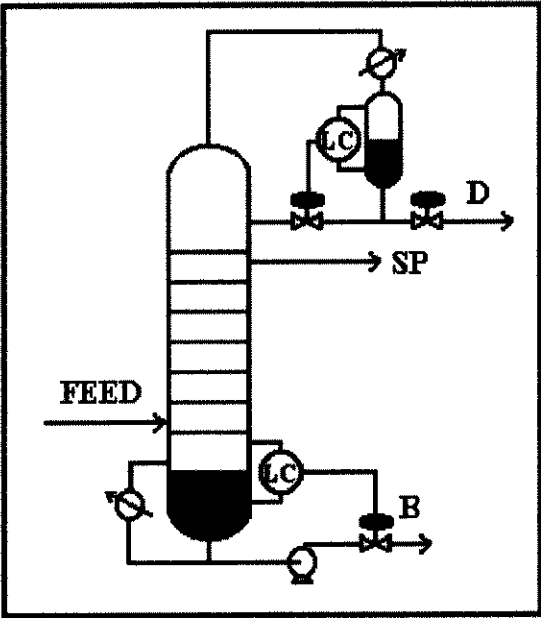


Figure 6.32 Different Setting of Base Level Control Loop

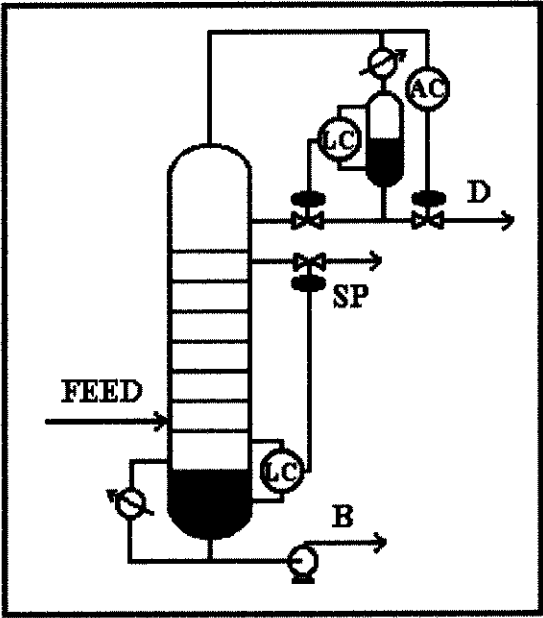


Figure 6.33 Additional Quality Control Loop

5. Conclusion

To narrow the gap between theory and application, the real plant implementation of the switchability and operability analysis is considered throughout this chapter. From a simple plant consisting of two CSTRs in series to a more complicated unit dealing with multicomponent separation, a good model can always predict well the plant behavior. Based on the model equations of the plant, feasible operating conditions subject to possible disturbances and uncertainties are found. An optimal switching policy is essential for a plant to move safely and smoothly between operating states without upsetting the downstream unit. These policies can be solved off-line by two different techniques. For the Distributed Control System that cannot automatically adjust the set point, the sequential optimization technique provides a step policy, which is more convenient to be manually fed back to the DCS as the set point. For the more advanced DCS, the simultaneous optimization and integration technique provides a curve or rather a series of tiny steps, which can only be automatically fed back to the DCS. An improvement of control strategy for each plant is proposed at the end of each section. These control schemes might increase the reaction rate of the reactors, improve the inferential control performance or increase the production rate, the quality of the product and the safety of the operation. The implementation of these schemes is left as the coming project in the department.

