

PROCESS DESIGN FOR CONTROLLABILITY OF  
NONLINEAR SYSTEMS WITH MULTIPLICITY

Keming Ma



A thesis submitted for the degree of Doctor of Philosophy of the  
University of London

Department of Chemical Engineering  
University College London  
London WC1E 7JE

June 2002

ProQuest Number: 10016085

All rights reserved

INFORMATION TO ALL USERS

The quality of this reproduction is dependent upon the quality of the copy submitted.

In the unlikely event that the author did not send a complete manuscript and there are missing pages, these will be noted. Also, if material had to be removed, a note will indicate the deletion.



ProQuest 10016085

Published by ProQuest LLC(2016). Copyright of the Dissertation is held by the Author.

All rights reserved.

This work is protected against unauthorized copying under Title 17, United States Code.  
Microform Edition © ProQuest LLC.

ProQuest LLC  
789 East Eisenhower Parkway  
P.O. Box 1346  
Ann Arbor, MI 48106-1346

# Contents

<b>Abstract</b>	<b>5</b>
<b>Dedication</b>	<b>7</b>
<b>Acknowledgements</b>	<b>8</b>
<b>1 Introduction</b>	<b>9</b>
1.1 General Overview . . . . .	9
1.2 Objectives . . . . .	14
1.3 Outline of the Thesis . . . . .	14
<b>2 Literature Review</b>	<b>16</b>
2.1 Basic Concepts and Properties of Nonlinear Systems . . . . .	17
2.1.1 Fundamentals . . . . .	17
2.1.2 Properties of Solutions . . . . .	18
2.1.3 The Concept of Bifurcation Analysis . . . . .	20
2.2 The Concept of Controllability in Process Engineering . . . . .	23
2.3 Limitations on Controllability . . . . .	27
2.3.1 The Concept of Zeros and Zero Dynamics . . . . .	27
2.3.2 Perfect Control . . . . .	30
2.3.3 Ideal ISE Optimal Control . . . . .	33

2.3.4	Control Problems Associated with Unstable Inversion . . .	35
2.4	Input Multiplicity and Controllability . . . . .	36
2.4.1	Input Multiplicity and RHP Zeros . . . . .	38
2.4.2	Control Problems Associated with Input Multiplicity . . .	40
2.5	An Overview of Controllability Analysis Techniques and Process Design Methods for Improved Controllability . . . . .	43
2.5.1	Definitions . . . . .	43
2.5.2	Techniques for Controllability Analysis . . . . .	44
2.5.3	Design Methods for Improved Controllability . . . . .	48
2.6	Conclusions . . . . .	53
<b>3</b>	<b>A New Analysis Method</b>	<b>55</b>
3.1	Introduction . . . . .	56
3.2	Bifurcation Analysis . . . . .	57
3.3	Problem Formulation . . . . .	60
3.4	Solution Method . . . . .	64
3.5	Illustration: van de Vusse Reactor Example . . . . .	66
3.5.1	Analysis for the van de Vusse Reactor . . . . .	68
3.5.2	Comparison with Analytical Solutions . . . . .	69
3.5.3	Summary . . . . .	75
3.6	Conclusions . . . . .	75
<b>4</b>	<b>Process Modification for Improved Controllability</b>	<b>76</b>
4.1	Introduction . . . . .	77
4.2	Process Modification Methodology for Improved Static Controllability . . . . .	77
4.2.1	Economically Optimal Design . . . . .	78
4.2.2	Controllability Analysis for the “Base-Case” Design . . . .	79

4.2.3	Design Modification Algorithm . . . . .	79
4.3	Illustrative Example: An Exothermic CSTR . . . . .	82
4.3.1	Process Description . . . . .	83
4.3.2	Analysis for the Given Process . . . . .	84
4.3.3	Process Design Modifications . . . . .	88
4.3.4	Closed-Loop Simulations . . . . .	90
4.4	Conclusions . . . . .	95
<b>5</b>	<b>Case Studies</b>	<b>96</b>
5.1	Case Study I:	
	A Reactor-Separator System with Recycle . . . . .	98
5.1.1	Introduction . . . . .	98
5.1.2	Process Description . . . . .	99
5.1.3	Process Model Equations . . . . .	100
5.1.4	Controllable Analysis for the Base Case Design . . . . .	105
5.1.5	Process Design Modifications . . . . .	107
5.1.6	Simulations . . . . .	113
5.1.7	Summary . . . . .	118
5.2	Case Study II:	
	An Industrial Polymerization Reaction . . . . .	119
5.2.1	Introduction . . . . .	119
5.2.2	Process Model and Optimal Operation Design . . . . .	120
5.2.3	Analysis for the Base Case Design . . . . .	123
5.2.4	Effects of Design and Operation Parameters . . . . .	131
5.2.5	Process Design Modifications . . . . .	138
5.2.6	Closed-Loop Simulations . . . . .	140
5.2.7	Summary . . . . .	141

5.3	Conclusions . . . . .	144
<b>6</b>	<b>Conclusions and Future Work</b>	<b>146</b>
6.1	Summary of Findings . . . . .	146
6.1.1	New Method for Analysis . . . . .	146
6.1.2	Process Design Modifications for Improved Controllability	148
6.2	Key Contributions . . . . .	149
6.3	Recommendations for Further Work . . . . .	150
<b>A</b>	<b>Acronyms</b>	<b>153</b>
<b>B</b>	<b>Zero Dynamics</b>	<b>155</b>
B.1	Introduction . . . . .	155
B.2	Mathematical Preliminaries . . . . .	156
B.2.1	Lie Derivatives . . . . .	156
B.2.2	Lie Brackets . . . . .	156
B.3	Nonlinear Inversion: Zero Dynamics . . . . .	157
B.3.1	Relative Order . . . . .	158
B.3.2	Normal Forms . . . . .	158
B.3.3	Nonlinear Inversion . . . . .	161
B.3.4	Zero Dynamics . . . . .	162
<b>C</b>	<b>Numerical Techniques in Bifurcation Problems</b>	<b>165</b>
C.1	Introduction . . . . .	165
C.2	Continuation of Solutions . . . . .	166
C.2.1	Regular Solution Paths . . . . .	166
C.2.2	Folds . . . . .	167
C.2.3	Natural Parameter Continuation . . . . .	168
C.2.4	Pseudo-arclength Continuation . . . . .	169

C.3	Singular Points and Bifurcation . . . . .	171
C.3.1	Simple Singular Points . . . . .	171
C.3.2	Bifurcation Theorem . . . . .	171
C.3.3	Detection of Bifurcation Points . . . . .	172
C.4	Summary . . . . .	173

# List of Tables

2.1	Summary of the typical controllability analysis measures in the literature . . . . .	45
3.1	Parameters and values for van de Vusse reactor . . . . .	68
4.1	Parameters and values . . . . .	84
4.2	Process design modification results for the exothermic reaction . .	90
4.3	Parameters and operation values for the base-case and modified designs for the exothermic CSTR at steady state . . . . .	90
5.1	Parameters and values for the optimal design . . . . .	105
5.2	Modification results of the reactor-separator system for cost weights: $\mathcal{R} = 1$ , $\mathcal{Q} = 5$ , and $\mathcal{W} = 10$ . . . . .	112
5.3	Modification results of the reactor-separator system for cost weights: $\mathcal{R} = 0.15$ , $\mathcal{Q} = 0.55$ , and $\mathcal{W} = 1000$ . . . . .	113
5.4	Kinetic parameters . . . . .	124
5.5	Process design and operation parameter values . . . . .	124
5.6	Process design modification results . . . . .	140

# List of Figures

1.1	Illustrative example: van de Vusse reactor . . . . .	10
1.2	Steady-state solution relationship between input and output . . .	12
2.1	Two possible types of multiplicity. a) input multiplicity; b) output multiplicity. . . . .	36
3.1	Schematic diagram of the van de Vusse reactor . . . . .	66
3.2	Steady state solutions showing input multiplicity condition information for the van de Vusse reactor. Square: input multiplicity condition . . . . .	70
3.3	Steady state solutions showing input multiplicity condition with variation of $c_{A0}$ for van de Vusse reactor. Solid line: steady states for a fixed $c_{A0}$ ; dashed line: input multiplicity condition with variation of $c_{A0}$ . . . . .	70
3.4	Locus of input multiplicity condition between inlet flow rate $F$ and feed composition $c_{A0}$ . . . . .	71
3.5	Contour of input multiplicity conditions as inlet flow rate, output, and inlet concentration change for the van de Vusse reactor . . . .	71
3.6	Process gain as a function of inlet flow rate for the van de Vusse reactor . . . . .	74

3.7	Eigenvalue of zero dynamics as a function of inlet flow rate for the van de Vusse reactor . . . . .	74
4.1	Steady-state solutions showing input multiplicity condition with variations of inlet temperature. Square: input multiplicity condition; dashed line: input multiplicity condition with variation of inlet temperature . . . . .	86
4.2	Locus of inlet flow rate versus inlet temperature at input multiplicity condition . . . . .	86
4.3	Input multiplicity condition between the reactor temperature, inlet flow rate and inlet temperature . . . . .	87
4.4	Input multiplicity condition between the inlet flow rate, inlet temperature, and reactor volume . . . . .	87
4.5	The relationship between design parameter and disturbance rejection ability . . . . .	91
4.6	Profiles of input and output for the initial design, $V = 0.1 m^3$ , for disturbance rejection of inlet temperature: $-4 K$ and $-5 K$ . . . .	92
4.7	Profiles of input and output for the initial design, $V = 0.1 m^3$ , for rejection of $-5 K$ change in the inlet temperature . . . . .	92
4.8	Profiles of input and output for the initial design, $V = 0.1 m^3$ , for rejection of $-4 K$ change in the inlet temperature . . . . .	93
4.9	Profiles of input and output for the modified design, $V = 0.111 m^3$ , for rejection of inlet temperature changes: $-5 K$ and $-8 K$ . . . .	93
4.10	Profiles of input and output for the modified design, $V=0.111m^3$ , for the disturbance of the inlet temperature, $-8 K$ . . . . .	94
4.11	Closed-loop simulations for the original design, $V = 0.1 m^3$ , and the modified design, $V = 0.111 m^3$ , for a set-point change . . . . .	94

5.1	Schematic of the reactor-separator system . . . . .	99
5.2	Schematic of a distillation bottom reboiler . . . . .	102
5.3	Schematic of a distillation below feed tray . . . . .	102
5.4	Schematic of a distillation feed tray . . . . .	103
5.5	Schematic of a distillation above feed tray . . . . .	103
5.6	Schematic of a distillation overhead total condenser . . . . .	104
5.7	Steady-state solutions showing input multiplicity condition for the variation of the reflux $L$ for the base case design. Open square: input multiplicity condition. . . . .	106
5.8	Input multiplicity and output multiplicity for the base case with a larger recycle: $B=1.8$ kmol/min. Dashed line: unstable state . . .	108
5.9	Locus of output multiplicity conditions between reflux and recycle for the base case . . . . .	108
5.10	Locus of input multiplicity condition between reflux and recycle for the base case . . . . .	109
5.11	Relationship between reflux $L$ , recycle $B$ , and reactor volume $H$ at input multiplicity condition for the base case design . . . . .	109
5.12	Steady states of the design modifications for the reactor-separator system. Square: input multiplicity condition . . . . .	112
5.13	Steady states for the modified design, $H=65.40$ and $B=1.163$ , and the base case design. Open square: input multiplicity condition .	114
5.14	Step responses to 0.1% ( $t = 0$ ) and 0.12% ( $t \approx 6 \times 10^4$ ) changes in $y_{D,set}$ for the modified design $H = 65.40$ and $B = 1.163$ initially operating at (A) . . . . .	116
5.15	Details of output $y_D$ for time from 0 to 100 minutes of Figure ?? .	116

5.16	Step response to set point changes in $y_{D,set}$ for the modified design $H = 65.40$ and $B = 1.163$ initially operating at (B). Solid line: 0.1% change in $y_{D,set}$ ; dashed line: 0.12% change in $y_{D,set}$ . . . . .	117
5.17	Step response to set point changes in $y_{D,set}$ for the modified design $H = 65.47$ and $B = 1.155$ initially operating at point (B). Solid line: 0.2% change in $y_{D,set}$ ; dashed line: 0.21% change in $y_{D,set}$ . . .	117
5.18	Process flow diagram for the jacketed polymerisation CSTR . . .	123
5.19	Steady states of molecular weight number versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point . . . . .	125
5.20	Steady states of reaction temperature versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifur- cation point . . . . .	126
5.21	Steady states of jacket temperature versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifur- cation point . . . . .	126
5.22	Steady states of monomer concentration versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifur- cation point . . . . .	127
5.23	Steady states of initiator concentration versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifur- cation point . . . . .	127
5.24	Steady states of zeroth moment of molecular weight distribution versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point . . . . .	128

5.25	Steady states of the first moment of molecular weight distribution versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point . . . . .	128
5.26	Steady states of $MW_{av}$ showing input multiplicity condition. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point; open square: input multiplicity condition . . . .	132
5.27	Steady states of the jacket temperature showing input multiplicity condition. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point; open square: input multiplicity condition . . . . .	132
5.28	Trajectories of the output, input, and profile of the internal state for a step change in inlet temperature: $\Delta T_{in} = +3K$ . . . . .	133
5.29	Trajectories of the output, input, and profile of the internal state for a step change in inlet temperature: $\Delta T_{in} = +4K$ . . . . .	133
5.30	Pseudo-steady-state path followed by the process during such a destabilisation as depicted in Fig. ?? . . . . .	134
5.31	Locus of input multiplicity condition for the cooling water versus the inlet feed temperature . . . . .	136
5.32	Input multiplicity condition between jacket temperature, cooling water, and inlet feed temperature . . . . .	136
5.33	Locus of input multiplicity condition for the cooling water flow rate versus the reactor volume . . . . .	137
5.34	Input multiplicity condition between the jacket temperature, the cooling water flow rate, and the reactor volume. . . . .	138
5.35	Relationship between the cooling water flow rate $F_{cw}$ , inlet feed temperature $T_{in}$ , and reactor volume $V$ for the first input multiplicity condition . . . . .	139

5.36 Simulation for the base case design: $V = 0.1m^3$ and disturbance $\Delta T_{in} = +3K$ . . . . .	142
5.37 Simulation for the base case: $V = 0.1m^3$ and $\Delta T_{in} = +4K$ . . . . .	142
5.38 Simulation for the design modification: $V = 0.097m^3$ and distur- bance $\Delta T_{in} = +4K$ . . . . .	143
5.39 Simulation for the design modification: $V = 0.097m^3$ and distur- bance $\Delta T_{in} = +5K$ . . . . .	143
5.40 Simulation for the design modification: $V = 0.095m^3$ and distur- bance $\Delta T_{in} = +5K$ . . . . .	144
C.1 Schematics for pseudo-arclength continuation . . . . .	169

# Abstract

This thesis is concerned with the development of methods for controllability analysis leading to process design modifications of nonlinear chemical processes with input multiplicity. The first part of this thesis presents an approach to controllability analysis, based on bifurcation and continuation techniques, that can identify input multiplicity behaviour in the parameter space and give insights into the dependence of input multiplicity on the values of operating and design parameters. The algorithm developed incorporates the necessary condition for the existence of input multiplicity at a variety of steady states as an add-in subroutine into an available bifurcation analysis program, which is suitable for sizeable nonlinear processes. This allows one to study how operating conditions and design parameters influence input multiplicity behaviour, hence providing guidance to modify process designs to eliminate or avoid input multiplicity. The key features and application of the proposed approach are demonstrated through an exothermic continuous stirred tank reaction (CSTR) example and comparison made with the analytical results.