6. Nomenclature

B	: Base product, mol.s^{-1}
C	: Concentration, mol.l^{-1}
cool	: Removal heat from the reactor to the cooling jacket, l.Ks^{-1}
C_{pc}	: Coolant heat capacity, $\text{kJ} \cdot (\text{kg.K})^{-1}$
D	: Distillate, mol.s^{-1}
E	: Activation energy, l.atm.mol^{-1}
F	: Objective function or flexibility index
FL	: Feed flowrate, mol.s^{-1}
H	: Fraction of liquid over tank volume
H_L, H_V	: Enthalpy, kJ.s^{-1}
ko	: Arrhenius constant, s^{-1}
L	: Liquid flowrate, mol.s^{-1}
m	: Coolant flowrate = $(m_c C_{pc} / \rho_r C_{pr})$, l.s^{-1}
m_c	: Coolant flowrate, kg.s^{-1}
M	: Liquid holdup on the tray, kmol
Meff	: Murphree stage efficiency
Q	: Flowrate, l.min^{-1}
Q_{con}	: Condenser duty, kJ.s^{-1}
Q_{reb}	: Reboiler duty, kJ.s^{-1}

R_a	: Universal gas constant, l.atm.(K.mol) ⁻¹
Rate	: Rate of reaction, mol.s ⁻¹
RR	: Reflux ratio
SF	: Side product, ton.day ⁻¹
t	: Integration variable
T	: Temperature, K
u	: Vector of control (independent) variables
Ua	: Overall heat transfer coefficient/($\rho_r C_{pr}$), l.s ⁻¹
V	: Volume, l or vapor flowrate, mol.s ⁻¹
x	: Vector of state (dependent) variables or liquid composition
y	: Vapor composition
w	: Weighting function

Greek Letters

α	: Relative volatility
ΔH_r	: Heat of reaction, kJ.mol ⁻¹
ρ_r	: Density, kg.l ⁻¹

Superscripts and subscripts

1	: First CSTR
2	: Second CSTR
c	: Coolant
i, o	: Initial
L	: Lower bound
n	: Nominal value
s	: Steady state
f	: Final or feed
U	: Upper bound

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Appendix 6A

Details of the experimental works are presented in the following sections.

6A.1. Application 1: CSTRs in series

- ❖ Data including flowrate, temperature and level from the plant are collected through CITECT and written in EXCEL spreadsheets. The concentration information is obtained from direct titrations of samples at fifteen-minute intervals.
- ❖ The sample time is five seconds. The spans of the runs without reaction last one hour. The spans of the runs with reaction last three hours.
- ❖ Experimental data used in the figures, from 6.2 to 6.6 are selected from one representative run since all three runs are very similar.

6A.2. Application 2: Binary distillation column

- ❖ Data including flowrate, temperature, composition and level are collected through ABB MOD 300 DCS and written in data files.
- ❖ Data are recorded every thirty seconds. Ethanol compositions in the distillate, base product, feed and in some trays are recorded but the analyzer can take only one sample at a time. Hence, it takes more than 10 minutes to update composition information, and any change during that period can not be recognized.
- ❖ Experimental data plotted in Figure 6.13 are selected from three representative runs with three different feed rates of one, two and three liters per minute. The distillate rates and reflux ratios are also varied in each run to maintain the condition that the ethanol composition of the distillate is greater than 0.69 (mole fraction).
- ❖ Experimental data plotted in the figures, from 6.15 to 6.17 are selected from one representative run with the feed rate varied from one to two liters per minute. The distillate rates and reflux ratios are also varied in the run to maintain the condition that the ethanol composition of the distillate is greater than 0.69 (mole fraction).

6A.3. Application 3: Multicomponent distillation column

- ❖ Orica provides data used in Figure 6.30. They are collected from a normal run of the plant for seven days.

Chapter 7

Conclusions and Further Studies

1 Results and conclusions.....	7.1
1.1 A review of steady state and dynamic flexibility analysis of chemical processes with fixed design.....	7.1
1.2 Switchability and operability assessment in chemical processes.....	7.2
1.3 Switchability and controllability analysis - Predictive control approach.....	7.3
1.4 Solution method for switchability and operability analysis.....	7.4
1.5 Switchability and operability analysis of real processes..	7.4
2 Recommendations for further studies.....	7.5

Through five main chapters, the thesis has developed a new integrated and systematic approach for simultaneous flexibility, switchability and controllability analysis of chemical plants. The methodology starts with the determination of the operating conditions at the beginning and the end of the transition. The second step then searches for the optimal trajectories connecting the above states. Due to possible disturbances, uncertainties and imperfect control systems, the plant normally has to operate at the back-off conditions from nominal states. Furthermore if disturbances enter the process during a transition, following the optimal control profile does not guarantee no path constraint violations. As a result, if the dynamic plant is controlled, the profit loss due to the effect of disturbances and uncertainties on the process can be recovered and a feasible policy for an efficient switch can be found. For those reasons, the procedure of solving for the open loop and dynamic closed-loop back-off conditions as well as back-off trajectories has been focussed in the thesis. The closed-loop back-off problems are achieved first with proportional plus integral controllers then with linear and nonlinear model predictive control techniques. The latter technique is selected, since it has a general mathematical formulation very similar to that of a switchability problem. The proposed strategy is finally applied to three real processes.

The following issues have been discussed:

- ❖ An extensive review of steady state and dynamic flexibility analysis of chemical processes with fixed design
- ❖ Switchability and operability assessment in chemical processes
- ❖ Switchability and controllability analysis – Predictive control approach
- ❖ Solution method for switchability and operability analysis
- ❖ Switchability and Operability Analysis of Real Processes

1. Results and Conclusions

The originality of the thesis and main results can be extracted from each of the following chapters.

1.1. From Chapter 2: A Review of Steady State and Dynamic Flexibility Analysis of Chemical Processes with Fixed Design

Chapter 2 is not only a review of works done by Bahri (1995) and Landers (1997). Two minor features have been added.

- ❖ In addition to the basic algorithm, the KS modified form is also applied in the open loop back-off calculation.
- ❖ The chapter also introduces an extension of the algorithm to handle the dynamic situations, but the implementation is discussed in the following chapter since special techniques must be employed.

As a result, more complicated examples have successfully demonstrated the effectiveness of the algorithm in both steady state and dynamic situations. Through the case studies, the iterative procedure can also present two main issues:

1. Systematic analysis of the performance of the plant under different operating conditions and the effect of disturbances and uncertainties.
2. Ranking between different control schemes.

1.2. From Chapter 3: Switchability and Operability Assessment in Chemical Processes

The major novelty of the thesis is presented in this chapter.

- ❖ A new dimension has been added to the investigation of the operability in design or retrofit design of chemical processes. The switchability is expanded and incorporated in the operability concept, which becomes a well-established strategy for the analysis.
- ❖ A new formulation for the simultaneous flexibility, switchability and controllability analysis is established, which leads to an uncertain dynamic nonlinear programming problem.

As a result, sophisticated mathematical techniques must be employed to solve the optimization problems generated in the study. Two different techniques are selected in the case studies to compare the advantages and disadvantages of the solving methods. The sequential optimization approach converges slowly and handles constraints on state variables with difficulty. However, the technique is more practical for engineering

applications, since it can be used to solve large-scale problems. The simultaneous optimization and integration approach can properly handle path constraints and reduce computational time but cannot be used for large and complicated problems. Some results drawn from the case studies might be useful for similar investigations.

- ❖ The potential recovery of the profit loss caused by disturbances and uncertainties strongly depends on the control strategy. Controller gains, reset times and even set points can be included in the optimization problem as decision variables.
- ❖ Some factors affecting the feasibility and optimal solutions of a switchability problem include the number of degree of freedom in the system, the weighting factors and the control strategy.
- ❖ The switching problem involving feed changes accompanied by set point changes is lengthy to solve, since it is a mixture of regulator and servo problems. However, it can avoid abrupt changes in manipulated variables as well as path constraint violations.
- ❖ The optimal trajectories from solving the switchability problem subject to the worst condition might not be a feasible solution subject to other combinations of disturbances. Although it is tedious and time consuming, feasibility tests should always be carried out to guarantee a safe transition.

1.3. From Chapter 4: Switchability and Controllability Analysis – Predictive Control Approach

MPC, especially DMC are not the new advanced control techniques as they have been in use since the early 1970s. Although DMC is a linear MPC, the technique is selected as an alternative, because the on-line implementations of DMC to the pilot plant and the distillation unit in Chapter 6 are achievable. The NLPC technique on the other hand, is discussed in Chapter 4, since it has a general mathematical formulation very similar to that of a switchability problem. As a result the size of the simultaneous switchability and controllability problem does not increase, if it is achieved with MPC technique. This can avoid the size limitation of the software package and the solver itself, as discussed in the following chapter.