The second part of this thesis focusses on an approach to making process design modifications by using optimisation and bifurcation analysis. A process modification problem is formulated within an optimisation framework which aims at minimising design parameter adjustment to eliminate potential control difficulties associated with input multiplicity behaviour for a disturbance, and results in

a nonlinear programming (NLP) problem. Results are presented for its applications to a reactor-separator system with recycle and an industrial polymerization reaction.

# Dedication

To Hong & Tianran

# Acknowledgements

I would like to thank my supervisor David Bogle for his support, encouragement and guidance throughout the course of this work. He has not only taught me much, but has also given a continual source of encouragement. I am grateful to him in particular in the opportunities and support he has given me.

For the financial support of the project, I would like to thank the EPSRC.

Many thanks also go to Eric for his encouragement and support and all the people I have met during my time at UCL and the Centre for Process Systems Engineering (IC & UCL) for their friendship and support. I am also grateful to E. J. Doedel of Concordia University for help with the use of AUTO.

I would like to thank my parents in particular for their continual confidence in me.

Special thanks to my son, Tianran, who has suffered most as a result of this work.

Last but important, I must thank my wife, Hong, for her patience, encouragement, support and presence.

# Chapter 1

## Introduction

---

### 1.1 General Overview

Nonlinear systems possess distinguishing characteristics from linear systems. One important characteristic of a nonlinear system is the dependence on the initial conditions. For a linear system, identical input changes implemented at different operating steady-state conditions will give rise to output changes of identical magnitude and dynamic character. Many systems of engineering interest approximate this behaviour for small inputs, which accounts for the universal study and application of linear control system theory.

However, for a nonlinear system, qualitative properties can change under small perturbation of the system parameters and operating conditions. By qualitative properties we mean the existence of multiple steady-state solutions, instability of the solutions, limit cycles, and even chaotic behaviour. Such complex behaviour is known to impose difficulties in system control and to affect adversely the performance of the closed-loop system. But, with the increase of standards of product quality, stricter environmental regulations, and economic pressures, it is likely to

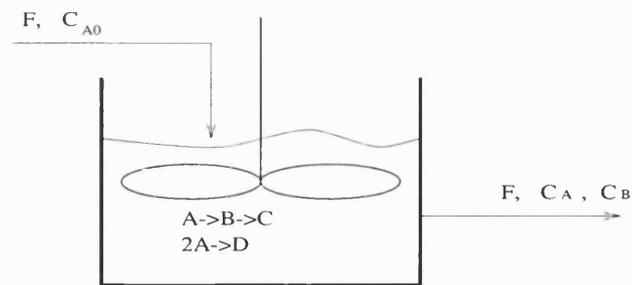


Figure 1.1: Illustrative example: van de Vusse reactor

push chemical process designs into regions where complex nonlinear behaviour occurs.

As an illustration of this, consider Figure 1.1 which is a reaction, known as the van de Vusse reaction taking place in an isothermal continuous stirred tank reactor (CSTR) (van de Vusse, 1964). This is the most popular nonlinear study example in the literature, and is frequently utilised to demonstrate control problems in nonlinear control design and optimisation (Daoutidis *et al.*, 1990; Sistu and Bequette, 1995; Doyle *et al.*, 1995).

The system illustrated has been designed with the maximum conversion of product  $B$  for the nominal conditions, and is operated at a steady-state point to control the concentration of  $B$ ,  $C_B$ , by manipulating the inlet flow rate,  $F$ . Although the process seems good from an economic point of view, it exhibits multiple steady-state behaviour as shown in Figure 1.2 which shows that more than one set of inputs exist for the same set of outputs, known as *input multiplicity*. The input multiplicity behaviour can cause control difficulties subject to the changing operation conditions, such as the changes of disturbances and setpoints. Thus, there are questions arising while assessing the ability to keep the process at the desired level in the face of the changing conditions. This attribute of a system is termed *controllability*.

In particular for this case, one might ask:

- How well can the process be controlled or is it a difficult control problem?
- How many variations in the set point change of the conversion of product  $B$  can the process actually tolerate?
- If the concentration of the reactant  $A$  is considered as a disturbance, how many changes in the disturbance can the process reject successfully?

and moreover

- How can the process be improved if it is not satisfied with the control requirements?

Such questions are clearly important, not only for examining and quantifying how controllable a process is, but also, more generally, for screening or comparing the process design alternatives at the process design stage.

*Input multiplicity* is one complex phenomenon that is encountered in chemical processes, and has been identified as a main cause of destabilisation of the control systems (Koppel, 1982; Dash and Koppel, 1989). Input multiplicity poses limitations on achievable dynamic performance and proves the need for complexity of control design (Morari, 1983; Skogestad and Postlethwaite, 1996; Sistu and Bequette, 1995). For instance, with reference to Figure 1.2, there exists no fixed feedback controller that can stabilise both a pair of steady-states 1 and 2, since the steady-state solutions 1 and 2 have different qualitative behaviour (i.e. different gain signs). A conventional controller with integral action only keeps one of these two steady states stable, and will become unstable for another because the sign change in the process gain causes the control system from the negative feedback system to a positive feedback one. Therefore, such a characteristic of the process should be identified and eliminated or avoided in the process design stage in order to make the process easily controllable.

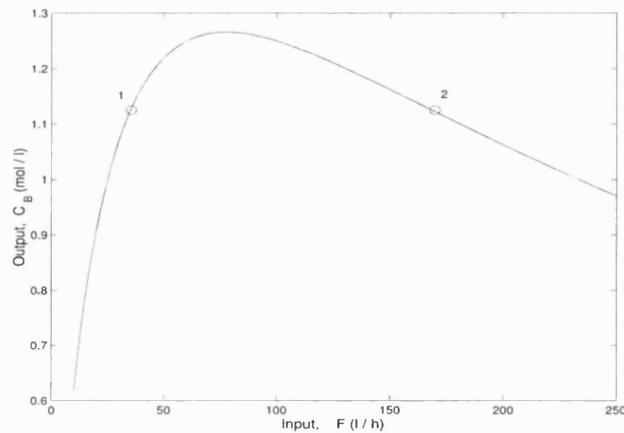


Figure 1.2: Steady-state solution relationship between input and output

Studies in the literature have been shown that the design of a process determines controllability and a controller only ensures the achievable performance (Morari, 1983; Skogestad and Postlethwaite, 1996). So, it is quite necessary to have a rough idea of what the inherent properties of the process are and how easy the process is to control at an early design stage. Controllability analysis could obtain insights into what the inherent properties of a process are and how they present limitations on the control performance of the process. Analysing the effects of these limitations early enough in the process design allows the opportunity to modify the design should the effects be critical to the dynamic performance of the process (Perkins *et al.*, 1996). Modifications of a process design itself, such as changing inputs or outputs, operating points, values of design parameters and even structure, can sometime affect the dynamics of the process significantly more than changes in the controllers (Morari, 1983).

Consideration of the controllability of a process at the very early phase of the process design is now being widely accepted in both academia and industry, as shown by a number of publications in the field (discussed in more detail in

Chapter 2). A growing amount of evidence points to the desirability of incorporating controllability consideration into all phases of the process design. It may be better in the long run to establish a process that has higher capital and energy costs if the process provides more stable operation and achieves less variability in product quality. A number of relevant techniques have been proposed, including optimisation-based approaches (Luyben and Floudas, 1994; Perkins and Walsh, 1996) and bifurcation-based analysis and design (Morari, 1992; Russo and Bequette, 1996, 1998).

In this thesis we present an approach to modifying a process design for improving controllability, using bifurcation analysis and optimisation. *Bifurcation analysis*, a method for studying how qualitative behaviour of a nonlinear system changes as the parameters vary, is recognised as a powerful tool in nonlinear system analysis and widely applied to chemical processes (Aris, 1979; Seider *et al.*, 1991; Sistu and Bequette, 1995). Morari (1992) suggested that bifurcation analysis should be employed in controllability analysis for nonlinear systems. Bifurcation analysis could be sufficient to obtain a qualitative picture of the solution space for a nonlinear process as a parameter of the process varies at the design stage when there is only limited information available. This can be used to identify the potential control difficulties determined by the process design, and to investigate the effects of the design and operating parameters and disturbances on them, hence providing the guidance to eliminate them by modifying the process design at the design stage.

## 1.2 Objectives

The primary aim of this thesis is to develop a methodology for modifying an existing process design with a fixed control structure for improving controllability over the operating regions in the face of a disturbance. In order to modify an existing process design for controllability it should be essential to understand what the potential control difficulties are and how the parameters under consideration affect them. Results from this analysis lead to a process modification so that such difficult control problems are eliminated or avoided by adjusting the design parameter values. The methods presented in this thesis dedicate to these purposes. The objectives are:

- to develop a methodology, based on bifurcation analysis, for determining potential control problems associated with inherent characteristics of a nonlinear process over the entire operating region of interest and analysing the parameter effects on these problems, and then
- to determine a method for modifying the process to improve controllability, while preserving modifications as small as possible.

## 1.3 Outline of the Thesis

The work in this thesis is broadly divided into two parts: the first part is concerned with the development of a new approach to controllability analysis of nonlinear systems with input multiplicity; the second part presents a static feedback optimisation formula as a trade-off between controllability and economics in process design modifications, and the applications of the proposed method to chemical process cases.

Chapter 2 serves as a brief literature review and background introduction to the methods used in this thesis. The main ideas on nonlinear systems, controllability, and bifurcation analysis are given. A brief review on controllability analysis and design techniques available in the literature is presented, while identifying potential limitations of these methods for nonlinear systems and addressing why the bifurcation-based approach as an appropriate one.

In Chapter 3, a new bifurcation-based analysis method for nonlinear processes with input multiplicity such as this described in Figure 1.2 in §1.1 is described and applied to an exothermic continuous stirred tank reaction (CSTR) that exhibits multiplicity as an illustrative example. The results are compared with analytical solutions.

Chapter 4 presents an optimisation-based approach to modifying an existing process design that has control difficulties associated with undesirable dynamic behaviour determined by the process design. A static feedback optimisation formulation is developed that can modify the process design to avoid the poor dynamics in the operating region while minimising changes to the process, namely producing a *feedback optimising design (FOD)*. An exothermic CSTR as an illustrative example demonstrates the features and application of this method.

Chapter 5 presents case studies to demonstrate the applications of these approaches in chemical processes. Two cases are given: one is a reactor-separator system including recycle and another is an industrial polymerisation reaction. In each case study, the control problems associated with the given process design and control structure are identified and how the input, disturbance and design parameters influence them is investigated; then the process design modifications are given; and closed-loop dynamic simulations follow in the final section.

In Chapter 6, the major findings and contributions of the work presented in this thesis are summarised and recommendations for future research are outlined.

# Chapter 2

## Literature Review

---

This chapter outlines the background of this thesis and serves as literature review. The main ideas on nonlinear systems and the concept of bifurcation analysis which is used in this thesis are briefly introduced. Process inherent limitations on controllability are discussed in the context of perfect control and process inversion. The relationship between multiplicity and controllability is discussed. A brief review on controllability analysis techniques and design methods for design and control available in the literature is presented, highlighting issues that need addressing.

## 2.1 Basic Concepts and Properties of Nonlinear Systems

### 2.1.1 Fundamentals

#### System Models

In this thesis we consider a continuous nonlinear dynamical system of the form:

$$\dot{x} = f(x, u), \quad (2.1)$$

where  $x \in \mathfrak{R}^n$  is the  $n$  dimensional state variable vector,  $u \in \mathfrak{R}$  is the manipulated variable, and  $\cdot$  denotes differentiation with respect to time  $t$ . The vector function  $f$  and its partial derivatives with respect to  $x$  and  $u$  are assumed to be continuous functions of  $x$  and  $u$ .

#### No Superposition Principle

The superposition principle states, in general, that the response of a linear system to a sum of inputs is the same as the sum of the responses of the individual inputs. That is, a linear combination of solutions

$$x = ax_1 + bx_2 \quad (2.2)$$

for a system with the form

$$\dot{x} = f(x) \quad (2.3)$$

only satisfies the system ( 2.3) if

$$f(ax_1 + bx_2) = af(x_1) + bf(x_2) \quad (2.4)$$

i.e. only if the system ( 2.3) is a linear one.

The superposition principle for a linear system does not apply to a nonlinear system.

### Dependence on Initial Conditions

The dynamic character of a linear system response to an input change is independent of the specific operating conditions at the time of implementing the input change. In other words, identical input changes implemented at different operating steady-state conditions will give rise to output changes of identical magnitude and dynamic character.

A nonlinear system response to a sum of inputs is not equal to a sum of the individual responses and the magnitude, and the dynamic character of the response to an input change are dependent on the initial operation conditions. A distinguishing characteristic of nonlinear systems that makes them differ from linear dynamic systems is that the qualitative properties of nonlinear systems could change under small perturbations of the system parameters.

## 2.1.2 Properties of Solutions

### Steady-state Solutions

For a fixed  $u$ , a steady-state solution  $\bar{x}$  of the dynamical system ( 2.1) is defined by the equation:

$$f(\bar{x}, u) = 0 \in \mathbb{R}^n, \quad (2.5)$$

i.e. a solution which does not change in time. There are other terms used for the “steady-state solution” such as “equilibrium solution” or “stationary point”. In this thesis these terms are alternatively used without distinction.

## Stability of Solutions

Stability is an important concept in system analysis, which is concerned with determining whether the resulting transient response ultimately settles and maintains a new steady-state when an input change is implemented on a system.

Qualitatively, a linear system that is described as stable if starting the system somewhere near its desired operating point implies that it will stay around this point. A linear system is said to be stable if and only if all the poles are in the left-half plane (LHP). Systems with poles on the imaginary axis are unstable from the above notion. The poles of a system with state space description:

$$\dot{x} = Ax \quad (2.6)$$

is defined as the eigenvalues of the constant matrix  $A$ , i.e. the roots of the characteristic equation:

$$\det(sI - A) = 0, \quad (2.7)$$

where  $\det(\cdot)$  stands for determinant. More general, the poles of a system with transfer function  $G(s)$  may be loosely defined as the finite values  $s = p$  where  $G(p)$  has a singularity (or is infinity). The stability of a linear system can be determined from its poles (eigenvalues). A linear feedback system is internally stable if and only if all its closed-loop transfer functions are stable.

For the stability of the nonlinear system ( 2.1), the linearly stable notion is used, which is defined as follows (Wiggins, 1990):

**Definition 2.1** *Suppose all of the eigenvalues of  $Df(\bar{x})$  have negative real parts. Then the steady state solution  $x = \bar{x}$  of the nonlinear equation ( 2.1) is asymptotically stable.*

where  $Df(\cdot)$  is the derivative of function  $f$  from equation ( 2.1), which is defined

by

$$Df = \frac{\partial f_j}{\partial x_i}, \quad i, j = 1, \dots, n. \quad (2.8)$$

A steady state point  $\bar{x}$  is non-stable if at least one real part of the eigenvalues of  $Df(\bar{x})$  is positive.

### 2.1.3 The Concept of Bifurcation Analysis

One can draw conclusions about the local stability or instability of steady-state points for nonlinear systems based on the stability or instability of the linearised systems provided none of the eigenvalues of the linearised systems have zero real parts. The principle difficulty with cases where some of the eigenvalues of the linearised systems have zero real parts and are structurally unstable. A critical case occurs if some of the eigenvalues have zero real part and the other have negative real parts. That means that there are some of the eigenvalues crossing the imaginary axis. Below we provide a very brief introduction to the related concepts of bifurcation analysis used in this thesis which help to explain what happens when the critical case occurs. The text book by Iooss and Joseph (1990) provides more precise and complete description of these concepts.

The steady state solutions of the nonlinear system ( 2.1) depend on the values of  $u$ . It is often necessary to study the dependence of the steady state solutions of the system ( 2.1) on the values of  $u$ . For generality, let us assume now that  $u \in \mathfrak{R}$  is a parameter and set

$$\alpha = u \in \mathfrak{R}. \quad (2.9)$$

The system with the form ( 2.1) becomes

$$\dot{x} = f(x, \alpha). \quad (2.10)$$

A *branch of solutions* is defined as a continuous and uniquely dependent  $x(\alpha)$ . Uniqueness means that for every fixed  $\alpha \in (\alpha_0, \alpha_1)$  there exists an  $\epsilon > 0$  such that there exists no other solution  $x_1(\alpha)$  of equation ( 2.10) satisfying

$$\|x_1(\alpha) - x(\alpha)\| < \epsilon. \quad (2.11)$$

The branch of solutions can be continued in both directions until certain limit values of the parameter  $\alpha$ , say  $(\alpha_0, \alpha_1)$ , are reached and the uniqueness assumption no longer holds for these values. Such critical points will be called *branch points*. At the branch points the behaviour of the solutions of the dynamic system undergoes a qualitative change. This change includes multiple steady-state solutions, instability of the solutions, limit cycles, and so on. Such a kind of phenomenon is commonly called *bifurcation*.

Normally, a gradual variation of a parameter in a system corresponds to the gradual variation of the solution of the problem. However, there exists a large number of problems for which the number of the solutions changes abruptly and the structure of the solution manifold varies dramatically when a parameter passes through these values. In order to understand how the qualitative behaviour of a system changes under the variation of the parameter, *bifurcation analysis* is introduced. Bifurcation analysis is a method for studying such qualitative changes in the behaviour of the nonlinear system when the parameters vary.

For the nonlinear system with the form of ( 2.10), if the steady-state  $\bar{x}$  is a regular steady-state point where all the parts of the eigenvalues of the Jacobian matrix  $Df(\bar{x})$  are nonzero, a small perturbation in the parameter will not change the qualitative behaviour of the system. Bifurcations occur when some of the eigenvalues approach the imaginary axis in the complex plane. The simplest bifurcation is associated with a single real eigenvalue  $\lambda_1$  becoming zero ( $\lambda_1 =$

0) or a pair of complex conjugate eigenvalues  $\lambda_{1,2}$  crossing the imaginary axis ( $\lambda_{1,2} = \pm i\omega_0$ ,  $\omega_0 > 0$ ). The bifurcation where  $\lambda_1 = 0$  is called a *fold (turning or limit point) bifurcation*. The bifurcation where  $\lambda_{1,2} = \pm i\omega_0$ ,  $\omega_0 > 0$  is called *Hopf bifurcation*. These are the most common bifurcations encountered in nonlinear systems. A *fold bifurcation* usually is the cause of multiple steady states. *Hopf bifurcations* are responsible for the appearance and disappearance of periodic solutions. The stability of the system must change at each bifurcation point, and only at such a point (Iooss and Joseph, 1990).

If the other parameter effects on the bifurcation points are considered, we have a picture of the solution dependence on the parameters, which is called a *bifurcation diagram*. This diagram can be used to determine how the system behaves under changing conditions, and then could provide a guideline to modify the system to avoid bifurcations.

Bifurcation analysis can obtain insights into what the dynamics of a nonlinear process is and how parameters influence them and is used to investigate the behaviour of the process in terms of parameter-dependent branches of steady-state solutions. Several decades ago, bifurcation analysis was applied to chemical processes. In the 70's, Aris (1979) applied bifurcation theory to discuss some complex phenomena in chemical reactors and Chang and Calo (1979) presented a bifurcation-approach to determining the regions of unique and multiplicity solutions to chemical reaction. Recently, bifurcation analysis is recognised as a powerful tool and widely applied to nonlinear chemical process analysis (Seider *et al.*, 1991; Pinto *et al.*, 1995; Russo and Bequette, 1996, 1997, 1998; Pushpavanam *et al.*, 2001; Zhang and Henson, 2001). Using bifurcation analysis was also suggested in process design (Seider *et al.*, 1991; Morari, 1992). Bifurcation analysis to aid in redesigning processes has been proposed (Russo and Bequette, 1995).

The continuation technique, a numerical technique to obtain one or more branches of steady-state solutions mutually connected at bifurcation points, has been developed and is widely used for bifurcation analysis (Keller, 1977; Kubíček and Marek, 1983). With advanced computational techniques and computer's power, continuation and bifurcation analysis software packages available, such as AUTO (Doedel *et al.*, 1998), can allow one to carry out bifurcation analysis for large nonlinear systems.

## 2.2 The Concept of Controllability in Process Engineering

Qualitative changes of nonlinear processes resulting in the complex behaviour have been briefly discussed in last section and bifurcation analysis provides a method for exploring the complex solution spaces for a nonlinear process as a parameter of the process varies. When a nonlinear process exhibits complex characteristics, the control performance of the process might be adversely affected or possibly the process cannot be controlled. This section is concerned with the issue of controllability, which describes the achievable dynamic performance (set point following and disturbance rejection) for a process in control.

In the literature, there are many different definitions about controllability. Ziegler and Nichols (Ziegler and Nichols, 1943) first defined controllability as “the ability of the process to achieve and maintain the desired equilibrium value”. Later the term “controllability” became synonymous with the rather narrow concepts of state controllability, which was introduced by Kalman in the 60's. *State controllability* is defined as the ability to bring a system from a given initial state to any final state within a finite time. State controllability is still a widely used

criterion for controllability in the control system community but not necessarily the most appropriate for chemical process control. This is because state controllability is concerned only with the value of the states at discrete values of time, while in most cases we want the outputs to stay close to some desired values (trajectory) for all values of time, and without using inappropriate control inputs.

An alternative is *functional controllability*, defined by Rosenbrock (1970). A system with polynomial transfer function matrix  $G(s)$  is called functionally controllable if it satisfies the following condition (Rosenbrock, 1970). Given any trajectory output which is zero for time  $t = 0$  and which satisfies certain smoothness conditions, there exists an input trajectory  $u$  defined for time  $t > 0$  which generates the output  $y$  from the initial condition  $x(0) = 0$ .

Rosenbrock stated that a system with transfer function  $G(s)$  is functionally controllable if and only if  $G(s)$  is nonsingular. Sufficiency of this condition is obvious because the expression

$$u(s) = G^{-1}y(s) \quad (2.12)$$

has input trajectories which generate the required output trajectories.

Functional controllability has some advantages over state controllability for the evaluation of controllability of chemical process as indicated in Russell and Perkins' paper (1987). State controllability does not guarantee that it is possible to independently specify arbitrary trajectories of the selected set of output variables, whereas functional controllability does (subject to smoothness conditions). This is important since the main goal of regulatory control is usually to maintain the plant at some steady state.

Rosenbrock (1970) stated that "most industrial plants are controlled quite

satisfactorily though they are not (state) controllable”. An example of tanks in series was given by Skogestad and Postlethwaite (1996). As the result of this example, it is seen that the property of state controllability may not imply that the system is controllable in a practical sense.

Functional controllability depends on the invertibility of the transfer function. Thus an examination of the properties of the system which prevent the inversion of the system will provide a valuable tool for controllability analysis and therefore control system synthesis.

To avoid confusion with state controllability, Morari (1983a) also introduced the concept of “*dynamic resilience*”, which describes the quality of control behaviour that can be obtained for a plant by feedback. This term does not capture the fact that it is related to control design.

Recently, the concept of *input-output controllability* is introduced. Skogestad and Postlethwaite (1996) defined the input-output controllability as “the ability to achieve acceptable control performance” and then followed an explanation “to keep the outputs ( $y$ ) within specified bounds or displacements from their references ( $r$ ), in spite of unknown but bounded variations, such as disturbances ( $d$ ) and plant changes, using available inputs ( $u$ ) and available measurements ( $y_m$ ) and ( $d_m$ )”.

The input-output controllability definition is more in tune with most engineers’ intuitive feeling about what controllability means, though only a structural property of a process is involved. In particular, for instance chemical processes, there are a lot of bounds, such as inputs, measurements, devices, and disturbances and uncertainties, and chemical processes are likely to exhibit strong nonlinear and complex behaviour subject to changing operation conditions and uncertainties. In this sense, the general notion of controllability, which follows the Skogestad and Postlethwaite’s definition, is used in this thesis, and simply referred to

as *controllability*.

Often the controllable performance of a system is assessed by exhaustive simulations, which requires a specified controller design. This implies that it is not possible to know from this kind of assessment if the behaviour is a fundamental property of the system, or if it is due to a specific controller used. By definition controllability does not depend on the controller but only on the system itself.

A potentially rigorous approach to controllability analysis is an optimisation-based test that formulates mathematically the control objectives, the class of disturbances, the model uncertainty, etc., and then attempts to synthesis ideal control to see whether the performance objectives can be met (Perkins and Walsh, 1996). This could be applied to processes without detailed control designs on controllability assessment and much progress has been made in this area (see § 2.5.3).

So, there are many different ways to definite and assess the controllability of a process. What is ultimately of interest is the dynamic performance of the process subject to disturbances, model parameter and operating condition changes, and other changes in its environment, and what is more desirable is to have a few simple tools which can be used to obtain a rough idea of how easy the process is to control. The methods should be independent of detailed controller designs so that the inherent limitations on controllability by the process design itself, which no control system, whatever sophisticated, will be able to overcome, can be identified; and the methods should enable to effectively analyse the effects of these limitations, which could lead an modified process with improved controllability. It is some of importance, as stated by Perkins *et al.* (1996), that analysing the effects of these limitations early enough in the design process allows the opportunity to modify the design should the effects be critical to performance.

This thesis will focus on developing an analysis methodology for process modifications, rather than only for controllability evaluation as the majority work had been concerned with in this area.

## 2.3 Limitations on Controllability

Controllability describes the achievable dynamic performance of a process independent of controller design. In order to analyse controllability, it is desirable to understand what imposes limitations on controllability and how the process behaves subject to changing conditions. It has been identified that some process characteristics will limit the control performance and pose control difficulties for controller design, such as input constraints, time delays, right half plane (RHP) zeros, and a number of techniques are now available to evaluate their potential impact on closed-loop performance mainly for linear systems (see Morari, 1983; Skogestad and Postlethwaite, 1996).

In this section the limitations on the control performance and difficult control design problems associated with the inherent characteristics of a process such as RHP zeros are addressed. Several concepts related to control system design and analysis are given. The definitions and ideas for linear systems are briefly described in order to explain the nonlinear approaches for nonlinear systems.

### 2.3.1 The Concept of Zeros and Zero Dynamics

A controller generates an approximate inverse of the process in an implicit or explicit form (Morari, 1983). This implies that the inverse characteristics of the process will determine if the control is easily realised or not. In order to study the inverse behaviour of a nonlinear process, the concept of zero dynamics is introduced, which is analogous to the notion of the zeros of a linear system.

## Zeros

For a single input single output (SISO) linear system with input-output transfer function  $G(s)$ , the zeros  $z_i$  are the solutions to  $G(z_i) = 0$ , as in the following definition:

**Definition 2.2** (*Zeros*) *The zeros of a linear system with the state space form:*

$$\dot{x} = Ax + Bu \quad (2.13)$$

$$y = Cx \quad (2.14)$$

*are the roots of the numerator polynomial of its transfer function:*

$$\begin{aligned} G(s) &= C(sI - A)^{-1}B \\ &= \frac{C \operatorname{adj}(sI - A)B}{\det(sI - A)}, \end{aligned} \quad (2.15)$$

*i.e. the roots of  $C \operatorname{adj}(sI - A)B$  (Kravaris and Kantor, 1990a).*

The definition of zeros is based on a transfer function description, which is a minimal realisation of a system.

There will be additional zeros found if the description is not minimal. Those additional zeros arise from hidden pole/zero cancellations in the non-minimal order description. A minimal order realisation of the system will, however, lead to the same zeros as the transfer function description (Kravaris and Kantor, 1990a).