The new feature in this chapter is not the control technique itself, but the incorporation of the MPC technique in the switchability problem. The main results from the replacement of PI by MPC techniques include:

- ❖ In a regulator control problem designed for the SISO case, DMC does not offer significant advantages over PI controllers. In more complicated control and switchability problems such as a mixed servo regulator problem designed for the MIMO case, the well-tuned DMC can handle much better these situations.
- ❖ The selection of tuning parameters is a time consuming job. As a result, DMC is more practical for multivariable systems, especially for distillation processes.

1.4. From Chapter 5: Solution Method for Switchability and Operability Analysis

Chapter 5 reviews solution techniques as well as the usage of software packages in solving standard and dynamic optimization problems generated by the flexibility, switchability and controllability analysis. The main result from this chapter is

- ❖ The simultaneous integration and optimization technique applied in GAMS is a promising tool for dynamic optimization. It can certainly solve the optimal control problem better and faster than the sequential optimization technique applied in SPEEDUP or MATLAB. Therefore, it is used in solving the NLPC control problem in Chapter 5 for the optimal set of control actions. Unfortunately the approach cannot be used for large and complicated problems due to the size limitation of the software package and the solver. The sequential optimization technique in SPEEDUP is used instead to optimize the whole flowsheet including many operation units.

1.5. From Chapter 6: Switchability and Operability Analysis of Real Processes

The aim of Chapter 6 is to verify the simultaneous formulation for flexibility, switchability and controllability analysis. The formulation is applied in three real plants:

1. The two CSTRs in series produce acetic acid and ethanol from ethyl acetate over catalyst.

2. The binary distillation column separates ethanol from water.
3. The industrial multicomponent distillation column separates high-grade olefin oxide from impurities.

There is no new feature but some useful results can be extracted from this chapter for further investigations.

- ❖ Mathematical models used with different software packages, which describe well steady state and dynamic behaviors of each plant, have been developed.
- ❖ As discussed before, the simultaneous integration and optimization technique applied in GAMS is the best tool for the CSTR plant. The technique guarantees convergence in solving for operating states at different conditions, trajectories connecting operating states and improvements of the control performance. However, it cannot be used for the distillation applications because of the size limitation of the package and the solver. The sequential optimization technique in SPEEDUP is used in spite of lengthy computational time.
- ❖ Compartmental models are commonly used for large size columns. However, the issue of replacing rigorous by compartmental models has to be considered with care, especially for the case in which the impurities appear in trace quantities.
- ❖ Using mixed integer and nonlinear programming technique, the optimum feed and product locations can be included as decision variables in the flexibility problem.
- ❖ In order to avoid large dead time, an algorithm has been developed for the on-line-implementation of MPC technique to control the binary distillation column.

The above applications have proved the theories to be successfully applicable to real plants, but there are still some useful extensions that must be considered in the research.

2. Recommendations for Further Studies

The effectiveness of the simultaneous switchability and operability analysis has been demonstrated throughout the thesis. However, a number of potential areas should be addressed for further investigations.

- ❖ Further development is needed for the efficient large-scale use of the proposed methodology. This is particularly true for the simultaneous flexibility, switchability and controllability study, since the analysis leads to dynamic optimization problems, on-line applications and design problems with complex models. These are considered more frequently by industry. The next challenge in the future is to maintain the reliability and efficiency of the optimization approach, as more difficult and large problems are solved.
- ❖ A strategy is required to incorporate the reliability and safety concepts in design and operation of chemical processes, using the same proposed methodology.
- ❖ Up to the present the approach has been applied to the systems, which require only the average (or best-known) value and an estimate range of variation for each single parameter subject to uncertainties. An extension of the approach should be considered to apply to the systems, in which disturbances and uncertain parameters are defined by probabilistic distribution functions.

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