For a multivariable system, the following definition of the zero of a multivariable systems is used:

**Definition 2.3** (*Zeros*) *The zeros of a linear multivariable system,*

$$\begin{aligned} \dot{x} &= Ax + Bu, \\ y &= Cx, \end{aligned} \tag{2.16}$$

*are the roots of the determinant of its transfer function matrix, i.e.*

$$|C \operatorname{adj}(sI - A)B| = 0, \tag{2.17}$$

*where the transfer function matrix is square (MacFarlane and Karcanias, 1976).*

When the transfer function matrix is not square, it is no longer possible to define the zeros in terms of determinants. The more general definition of the zeros of a multivariable system resulting from the generalization of the notion of the determinant of a square matrix is expressed as: those values of  $s$  for which the rank of the transfer function matrix  $G(s)$  is reduced are called the zeros of  $G(s)$ .

**Remark 2.1** *It is possible for a multivariable system to have poles and zeros in the same location. In evaluating the zeros of a multivariable system from the determinant of its transfer function matrix, it is therefore utmost important to ensure that the denominator polynomial contains all the system poles, i.e. ensure that there has been no pole-zero cancellation when forming the determinants (see Morari and Zafiriou, 1989).*

An alternative interpretation of the zeros of a system is to view them as the poles of the inversion of the system. This view makes it easier to move to nonlinear systems and the notion of the zero dynamics.

## Zero Dynamics

For a linear system, the zeros are the roots of numerator polynomial and, in other words, are the poles of the inverse of its transfer function. The zeros of a linear system are completely determined by the characteristics of its inverse. For a nonlinear system, transfer function, on which linear system zeros are based, cannot be defined, and therefore cannot have zeros as a set of numbers. A notion, *zero dynamics*, is imported, which is analogous to the right half plane (RHP) zeros of a linear system. The zero dynamics for a nonlinear system is defined to be the internal dynamics of the system when the system output is kept at zero by the input (Isidori, 1995; Slotine, 1991). In order not to disrupt the whole flow of this thesis, the more details about zero dynamics is given in Appendix B.

Regarding the stability of the zero dynamics, the terms of the minimum phase (MP) and nonminimum phase (NMP) are used and defined as:

**Definition 2.4** *A system is termed minimum phase (MP) at a steady state point  $\bar{x}$  if its zero dynamics are stable at  $\bar{x}$ , otherwise, it is nonminimum phase (NMP).*

### 2.3.2 Perfect Control

#### Perfect Control of Linear Systems

Let the process model be:

$$y = G u + G_d d, \quad (2.18)$$

where  $G$  and  $G_d$  are the process and disturbance transfer functions, respectively.

“Perfect control” is achieved when the output is identically equal to the reference, i.e.  $y = y_{ref}$ . To find the corresponding process input, let us set  $y = y_{ref}$  and solve ( 2.18) for  $u$ :

$$u = G^{-1}y_{ref} - G^{-1}G_d d, \quad (2.19)$$

which represents a perfect feedback controller, where  $G^{-1}$  is the inverse of the process. When proportional feedback control

$$u = K(y_{ref} - y) \quad (2.20)$$

is used, we have the form:

$$u = (I + KG)^{-1}Ky_{ref} - (I + KG)^{-1}KG_d d. \quad (2.21)$$

If we make  $K$  “large” then we see qualitatively that ( 2.21) becomes

$$u \approx G^{-1}y_{ref} - G^{-1}G_d d. \quad (2.22)$$

An important lesson therefore is that perfect control requires the controller to somehow generate an inverse of  $G$  (Morari, 1983). From this perfect control cannot be achieved if

- $G$  contains RHP-zeros (since then  $G^{-1}$  is unstable);
- $G$  contains time delays (since then  $G^{-1}$  contains a prediction);
- $G$  has more poles than zeros (since then  $G^{-1}$  is unrealizable).

### Perfect Control of Nonlinear Systems

Consider a nonlinear system with the following form:

$$\begin{aligned} \dot{x} &= f(x, u), \\ y &= h(x), \end{aligned} \quad (2.23)$$

where  $x \in \mathfrak{R}^n$ ,  $u \in \mathfrak{R}$ , denote the state variable vector and the manipulated variable, respectively, and  $f$  denotes smooth vector fields on  $\mathfrak{R}^n$ ,  $h$  is a smooth scalar function on  $\mathfrak{R}$ . The system ( 2.23) can, more generally, be described by the input/output nonlinear operator implied by the model:

$$y = P[u], \quad (2.24)$$

where  $P$  is a general nonlinear operator that maps the input  $u$  into the output, or response,  $y$ . If  $\tilde{y}$  represents the actual measurement of the plant output then the model error obtained as

$$e = \tilde{y} - y \quad (2.25)$$

enables us to express

$$\tilde{y} = P[u] + e \quad (2.26)$$

as the relationship between the input and the actual plant output.

Given  $y_{ref}$  as the desired trajectory for the actual plant output  $y$  to follow, the control action  $u$  that satisfies the objective

$$\min_u = \|y_{ref} - \tilde{y}\| \quad (2.27)$$

is obtained as

$$u = P^{-1}[y_{ref} - e], \quad (2.28)$$

provided that the inverse of  $P^{-1}$  exists. If  $y_{ref}$  is selected as the set-point  $y_{set}$  for  $y$ , then

$$u = P^{-1}[y_{set} - e]. \quad (2.29)$$

It is noted here that nominal stability is concerned with the case  $e = 0$ , for which

( 2.29) implies an open-loop control policy, and feedback appears only in the presence of the existence of the error, i.e.  $e \neq 0$ .

It is clear that ( 2.29) results in so called “perfect control” when  $P^{-1}$  exists (and is realisable). For a nonlinear operator the  $P^{-1}$  may not exist. If this is the case, it cannot be realisable. For nonminimum phase systems, the problem is analogous to the linear case; the inverse of a time delay system is not realisable due to the necessity of producing predictions.

### 2.3.3 Ideal ISE Optimal Control

As stated in the previous section, perfect control is not possible for all systems. A way to have insight into the “best” control performance is to consider an ideal controller which is integral square error (ISE) optimal. For invertible system, this is equivalent to considering perfect control as above, but for non-invertible systems this approach makes it possible to determine the “best” possible controller (in terms of ISE). For a given output trajectory (which is zero for time  $t < 0$ ), the ideal controller is the one that generates the plant input  $u(t)$  (zero for time  $t < 0$ ) which solves the following:

$$\min ISE = \frac{1}{2} \int_0^{\infty} \|y_{ref} - y\|^2, \quad (2.30)$$

subject to

$$\begin{aligned} \dot{x} &= f(x, u), \\ y &= h(x), \\ x(0) &= x_0, \end{aligned} \quad (2.31)$$

where  $u$  is the input,  $y$  is the output,  $x$  is the state vector,  $y_{ref}$  is the reference output,  $f$  and  $h$  are the plant model equations, and  $x_0$  is the vector of the initial states. This controller is ideal in the sense that it may not be realisable in practice because the cost function includes no penalty on the input  $u(t)$ . The perfect control ( $ISE = 0$ ) represents the inverse of the process.

For a SISO stable plant with real RHP zeros at  $z_i, i = 1, \dots, m$ , the ideal ISE value for a step change in the reference is given by (Morari and Zafiriou, 1989):

$$ISE = \sum_{i=1}^m \frac{2}{z_i} \quad (2.32)$$

or with complex RHP zeros  $z = x \pm jy$

$$ISE = \frac{4x}{x^2 + y^2}. \quad (2.33)$$

Thus, as for SISO linear systems, RHP-zeros close to the origin imply poor control performance. Therefore, to relocate the zero positions can improve the control performance (Skogestad and Postlethwaite, 1996).

**Remark 2.2** For a MIMO linear plant with RHP transmission zeros at  $z_i$ , the ideal ISE value for a step disturbance or reference is also directly related to  $\sum_{i=1}^m \frac{2}{z_i}$  (Qiu and Davison, 1993).

For nonlinear systems having nonminimum phase behaviour the problem (2.31) cannot be solved numerically due to two major problems:

- An infinite time horizon is not implementable in a nonlinear setting
- The solution  $ISE = 0$  (a representation of the inverse of the process) is unstable for NMP systems

Thus unstable zero dynamics impose unavoidable limitations on the closed-loop performance of nonlinear systems (Seron *et al.*, 1997).

### 2.3.4 Control Problems Associated with Unstable Inversion

Unstable inverse behaviour of a system has been identified as one of the system inherent limitations on control performance. Such a characteristic also presents hard problem for the stability of the controller. Concerning the realisation of a controller for a linear system RHP zeros contribute additional phase lags to the system when compared to that of a minimum phase system with the same gain. A larger phase lag brings the system closer to its stability margin (Stephanopoulos, 1984). The extra phase lag also causes a limited speed of response by limiting the obtainable bandwidth. The upper bound on the bandwidth  $\omega$  for a SISO system is approximated by  $\omega < z/2$  ( $z$  is a real RHP zero) (Skogestad, 1996).

For the control of a nonlinear system with NMP behaviour has a similar effect (Seron *et al.*, 1997). The presence of unstable zero dynamics forbids the implementation of any controller from the class of nonlinear inversion-based controllers since such a controller is unstable.

**Remark 2.3** *A NMP system could be stabilised either with longer prediction horizons or by putting a penalty on the input in the objective function within the framework of optimal control such as nonlinear model predictive control (NMPC). However, an offset-free performance (i.e. ideal optimal control) cannot be achieved in the presence of a disturbance when the input is penalised in the objective function (Sistu and Bequette, 1995; Seki and Morari, 1998).*

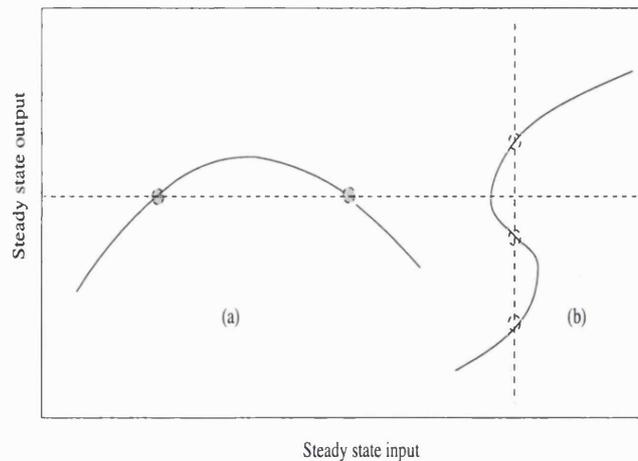


Figure 2.1: Two possible types of multiplicity. a) input multiplicity; b) output multiplicity.

## 2.4 Input Multiplicity and Controllability

In the previous sections, we have discussed difficult characteristic of a system with respect to the closed loop stability and performance. A stable and invertible process is very desirable from a control design standpoint. However, for a nonlinear process, the characteristic behaviour of the system and its inverse such as stability may change with changes in operating conditions, resulting in difficult control problems.

A multiple steady-state phenomenon, namely multiplicity, is often found in nonlinear chemical processes, which shows multiple solutions and changes in the stability of the solutions. Chemical processes have been known to exhibit such nonlinear behaviour. A number of the papers published have reported multiplicity found in reactions, distillation columns, polymerisation reactions, etc. (Amundson and Aris, 1958; Uppal *et al.*, 1974; Balakotaiah and Luss, 1981; Dash and Koppel, 1989; Gani and Jørgensen, 1994; Sistu and Bequette, 1995; Ray and Villa, 2000).

There are two typical types of multiplicity as illustrated in Figure 2.1: *input*

*multiplicity and output multiplicity.* *Input multiplicity* refers to the case where there exist more than one steady state solutions when the output is specified (curve (a) in Fig. 2.1); *output multiplicity*, the most common form, refers to the case where one input can produce more than one distinct outputs (curve (b) in Fig. 2.1).

Uppal *et al.* (1974) and Aris (1979) have presented multiplicity behaviour found in chemical reactors and Koppel (1982) have studied the effect of input multiplicity in control systems. Dash and Koppel (1989) have shown a number of chemical process examples with input and output multiplicity and demonstrated that input multiplicity can be a main cause of “sudden destabilisation” of the controlled system with integral action. Recently, Sistu & Bequette (1995) and Seki & Morari (1998) demonstrated the control performance and control problems imposed by input multiplicity behaviour under nonlinear model predictive control (NMPC). A process having input multiplicity behaviour is difficult to control because there exists more than one steady state manipulated variable value associated with a given output. A process with input multiplicity behaviour also places a limitation on the structure of the feedback controller (Koppel, 1982) and poses the feedback performance limitations since there must exist unstable zero dynamics on one “side” of the steady-state operating curve under some mild assumptions (Russo and Bequette, 1996). Therefore, the attention in this thesis focuses on processes with input multiplicity.

### 2.4.1 Input Multiplicity and RHP Zeros

In this subsection the combination between input multiplicity and RHP zeros or zero dynamics of processes will be discussed. It has demonstrated for SISO systems that models having input multiplicity behaviour will, under some assumptions have RHP zeros (Sistu and Bequette, 1995). This implies that a process with input multiplicity will have stability changes in its inverse.

Consider the SISO continuous nonlinear system with the form ( 2.23). The steady state solution to the system ( 2.23) is obtained by solving the equations of the form:

$$0 = f(x_s, u_s), \quad (2.34)$$

$$y_s = h(x_s), \quad (2.35)$$

where the subscript  $s$  indicates steady state values.

If the equation ( 2.35) has multiple steady-state solutions then the steady-state input-output relationship could be depicted by the curve (a) or (b) shown in Figure 2.1. A process having output multiplicity can reach a nonunique output  $y_s$  for a given input  $u_s$ , depending on the initial conditions. On the other hand, a system with input multiplicity behaviour can have more than one steady-state input  $u_s$  for a specified output  $y_s$ . It is noted from the curve (a) that the steady-state gain changes its sign in the operating region.

Mathematically, the condition for the existence of the steady state input multiplicity is (Koppel, 1982):

$$G(0) = -CA^{-1}B = 0, \quad (2.36)$$

where  $G(0)$  is the steady state process gain (Morari, 1983, Jacobsen, 1994),  $A$ ,

$B$ , and  $C$  represent the gradients of function  $f(x, u)$  with respect to  $x$ ,  $f(x, u)$  with respect to  $u$ , and  $h(x)$  with respect to  $x$  at the steady state operating point, respectively.  $A$ ,  $B$ , and  $C$  are obtained by linearising ( 2.23) around the steady state point  $(x_s, u_s)$ :

$$A = \left. \frac{\partial f}{\partial x} \right|_{x_s, u_s}, \quad (2.37)$$

$$B = \left. \frac{\partial f}{\partial u} \right|_{x_s, u_s}, \quad (2.38)$$

$$C = \left. \frac{\partial h}{\partial x} \right|_{x_s, u_s}. \quad (2.39)$$

Inserting the equations ( 2.37), ( 2.38) and ( 2.39) into the equation ( 2.36) gives the following equation:

$$\begin{aligned} G(0) &= CA^{-1}B \\ &= \left. \frac{\partial h}{\partial x} \frac{\partial x}{\partial f} \frac{\partial f}{\partial u} \right|_{x_s, u_s} \\ &= - \left. \frac{\partial h}{\partial u} \right|_{x_s, u_s} \\ &= 0 \end{aligned}$$

Thus  $G(0) = 0$  at the point  $(x_s, u_s)$  implies that the output is at the potential maximum or minimum point. If one wishes to control at the maximum or minimum output, a control problem arises since the steady state gain is zero. However, even at points away the maximum or minimum output there may be limitations in the achievable control performance due to unstable zero dynamics. Sistu and Bequette (1995) state in their **Lemma 1**:

*If the open loop steady state gain of a SISO nonlinear system changes sign in an operating region, then there is at least one zero of the linearised process crossing the imaginary axis under the following assumptions:*

1. *There is no simultaneous change in the relative order of the linearised process.*
2. *The linearised process dynamics are described by a strictly proper transfer function with at least one finite zero.*

This implies that if the inverse of the system is stable on one side of the maximum in the steady state curve it must be unstable on the other side, and vice versa. It will be sufficient to note that whenever the equation ( 2.36) is true one must consider the possibility of the existence of input multiplicity and cannot be confident of the unique behaviour (exchange of stability) of the inverse of the system (Koppel, 1982). Defined by the mathematics of bifurcation theory, the equation ( 2.36) has its significance that can be referred to as a bifurcation condition in bifurcation analysis (discussed in Chapter 3).

### **2.4.2 Control Problems Associated with Input Multiplicity**

Input multiplicity implies a change in the steady state gain of a system which imposes difficult control problems in control system designs. The potential control problems associated with input multiplicity in several common control design techniques are discussed as follows.

When a process gain sign changes, the process with a fixed conventional controller having integral action will result in a positive feedback loop and become unstable (Koppel, 1982). In addition systems with input multiplicity may be nonminimum phase in a region of the operating range - one of the major limitations on controllability. Especially at operating points close to the maximum of the steady state curve, nonminimum phase behaviour can be expected to be

detrimental to control performance because the linearised zero is situated close to the origin (Morari, 1983).

Within the framework of *robust control* (Morari and Zafiriou, 1989) this has been formulated as follows. It is possible to design a linear feedback controller which guarantees zero tracking error for steps, if and only if the steady state gain uncertainty does not exceed 100 %, i.e. the process steady state gain does not change sign.

Using *input/output linearisation* controller design techniques by employing differential geometry methods for nonlinear process control have been proposed (Isidori, 1995; Kravaris and Kantor, 1990a; Slotine, 1991). However, stability of the zero dynamics is necessary condition for the input/output linearised controller to yield an internally stable closed-loop system (Isidori, 1995). At the maximum (or minimum) of the steady state of the system the controller following exact linearisation techniques generates infinite control moves due to zero process gain. Henson and Seborg (1992), who applied *input/output linearisation* controller design technique to a particular continuous fermenter process having input multiplicity behaviour, demonstrated the control problems caused by instability of the zero dynamics. An ad hoc method for exact linearising controller design for improving the control performance of the system was proposed to avoid breaching input multiplicity condition by holding the manipulated variable constant near the maximum, provided that the maximum is known.

Sistu and Bequette (1995) analysed the application of a *nonlinear model predictive controller* (NMPC) on processes with input multiplicity. Their work demonstrated problems caused by the instability of the employed controller in the nonminimum phase region, which resulted in the process moving to another steady state solution in the minimum phase region, where the controller is stable.

Seki and Morari (1998) employed *receding horizon control* (RHC) techniques

(same as MPC in principle) for nonlinear processes which exhibit input multiplicity behaviour. An infinite-time horizon linear quadratic optimal problem was formulated with penalty on the control input as well as on its time-derivative in the performance index, based on local linearisation of the nonlinear process model around its trajectory. They showed that the input penalty in the performance index made it possible to handle SISO processes with input multiplicity. However, the offset removal could not be achieved due to the penalty on the input, and the tuning parameters must be carefully chosen to have a local closed-loop stability.

In general the following problems concerning the control of a process associated with input multiplicity can be expected. At the maximum of the steady state curve the process is not controllable due to the zero steady state gain. In addition, systems with input multiplicity may have unstable zero dynamics which poses inherent limitations on the control performance and potentially internal instability problems.

When we consider a process having input multiplicity in an inverse-based control system framework, we could probably refer the occurrence of input multiplicity condition in equation ( 2.36) (see § 2.4.1), namely vanishing of the determinant of the process gain matrix, to as a bifurcation condition. When equation ( 2.36) is true, we cannot be confident the inverse of the control system exists as a one-to-one mapping from values of outputs to values of inputs and there exist more than one input for a specified output (Koppel, 1982), probably resulting in a big move in input or dramatic change in the control system.

Input multiplicity gives rise to a cause for considerable concern in control system design and complexity of controller designs (Morari and Zafiriou, 1989; Sistu and Bequette, 1995).

## 2.5 An Overview of Controllability Analysis Techniques and Process Design Methods for Improved Controllability

In this section, an overview is presented of the principle, published methods for controllability analysis and integration of process design and control. Rather than going into specific details of the approaches, the focus is on investigating the classes of problems that they are able to treat. Much of this work in the literature has focussed on the development of analysis tools that provide some measures of the controllability of a process and that could allow design alternatives to be screened or compared on a common sense. There exist comprehensive review papers on this subject (Perkins, 1989; Morari, 1992; Perkins & Walsh, 1996).

### 2.5.1 Definitions

In order to clarify the following discussions it seems necessary to define a number of terms. There are other definitions around but these ones will be used in this thesis.

- *Controllability* concerns the dynamic performance of a process and its ability to cope with variability and uncertainty (setpoint following and disturbance rejection) subject to feedback control independent of the controller design.
- *Flexibility* concerns the ability to accommodate uncertainty at steady state.
- *Operability* concerns the ability of a process to deal with uncertainty and disturbance and also with issue of reliability and maintenance.

- *Switchability* is the ability of a process to cope with changes of operation between operating points.
- *Dynamic resilience* concerns the quality of the control system behaviour (setpoint following and disturbances rejection) that can be obtained for a process by feedback.

## 2.5.2 Techniques for Controllability Analysis

The major works on controllability analysis are summarised in Table 2.1. In general, these measures are broadly classified into two main sets: linear model based approaches and nonlinear model based approaches.

### Linear Methods

Commonly used controllability measures for linear systems include the relative gain array (RGA) (Bristol, 1966) and the minimised condition number (CN) (Nguyen *et al.*, 1988), both of which rely on a linear model describing the effect of control variables on the process outputs (structural controllability). Typical resilience measures are the disturbance condition number (Skogestad and Morari, 1987), the disturbance cost (Weitz and Lewin, 1996) and the relative disturbance gain array (Chang and Yu, 1992), which require input-output control structure as well as an additional disturbance model that describes the effect of the disturbance on the process outputs. A review and a procedure for controllability analysis for linear systems is demonstrated in Skogestad and Postlethwaite (1996). The principle is to consider the effect of the different limitations separately and then to conclude whether or not controllability is sufficient for a given task and also to rank order different design alternatives. It is also one of major problems in controllability analysis to date since there are many different aspects resulting from

Table 2.1: Summary of the typical controllability analysis measures in the literature

Authors	Merits	Model
Morari (1983)	IMC: RHP Zeros, time delay	LD
Holt and Morari (1985)	RHP Zeros	LD
Perkins and Wong (1985)	Time delay, CN, RHP Zeros	LD
Palazoglu <i>et al.</i> (1985)	CN	LD
Morari <i>et al.</i> (1987)	RHP Zeros	LD
Russell and Perkins (1987)	Time delay	LD
Skogestad and Morari (1987)	CN	LD
Bogle and Rashid (1989)	CN	LD
Naraway and Perkins (1991)	Economic back-off	LD
Skogestad <i>et al.</i> (1991)	Frequency-dependent RGA, CLDG	LD
Elliot and Luyben (1995)	Off-specified product time	LD
Weitz and Lewin (1996)	Disturbance Cost	LD
Sorough (1996)	Time delay	LD
Zafiriou and Chou (1996)	Process Zeros	LD
Cao <i>et al.</i> (1996)	Output deviation	NLD
Young <i>et al.</i> (1996)	Economic back-off	LD
Kuhlmann and Bogle (1997)	NMP performance	NLD
Gal <i>et al.</i> (1998)	Structural controllability	LD
Chenery and Walsh (1998)	Output deviation	LD
Zheng <i>et al.</i> (1999)	Surge tank	LD
Vinson & Georgakis (2000)	Achieved output space	NLD
Kim <i>et al.</i> (2000)	Structural controllability	NLD
Kuhlmann and Bogle (2001)	NMP performance	NLD

IMC = Internal Model Control; RHP = Right half Plane; NMP = Non-Minimum Phase;  
 CN = Condition Number; RGA = Relative Gain Array; LD = Linear Dynamics;  
 NLD = Non-Linear Dynamics; CLDG = Closed-Loop Disturbance Gain,

such analysis. It is the reason that many researchers now develop optimisation-based integration methods for controllability tests where a single value connected to the economics of the process is generated that allows for realistic use to rank alternative designs (Luyben *et al.*, 1992, 1994; Perkins and Walsh, 1996; Chenery and Walsh, 1998; Ellito *et al.*, 1995; Zheng *et al.*, 1999; McAvoy, 1999; Kookos and Perkins, 2002).

As can be seen from Table 2.1, most tools rely on the use of steady-state or linear dynamic models, and the use of such models may be adequate in some cases. But, in general, it is quite unpredictable whether the conclusions drawn are correct, particularly in the face of process nonlinearities. Often, the final evaluation of the controllability of a system has to go through simulations, in particular when nonlinear characteristics are important. Moreover, while a dynamic simulation is used, several limitations can be identified:

- It is inefficient and potentially not inclusive, especially when the process possesses fast and slow modes;
- It is incomplete since only a limited number of simulation tests can be performed, and important and complex dynamic behaviour may not be observed for the specified conditions.

### **Nonlinear Methods**

In most cases, it appears that a controllability evaluation based on a linearised model for a nonlinear system by using controllability criteria as described above suffices (Perkins, 1989; Morari, 1992). Often, it is quite easy to design simple static nonlinear compensators which remove most of the process nonlinearity. The compensated system can then be analysed with linear techniques. This is true for the regulatory performance around a specified steady state point but fails

for problems with the high degree of nonlinearity, ranged throughout the entirely operating regions. The reliability of the controllability analysis conclusions from these linearised methods is only around the specified conditions, which is main drawback of employing linear analysis methods for nonlinear systems.

But very important instances, processes can exhibit nonlinear behaviour which is not easily correctable with simple nonlinear transformations. These nonlinear characteristics may have adverse effects on the dynamic performance of the systems. Therefore, it is of some importance to understand complex nonlinear behaviour of a process and to analyse the effects of the parameter and operation conditions on it.

The complex behaviour of a nonlinear process and its dependence of the parameters and conditions can be analysed by utilising nonlinear techniques such as bifurcation analysis. If this is done early enough at the design stage, the potential control problems associated with the characteristics could be eliminated or avoided by modifying the process design itself (Morari, 1992).

It is argued that as long as the dynamics are known to the control engineers, modern nonlinear control algorithms that allow one to deal with almost any difficult control situation, and consequently regions of usual dynamic behaviour should not be avoided in process design, such as nonlinear predictive control could handle with difficult control problems. Carried to the extreme, one could conclude that such a nonlinear analysis is not needed at all at the design stage since any complex nonlinear behaviour can be fixed later on by the control algorithm (Seider *et al.*, 1990). This may be true for controller design but is not satisfactory for analysing the controllability of a system since it is necessary to fully identify all potential problems associated with the complex behaviour and to assess how easy the design is to control when the design alternatives are considered at the design stage.

### 2.5.3 Design Methods for Improved Controllability

Consideration of the controllability of a process at an early phase of the process design is now being widely accepted in both academia and industry. A number of methodologies and tools have been reported for taking account of the interactions between process design and process control. A class of approaches that include the question of controllability into the design problem formulation are the optimisation based methods for synthesis and design. The first approach employing optimisation is the steady-state flexibility approach by Grossmann *et al.* (1983). Here feasible operation is checked for a range of operating conditions including uncertainties and the design variables are determined accordingly. A formulation is used that includes operating variables that are allowed to be varied in order to compensate for the uncertainties at steady state. This work has been extended by Swaney and Grossmann (1985) in order to measure the flexibility of a process by maximising a scalar value called the flexibility index. Both measures evaluate the flexibility of a process at steady state. Dimitriadis and Pistikopoulos (1995) extended this approach for dynamic systems. Mohideen *et al.* (1996) further extended this work by employing an economic objective. They formulated the process and control design within an integrated optimisation framework, where process characteristics and control system parameters were determined simultaneously. Rigorous dynamic models, pre-specified disturbance and PID controllers were used while significant economic benefits were reported. Further work following this measure has been presented by Bansal *et al.* (2000a).

Narraway and Perkins (1993) presented a method for selecting of the economically optimal control structure of a process without designing the process controller, while preserving good controllability characteristics. Assuming perfect disturbance rejection by the control system and a linear dynamic model for

the process, a systematic economic evaluation of the candidate control structures was performed using a mixed-integer linear programming technique. Recently, Kookos and Perkins (2002) presented a modification to the previous work of Naraway and Perkins (1993). In their work, the control objectives are posed in terms of economic penalties associated with the effect of disturbance on key process variables aiming to identify optimal control structure selection for static output feedback controllers.

Luyben and Floudas (1994a) approached the design problem taking into account dynamic control performance characteristics in the form of matrix merits within a multi-objective optimisation framework.

White *et al.* (1996) proposed an approach to evaluate switchability of a process design, or its ability to move between operating points. Their approach was based on determining the optimal switching trajectory for the plant by setting up and solving an optimal control problem. One feature of this approach is the ability to include parameters characterising the design of the plant as decision variables.

Bahri *et al.* (1996) presented a back-off optimisation formulation to examine the disturbance rejection capability of the given design and find a back-off optimal design in order to reject the specified disturbance at steady state. One feature of optimisation formulation of Bahri *et al.* is the ability to include parameters characterising the design of the plant as decision variables without control design. In their later work, Bahri *et al.* (1997) extended their work in dynamic situation. In this work dynamic performance was evaluated dependent on detailed control design.

Zheng *et al.* (1997) based the selection of the controlled and manipulated

variable set on the sensitivity of the optimal economic potential to process disturbances in a hierarchy approach for plantwide control system synthesis. Relative gain array (RGA) and singular value were utilised in the selection of proper variable pairing. A controllability index introduced by Zheng and Mahajanam (1999) accounted for the minimum additional surge capacity required for a given structural process and control design to achieve the dynamic objectives of the control system.

McAvoy (1999) presented a methodology for the design of plantwide control systems for a given set of controlled variables that satisfied certain safety requirements and product quality control specifications. A set of manipulated variables was selected, which required the least changes to anticipate the effects of a specified step disturbances. A linear process model was incorporated and the resulted control scheme were deemed viable or not with the assistance of an integration analysis employing the relative gain array for the MIMO control system. This work was extended to a dynamic system (Wang and McAvoy, 2001).

The complete and combined approaches of rigorous and systematic screening of alternative process design with embedded control structure characteristics based on control and economic performance have been given proper attention (Mohideen *et al.*, 1996; Zheng *et al.*, 1999; Skogestad, 2000; Kookos and Perkins, 2002). The full count of all possible combinations between potential manipulated and controlled variables may become large, especially for plantwide control system design. Thus, the complete enumeration of all possible sets of control structure for a number of disturbances incorporating the dynamic behaviour of the system within an optimisation framework would require great computational effort. Furthermore, use of the merits such as singular value and condition number of the system's transfer function and interaction measures for the quality (Luyben and Floudas, 1994a,b) in the design of process and control systems may

become prohibitive.

In general, the integrated design methods in the literature can be classified as having two different perspectives. The first set of approaches consider steady-state operation to be most desirable. They then seek to develop the steady-state designs that are economically optimal but are also dynamically operable in a region around specified steady-states. This is usually implemented by using trade-off between an economic performance measure and a controllability performance index at steady-state, using one of merits listed in Table 2.1. The final decision as to what constitute the “best” design is often somewhat arbitrary in the sense that it depends on the relative weights used for the conflicting objectives. Furthermore, these approaches suffer from the inherent weaknesses of the performance indexes used, namely that the controllability indicators may not directly and unambiguously relate to real performance requirements. The main drawback is that the solutions are only reliable around the specified steady-states. In order to check the validity of the conclusion drawn, closed-loop dynamic simulations are usually required.

The second set of approaches are dynamic approaches (Mohideen *et al.*, 1996; White *et al.*, 1996; Bahri *et al.*, 1997; Bansal *et al.*, 2000a,b) that take the view that all processes are inherently dynamic, and that dynamic operation is inevitable or in some cases preferable to steady-state operation. They therefore explicitly consider the dynamic performance at the design stage through the use of the dynamic models. The ambiguity associated with controllability performance is thus avoided. These methods are not restricted to a small operating envelope around steady-states, thus the final decision drawn are reliable over a large region of the operation in the face of the disturbances. However, the optimal controller parameters strongly depend on the detailed dynamic process models of the process systems. The uncertainty (e.g. disturbances) seems to be solved at design stages.

Uncertainty of the models will arise in practice. Moreover, the methods of the integrated process design and control optimisation, although they are reasonable and applicable from a mathematical point view, are not likely to be used in practice. One important reason is the cost of obtaining a “detailed” dynamic model.

Therefore, it is desirable that a method should be one that only use open-loop steady-state data while considering dynamic characteristics of a process design, i.e. information is independent of a detailed controller design, and could eliminate the design candidates for which a controller that achieves the control objectives in the face of disturbances does not exist, whatever controller design method is used. Bifurcation analysis can be one of the suitable nonlinear analysis tools that captures complex nonlinearity by using only steady-state data and applies to process design.

Bifurcation analysis proves its power in nonlinear system analysis and a few applications to process design have been reported. Ray (1989) demonstrated a limit cycle that occurs at typical operating conditions in emulsion polymerisation of vinyl acetate taking place in a CSTR. This limit cycle can be avoided either by increasing the solvent fraction or by decreasing the solvent volume fraction and increasing the initiator feed concentration. Russo and Bequette (1996, 1998) studied the influence of design parameters on the multiplicity behaviour of jacketed exothermic CSTRs. Morud and Skogestad (1998) discussed the dynamics of an industrial multibed ammonia reactor, where positive feedback due to heat integration led to oscillatory behaviour. They demonstrated that instability occurs at a Hopf bifurcation point. Khinast *et al.* (1998) analysed the continuously stirred decanting reactor. They computed loci of the singular point, which divided the space of the design parameters into regions having different steady-states and bifurcation behaviour, and therefore desirable regions of operation and potential

stability or operability issues were identified.

Bifurcation analysis does give a guideline to modify a process to avoid the undesirable behaviour and optimisation as a promising tool for design/control integration (Perkins and Walsh, 1996) is widely recognised. In this thesis, an approach to modifying process design for improved controllability is developed, using optimisation and bifurcation analysis.

## 2.6 Conclusions

This chapter served to introduce the background of this thesis. Bifurcation analysis that provides a tool for analysing nonlinear system in the parameter space was discussed. The ideas of the inherent limitations on controllability and difficult control characteristics of a system were introduced by the means of perfect control and process inversion. It was shown that a system with complex behaviour such as input multiplicity is very difficult to control and the closed-loop system with respect to stability and performance will be limited.

Various analysis tools and design methodologies have been critically reviewed with reference to features that a general controllability analysis and design approach should possess. The linearisation-based measures of controllability analysis are limited in their use for nonlinear systems since the results obtained from the linearised models are only reliable around the specific conditions, not through a large operating region, which is also main drawback of steady-state optimisation-based methods. Dynamic optimisation-based methods are strongly dependent on the detailed controller designs so that the results from these kinds of methods are not comparable. The controller-dependent methods are inefficient when prior controller design are required since controllability is determined by the process itself.

Continuation combined with bifurcation theory has been identified as the most appropriate tool in nonlinear system analysis and the results of this analysis could be used to guide the process modification at the design stage.

Bifurcation analysis as a powerful tool in nonlinear system analysis ( Seider *et al.*, 1991; Moari, 1992; Sistu and Bequette, 1996) and optimisation as a promising tool for design/control integration (Perkins and Walsh, 1996) have been recognised. In Chapters 3 and 4, we will show how these kinds of approaches can be used to analyse an existing process design with input multiplicity and then to modify the process to eliminate the control difficulties associated with input multiplicity in the operating regions of interest.

# Chapter 3

## A New Analysis Method

---

This chapter presents a bifurcation-based approach to studying potential control problems associated with input multiplicity. An algorithm is developed by augmenting the open-loop system with the necessary condition for the existence of input multiplicity that is incorporated as an add-in subroutine to a bifurcation analysis software code available. This allows one to identify input multiplicity behaviour in the parameter space and to investigate the dependence of input multiplicity on the values of the parameters of interest. The computational aspect of bifurcation analysis are briefly discussed in section 2 and a formulation is presented in section 3. The solution method for a SISO system is described in section 4. An isothermal CSTR, as an illustrative example of application, is given to demonstrate the key features and applications of this proposed method, and results are compared with the analytical solutions.

### 3.1 Introduction

The literature survey in Chapter 2 indicates that continuation computational method combined with concepts of stability and bifurcation theory is now recognised as a powerful tool and widely applied to chemical process analysis.

In principle, bifurcation analysis is a method for studying qualitative behaviour changes of a process under parameter variations. The critical points or bifurcation points at which qualitative behaviour of the process changes are detected and located in the parameter space. The behaviour of the process is studied in terms of parameter-dependent branches of steady-state solutions. The characteristics of the process under disturbances and uncertainties such as operation condition and model parameter changes can be highlighted. Bifurcation analysis does give insight into the qualitative aspects of the dynamic behaviour of a process such as multiplicity, and possibly leads to improved dynamic behaviour in the process (Aris, 1979; Seider, 1991; Teymour and Ray, 1989; Russo and Bequette, 1995).

The bifurcation-based approaches that have appeared in the literature are mainly concerned with open-loop characteristics of processes even though few bifurcation studies of systems subject to control have been performed (Chang and Chen, 1984, Ginona and Paladino, 1994, Russo and Bequette, 1996). It is of some of interest to study the properties of a control-related process.

The properties of a feedback system with respect to its stability and control performance limitations are directly related to the characteristics of the process gains as stated in Chapter 2, if a specified control strategy is considered. It is the nature of nonlinear systems for characteristic process parameters to be different at different steady-state operating conditions. Thus, while the process gains for a linear system consist of constant elements, the process gains for nonlinear system

are the functions of process operating conditions and will therefore change as these operating conditions change. Hence, the linear-based methods, such as relative gain array (RGA), condition number (CN), etc, are inadequate for nonlinear systems. Carried to the extreme, no information is available from these methods when a process gain matrix vanishes, i.e. the determinant of the process gain matrix is zero. For instance, the inverse of a process gain matrix is used in RGA calculations. When the determinant of the process gain is zero, the inverse does not exist.

Defined by the mathematics of bifurcation theory, the zero of a process gain has significance, which can be one of the tests used by nonlinear analysis to detect the possible existence of input multiplicity for a SISO system so that the control difficulties caused by the input multiplicity can be investigated.

In this chapter, a formula for a SISO system is developed by augmenting an open-loop process with its gain, that can be incorporated as an add-in subroutine to a bifurcation analysis software code available, AUTO (Doedel *et al.*, 1998). Thus, the occurrence of the existence of input multiplicity can be automatically detected by utilising bifurcation analysis. Hence, the properties of the process gain can be studied in the parameter space. The results from this analysis are then used to guide process modifications to eliminate or avoid input multiplicity, which will be discussed in Chapter 4.

## 3.2 Bifurcation Analysis

In § 2.1.3, the concept of bifurcation analysis was introduced. In this section, the computational aspect of determination of bifurcation points is discussed.

Consider a continuous nonlinear system, which is expressed by

$$\dot{x} = f(x, u), \quad (3.1)$$

where  $x \in \mathfrak{R}^n$  is an  $n$  dimensional vector of the state variables;  $u \in \mathfrak{R}$  is a manipulated variable;  $f(x, u)$  is an  $n$ -dimensional vector of smooth nonlinear functions.

For a given  $u$ , an open-loop steady-state solution of the equation ( 3.1) is a point such that:

$$0 = f(x, u). \quad (3.2)$$

The behaviour of the open-loop steady-states can be evaluated by the Jacobian matrix of the system,  $J$ , which is expressed as:

$$J = \begin{bmatrix} \frac{\partial f_1(x, u)}{\partial x_1} & \frac{\partial f_1(x, u)}{\partial x_2} & \dots & \frac{\partial f_1(x, u)}{\partial x_n} \\ \frac{\partial f_2(x, u)}{\partial x_1} & \frac{\partial f_2(x, u)}{\partial x_2} & \dots & \frac{\partial f_2(x, u)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n(x, u)}{\partial x_1} & \frac{\partial f_n(x, u)}{\partial x_2} & \dots & \frac{\partial f_n(x, u)}{\partial x_n} \end{bmatrix}. \quad (3.3)$$

Eigenvalues  $\lambda$  of the Jacobian matrix  $J$  satisfy the equation:

$$\det(J(x, u) - \lambda I) = 0. \quad (3.4)$$

If all the eigenvalues of  $J$  have negative real parts, then the steady-state solution of the nonlinear system is asymptotically stable. A steady state point is unstable if at least one real part of the eigenvalues of  $J$  is positive. There may exist some branch points at which the stability of the system changes. Bifurcation

theory is used to analyse the stability changes of the steady-state solutions and to understand what happens when a part of the spectrum of the matrix  $J$  moves from the left hand plane (LHP) into the right hand plane (RHP) or vice versa when the parameter  $u$  changes. The term *bifurcation point* refers to branch points in general and is used in the foregoing discussion to mean the branching of the solutions.

The necessary condition which determines a bifurcation point for the system at steady-state, from the implicit function theorem, is described by (Kubíček and Marek, 1983):

$$f(x, u) = 0, \quad (3.5)$$

$$\det(J) = 0. \quad (3.6)$$

The eigenvalues  $\lambda$  of the Jacobian matrix  $J$  satisfy the equation (3.4). The equality is therefore equivalent to the statement that at least one of the eigenvalues of  $J$  is zero. At a bifurcation point, the stability of the solutions in the transient sense can change.

Numerical solutions for the dependence of steady-states on  $u$  can be solved by using an iterative procedure known as continuation. Typically, one parameter is varied to allow the continued calculation of solutions as a function of this parameter. At each iteration, a step in the parameter is taken and a predictor-corrector method is utilised to locate the solution. The step size of each iteration is controlled by a convergence criterion. The procedure is repeated until a desired range of the parameter values has been evaluated. Bifurcation points can be detected and located. Branches of the steady-state solutions at the bifurcation points can be traced out in the parameter space. Therefore, continuation can provide a “complete” picture of the nonlinear behaviour.

The results of the continuation calculations are typically presented as a bifurcation diagram where the behaviour of a key variable is shown as a function of the bifurcation parameters.

A number of software packages have been developed for bifurcation analysis of nonlinear systems. AUTO, a continuation and bifurcation analysis package developed by Doedel *et al.* (1998), is perhaps, to the author's knowledge, the most widely used numerical bifurcation code. AUTO can perform bifurcation analysis of nonlinear systems described by algebraic equations, ordinary differential equations, and partial differential equations. In addition to the simple limit and Hopf bifurcations that commonly occur, more complex bifurcation behaviour such as tori and period doubling bifurcation as a function of two or more parameters can be solved. AUTO also includes a graphical user interface (GUI) which simplifies specification of computational parameters required by the continuation code. For these reasons, the AUTO package is utilised to conduct bifurcation analysis in this thesis.

The basic numerical techniques of continuation and bifurcation employed in the AUTO package are given in Appendix C and the details can be found in the published papers (Keller, 1977, 1987; Doedel *et al.*, 1991a, b)

### 3.3 Problem Formulation

Consider a SISO process described by the following modelling equations:

$$\begin{aligned}\dot{x} &= f(x, u), \\ y &= h(x),\end{aligned}\tag{3.7}$$

where  $x \in \mathfrak{R}^n$  is an  $n$  dimensional vector of the state variables;  $u \in \mathfrak{R}$  is a manipulated variable;  $f(x, u)$  is an  $n$ -dimensional vector of smooth nonlinear functions;  $h$  is smooth function on  $\mathfrak{R}$ . For the given SISO system, the process gain at steady state is expressed by:

$$G(0) = -CA^{-1}B, \quad (3.8)$$

where  $G(0)$  is the steady state process gain and  $A$ ,  $B$ , and  $C$  represent the gradients of function  $f(x, u)$  with respect to  $x$ ,  $f(x, u)$  with respect to  $u$ , and  $h(x)$  with respect to  $x$  at the steady state operating point, respectively.

Mathematically, the necessary condition for the existence of steady state input multiplicity (Koppel, 1982) is:

$$G(0) = -CA^{-1}B = 0. \quad (3.9)$$

Whenever equation ( 3.9) is true, one must consider the possibility of the existence of input multiplicity behaviour and cannot be confident that the inverse of the system exists as a one-to-one mapping from the values of the output to the values of the input, resulting in a large move of the input for an inverse-based control framework. Therefore, equation ( 3.9) can be referred to as a bifurcation condition in bifurcation analysis.

An artificial dynamic equation is then defined by using the process gain,  $G(0)$ , which is expressed as:

$$\dot{\nu} = G(0)\nu, \quad (3.10)$$

where  $\nu$  is an artificial state and the initial condition is assigned as 0 (the value of the  $G(0)$  is independent of the state  $\nu$ ).

Consider the system (3.10) where the eigenvalue of the system is  $G(0)$ . The

bifurcation condition for this particular system at steady-state is:

$$G(0) = 0. \quad (3.11)$$

Therefore, the necessary condition for the existence of input multiplicity characterises a bifurcation point for this dynamic equation. Exact satisfaction of equation (3.11) is of course unlikely in physical problems. A very small value of  $G(0)$  is also meaningless. However, for our purpose, it is sufficient to seek changes in the sign of  $G(0)$  to detect the occurrence of the input multiplicity at a variety of steady-states.

If the original dynamic system (3.7) is augmented with the dynamic equation (3.10), a new dynamic system is set up, giving the form:

$$\dot{x} = f(x, u), \quad (3.12)$$

$$\dot{\nu} = G(0)\nu, \quad (3.13)$$

or in short form:

$$\dot{X} = \mathcal{F}(X, u), \quad (3.14)$$

where  $X = [x, \nu]$  and

$$\mathcal{F}(X, u) = \begin{bmatrix} f(x, u) \\ G(0)\nu \end{bmatrix}. \quad (3.15)$$

The steady-state solutions of the new system are given by:

$$0 = \mathcal{F}(X, u). \quad (3.16)$$

The Jacobian matrix,  $\tilde{J}$ , of (3.16) with respect to  $X$  at steady state is:

$$\tilde{J} = \begin{pmatrix} J & 0 \\ 0 & G(0) \end{pmatrix}, \quad (3.17)$$

where  $J$  is Jacobian of the function  $f$  with respect to  $x$ . The eigenvalues of  $\tilde{J}$  are determined by:

$$\begin{aligned} \det(\lambda I - \tilde{J}) &= \det \left( \lambda \begin{pmatrix} I_1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} J & 0 \\ 0 & G(0) \end{pmatrix} \right) \\ &= \det \begin{pmatrix} \lambda I_1 - J & 0 \\ 0 & \lambda - G(0) \end{pmatrix} \\ &= \det(\lambda I_1 - J) \det(\lambda - G(0)), \end{aligned} \quad (3.18)$$

where  $I$  and  $I_1$  are  $(n+1) \times (n+1)$  and  $n \times n$  identity matrices, respectively. Eigenvalues  $\lambda$  of the Jacobian matrix  $\tilde{J}$  of the system (3.16) satisfy the equation:

$$\det(\lambda I - \tilde{J}(x, \nu, u)) = 0, \quad (3.19)$$

that is,

$$\det(\lambda I_1 - J) \det(\lambda - G(0)) = 0, \quad (3.20)$$

which represents the characteristic equation of the system (3.7) with the equation (3.10).

It is now possible to study the properties of the process and its process gain straight away by means of bifurcation analysis. Input multiplicity behaviour along with the open-loop characteristics of the process can be detected and located in the parameter space, in which the input multiplicity conditions are referred

to as additional bifurcation points. Branches of these bifurcation points can be traced out to determine the bifurcation regions and the parameter effects. The continuation techniques within the software package AUTO can handle the problems with additional small calculation expense of the process gain at a variety of steady states by an add-in subroutine.

### 3.4 Solution Method

The bifurcation analysis package AUTO (Doedel *et al.*, 1998), is utilised to solve the problem stated in the last section. An add-in FORTRAN subroutine that calculates the process gain at a variety of steady-states is incorporated with the AUTO software code so that input multiplicity condition can automatically determined along with the open-loop characteristics of the process.

AUTO, as do most numerical continuation algorithms, can deal with problems with only one degree of freedom, i.e. one independently varying parameter. This method can be straight away applied to a SISO control system. The manipulated variable of the SISO system is selected as the first bifurcation parameter and then bifurcation points are detected and located in the manipulated variable space. Bifurcation condition, i.e. bifurcation diagram, can be traced out if other considered parameter such as a disturbance or a design parameter is assigned as the second bifurcation parameter so that how the parameters influence the behaviour of the process can be studied.

Implementation of basic computation for the augmented system in AUTO is outlined as the following figure (see *AUTO 97* (Doedel *et al.*, 1998) for the details of the use of AUTO).

SUBROUTINE FUNC	⇒	Function subroutine in AUTO
$u = PAR(1)$	→	Bifurcation parameter definition
$x_1 = X(1)$	→	State variables
...		
$x_n = X(n)$		
$x_{n+1} = X(n + 1)$	→	New artificial state
$F_1 = f_1(x, u)$	→	Original dynamic equations
$F_2 = f_2(x, u)$		
...		
$F_n = f_n(x, u)$		
CALL sub-xfuhx	→	Add-in subroutine to calculate the derivatives, $f_x$ , $f_u$ and $h_x$
CALL sub-gain	→	Add-in subroutine to calculate gain, $G(0)$
$F_{n+1} = G(0)x_{n+1}$	→	New artificial dynamic equation
RETURN		
END		
SUBROUTINE STPNT	⇒	Starting point subroutine in AUTO
$PAR(1) = u_0$		
$X(1) = x_{1,0}$		
...		
$X(n) = x_{n,0}$		
$X(n + 1) = 0$	→	Initial condition of new artificial state
RETURN		
END		

Diagram of basic computation of the augmented system with AUTO

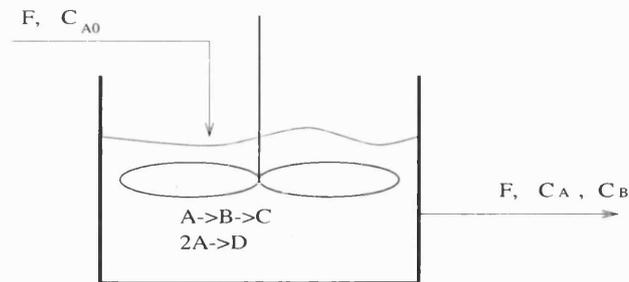
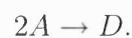


Figure 3.1: Schematic diagram of the van de Vusse reactor

### 3.5 Illustration: van de Vusse Reactor Example

In this section we consider the application of the proposed analysis method to the van de Vusse reaction taking place in an isothermal continuous stirred tank reactor (CSTR). A schematic diagram of the reactor considered here is shown in Figure 3.1. This example has been considered by a number of researchers as a benchmark problem in the literature for nonlinear process control and optimisation study (van de Vusse, 1964; Daoutidis *et al.*, 1990; Sistu and Bequette, 1995; Doyle *et al.*, 1995). It has been found that the reaction exhibits input multiplicity behaviour (see Figure 3.2).

The considered reaction kinetic scheme is:



The reaction rates with respect to A and B are:

$$r_A = -k_1 c_A - k_3 c_A^2, \quad (3.21)$$

$$r_B = k_1 c_A - k_2 c_B, \quad (3.22)$$

where  $k_1$ ,  $k_2$ , and  $k_3$  are the reaction rate constants. The feed stream consists of

pure A. The mass balances for A and B are given by:

$$\dot{c}_A = -k_1 c_A - k_3 c_A^2 + \frac{F}{V}(c_{A0} - c_A), \quad (3.23)$$

$$\dot{c}_B = k_1 c_A - k_2 c_B + \frac{F}{V}(-c_B), \quad (3.24)$$

where  $F$  is the inlet flow rate of A,  $V$  is the reactor volume,  $c_A$  and  $c_B$  are the concentrations of A and B inside the reactor, respectively, and  $c_{A0}$  is the concentration of A in the feed. The control problem focusses on regulating the concentration of component B,  $c_B$ , by manipulating the inlet flow rate  $F$ .

The equations by setting the state variables  $x_1 = c_A$ ,  $x_2 = c_B$ ,  $u = F$ , and  $y = c_B$  are expressed as:

$$\dot{x}_1 = -k_1 x_1 - k_3 x_1^2 + \frac{1}{V}(c_{A0} - x_1)u, \quad (3.25)$$

$$\dot{x}_2 = k_1 x_1 - k_2 x_2 - \frac{1}{V}x_2 u, \quad (3.26)$$

$$y = x_2, \quad (3.27)$$

or in the standard state space form:

$$\dot{x} = f(x, u), \quad (3.28)$$

$$y = h(x), \quad (3.29)$$

where

$$f(x) = \begin{pmatrix} -k_1 x_1 - k_3 x_1^2 + \frac{1}{V}(c_{A0} - x_1)u \\ k_1 x_1 - k_2 x_2 - \frac{1}{V}x_2 u \end{pmatrix}, \quad (3.30)$$

$$h(x) = x_2. \quad (3.31)$$

The parameters and values of the reaction are given in Table 3.1, which are

Table 3.1: Parameters and values for van de Vusse reactor

Parameters	Values	Units
$k_1$	50	$h^{-1}$
$k_2$	100	$h^{-1}$
$k_3$	10	$l \text{ mol}^{-1} h^{-1}$
$c_{A0}$	10	$\text{mol l}^{-1}$
$V$	1	$l$

referred to the published papers (Sistu and Bequette, 1995; Doyle *et al.*, 1995).

### 3.5.1 Analysis for the van de Vusse Reactor

Consider the system expressed by the equations from ( 3.25) to ( 3.27). The process gain  $G(0)$  as a function of the states is expressed by:

$$G(0) = -\frac{\partial h}{\partial x} \left[ \frac{\partial f}{\partial x} \right]^{-1} \frac{\partial f}{\partial u} \Big|_{x_s, u_s}. \quad (3.32)$$

We use the process gain to define a dynamic equation:

$$\dot{\nu} = G(0)\nu, \quad (3.33)$$

where  $\nu$  is an artificial state. An augmented dynamic system is set up as:

$$\dot{x}_1 = -k_1 x_1 - k_3 x_1^2 + \frac{1}{V} (c_{A0} - x_1) u, \quad (3.34)$$

$$\dot{x}_2 = k_1 x_1 - k_2 x_2 - \frac{1}{V} x_2 u, \quad (3.35)$$

$$\dot{\nu} = G(0)\nu. \quad (3.36)$$

The analysis for the new system is carried out by using AUTO (Doedel *et al.*, 1998), being incorporated to the add-in subroutine of calculating the determinant

of the process gain at a variety of steady state conditions. The steady-state solutions of the system with input multiplicity information are shown in Figure 3.2. The point indicated by the square in Figure 3.2 is an input multiplicity condition at which the value of the inlet flow rate  $F$  is:  $F \approx 77.5l/h$ . This condition is referred to as a bifurcation point of the augmented system in bifurcation analysis.

Having this bifurcation point, one can investigate the effects of the other concerned parameters on the input multiplicity behaviour. In this case, the feed composition  $c_{A0}$  as a main disturbance is taken into account to study how it influences the input multiplicity behaviour when it varies. Figure 3.3 shows the feed composition  $c_{A0}$  effect on the behaviour of the process as indicated by the dashed line. The locus of the input multiplicity condition is given in Figure 3.4, which indicates how the input multiplicity condition depends on the feed composition  $c_{A0}$  over the operating range of the inlet flow rate.

The relationship between the input  $u$ , the output  $x_2$ , and the disturbance  $c_{A0}$  at the input multiplicity condition can be obtained, as depicted in Figure 3.5. If the input moves to breach the input multiplicity condition in order to reject the disturbance of the feed composition during the operation, the input multiplicity behaviour will occur.

### 3.5.2 Comparison with Analytical Solutions

In section 2.4.1, we have discussed the combination of the existence of input multiplicity and process gain sign changes, resulting in the changes of zero dynamics behaviour. In this section it is shown for the van de Vusse example that the results from the proposed method and the analytic solutions are compatible.

For this equation system, it is possible to have the process gain at steady-state

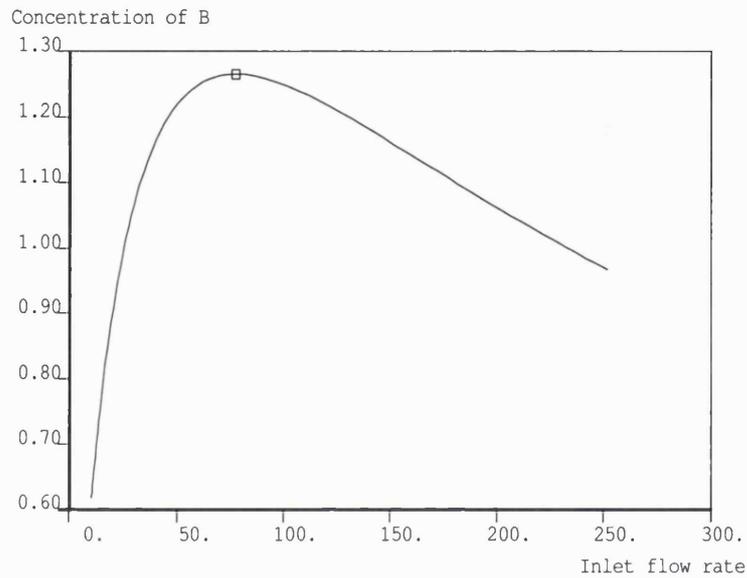


Figure 3.2: Steady state solutions showing input multiplicity condition information for the van de Vusse reactor. Square: input multiplicity condition

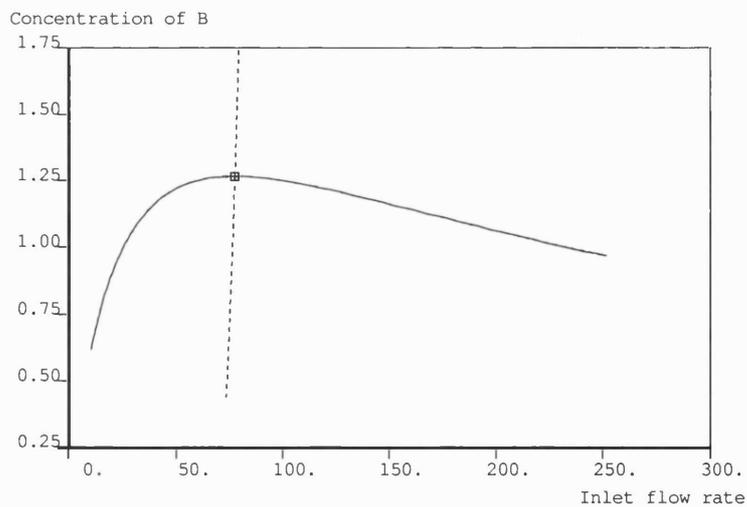


Figure 3.3: Steady state solutions showing input multiplicity condition with variation of  $c_{A0}$  for van de Vusse reactor. Solid line: steady states for a fixed  $c_{A0}$ ; dashed line: input multiplicity condition with variation of  $c_{A0}$

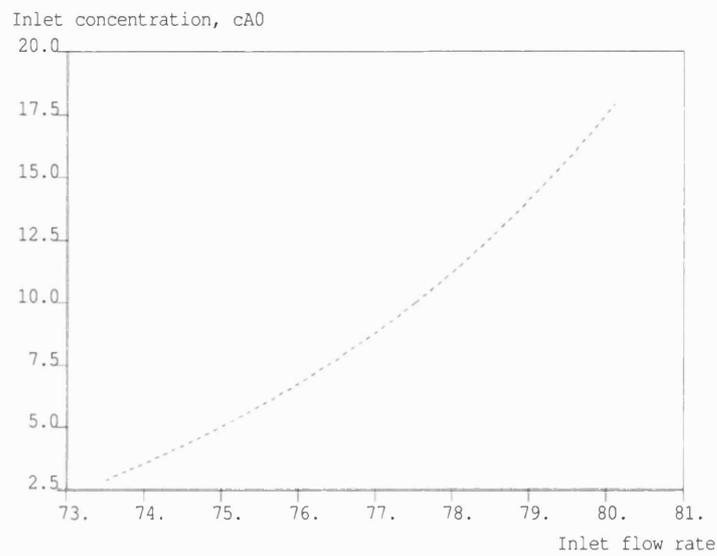


Figure 3.4: Locus of input multiplicity condition between inlet flow rate  $F$  and feed composition  $c_{A0}$

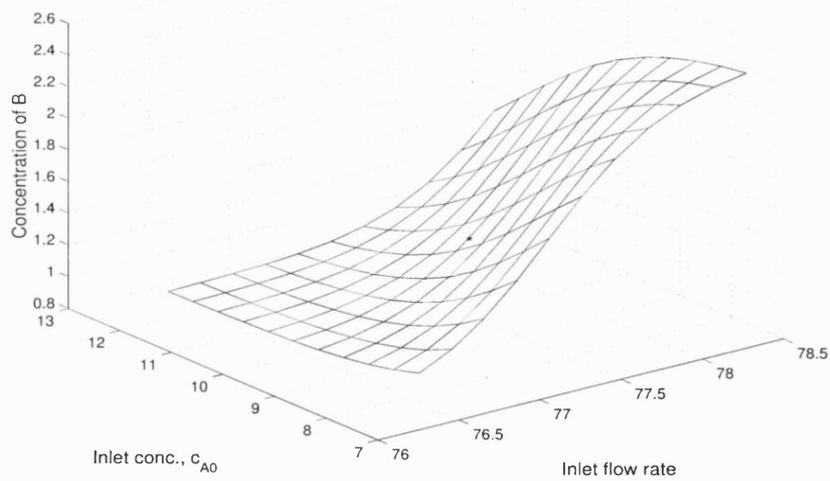


Figure 3.5: Contour of input multiplicity conditions as inlet flow rate, output, and inlet concentration change for the van de Vusse reactor

by calculating (Sistu and Bequette, 1995):

$$\frac{\partial f}{\partial x}\bigg|_{x_s, u_s} = \begin{pmatrix} -k_1 - 2k_3x_{1s} - \frac{1}{V}u_s & 0 \\ k_1 & -k_2 - \frac{1}{V}u_s \end{pmatrix}, \quad (3.37)$$

$$\frac{\partial f}{\partial u}\bigg|_{x_s, u_s} = \begin{pmatrix} \frac{1}{V}(c_{A0} - x_{1s}) \\ -\frac{1}{V}x_{2s} \end{pmatrix}, \quad (3.38)$$

$$\frac{\partial h}{\partial x}\bigg|_{x_s, u_s} = \begin{pmatrix} 0 & 1 \end{pmatrix}, \quad (3.39)$$

and therefore

$$\begin{aligned} G(0) &= -\frac{\partial h}{\partial x} \left[ \frac{\partial f}{\partial x} \right]^{-1} \frac{\partial f}{\partial u}\bigg|_{x_s, u_s} \\ &= -\frac{1}{V} \frac{-k_1(c_{A0} - x_{1s}) + x_{2s}(k_1 + 2k_3x_{1s} + u_s/V)}{(k_2 + u_s/V)(k_1 + 2k_3x_{1s} + u_s/V)}, \end{aligned} \quad (3.40)$$

where the index  $s$  indicates steady state values. The steady states of the concentrations as a function of the input are:

$$x_{1s} = \frac{-(Vk_1 + u_s) + \sqrt{(V^2k_1^2 + 2Vk_1u_s + 4Vc_{A0}k_3u_s + u_s^2)}}{2Vk_3}, \quad (3.41)$$

$$x_{2s} = \frac{k_1(-Vk_1 - u_s + \sqrt{(V^2k_1^2 + 2Vk_1u_s + 4Vc_{A0}k_3u_s + u_s^2)})}{2k_3(Vk_2 + u_s)}. \quad (3.42)$$

Substituting the equations (3.41) and (3.42) into equation (3.40), the process gain can be solved analytically. Figure 3.6 shows the process gain under the variation of the inlet flow rate for the given parameters. As can be seen, the process gain is zero at the value of 77.5l/h of the inlet flow rate  $F$  and changes its sign crossing this value, which is the same as the result from the proposed method given in the last section. This point was detected and referred to as a bifurcation point in the above proposed method (see Figure 3.2).

The sign change in the process gain indicates there exists a shift of the zero of the linearised process from LHP to RHP or vice versa as long as the relative order of the system is constant (Sistu and Bequette, 1995). Further to prove these statements, the zero dynamics of the system are given as follows.

**Zero Dynamics:** For this system, the relative order is shown to be  $r = 1$  by differentiating the output, i.e. one equation for the zero dynamics is expected. In this case, the zero dynamics can be directly determined from the model equations, as they are in the normal form. Setting the output and its derivative equal to zero in the equation ( 3.26), solving the remaining system and substituting  $u$  into equation ( 3.25) leads to zero dynamics:

$$\dot{x}_1 = -k_1x_1 - k_3x_1^2 + \frac{(c_{A0} - x_1)(k_1x_1 - k_2y)}{y}. \quad (3.43)$$

The eigenvalue  $\lambda$  of the zero dynamics of this system as the function of the states is expressed by:

$$\lambda = -k_1 - 2k_3x_1 + \frac{-k_1x_1 + k_2y + k_1(c_{A0} - x_1)}{y}. \quad (3.44)$$

If the steady state solution equations ( 3.41) and ( 3.42) are inserted into equation ( 3.44), an analytical expression for the eigenvalue of the zero dynamics as a function of the input in the whole operation region is obtained. The relationship between the eigenvalue of the zero dynamic and the input is depicted in Figure 3.7. The positive value of the eigenvalue of the zero dynamics indicates unstable zero dynamics. As can be seen, instability of the zero dynamics changes at the value of  $77.5l/h$  of the inlet flow rate, at which the process gain of the process is zero as shown in Figure 3.6. This case also gives a confirmation of the theory discussed in § 2.4.1.

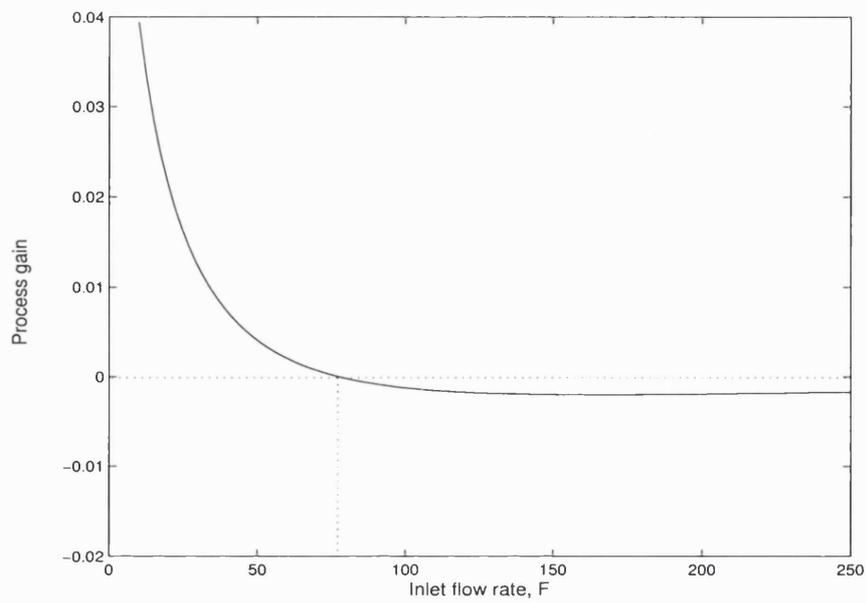


Figure 3.6: Process gain as a function of inlet flow rate for the van de Vusse reactor

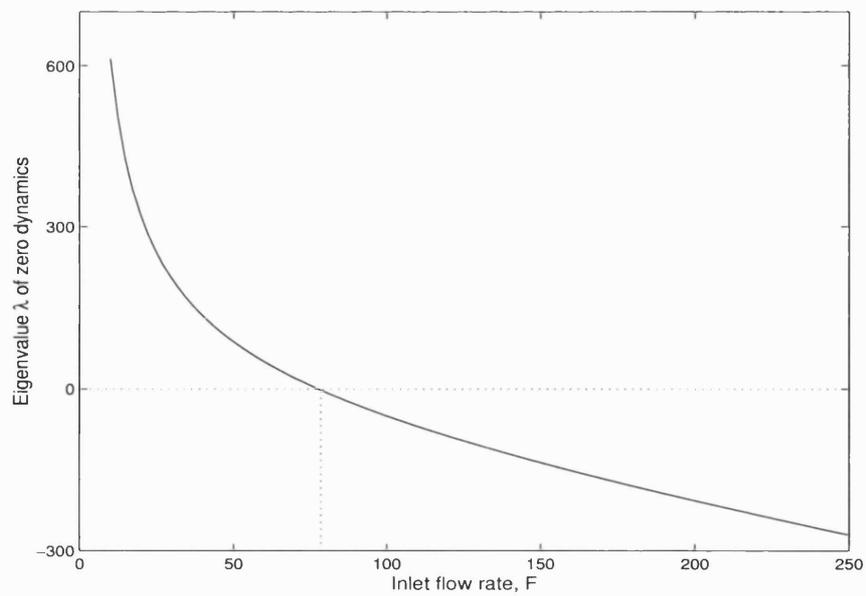


Figure 3.7: Eigenvalue of zero dynamics as a function of inlet flow rate for the van de Vusse reactor

### 3.5.3 Summary

An isothermal CSTR with input multiplicity behaviour has been analysed by using the proposed methodology. The results were compared with the analytical solutions. It was shown that the proposed method was capable of determining the input multiplicity characteristic and of studying the parameter effects on it. The proposed approach can straightaway detect input multiplicity behaviour and then conduct the studies of different parameter effects on the process behaviour for a large nonlinear system.

## 3.6 Conclusions

In this chapter a bifurcation-based method is presented for determining input multiplicity along with other open-loop characteristics of nonlinear processes. The foundation of the approach is to use bifurcation analysis techniques to investigate the qualitative behaviour changes of process gain matrices in terms of the possibilities of the existence of input multiplicity and to study the parameter effects on them. The necessary condition for the existence of input multiplicity as an add-in subroutine is incorporated with an available bifurcation package. This provides a way to identify potential control difficulties associated with input multiplicity in the parameter space for a given process design and control structure. This feature enables controllability in terms of qualitatively dynamic properties of the process to be analysed, independent of detailed controller design. The applicability and ease of calculation of this approach, compared to analytical methods, has been demonstrated through a process example. It is evident that the benefits offered by the bifurcation-based approach increase as the number of the considered parameter increases for large and complex nonlinear processes.

# Chapter 4

## Process Modification for Improved Controllability

---

This chapter presents a method for modifying an existing process design with input multiplicity to improve controllability. The static controllability (setpoint following ability and disturbance rejection) of the process design is considered in conjunction with economic criteria for the modification of the process design. The control and economic objectives are incorporated within a feedback optimisation framework that evaluates the required contribution of the input variable and process design parameters to alleviate the effects of an imposed disturbance on control performance. Bifurcation analysis is utilised to identify the potential control problems associated with input multiplicity behaviour and to determine the effects of the input, output, disturbance, and design parameters on them, hence providing the guide for the process modifications to eliminate or avoid such undesirable behaviour. Application of this method to an exothermic CSTR is given as an illustrative example.

## 4.1 Introduction

In the proceeding chapter a bifurcation-based approach to identifying the complex behaviour of a process has been developed. This method can determine the potential control difficulties for an existing process design with selected controlled and manipulated variables, and allow one to study the effects of the disturbances and design parameters on the behaviour of the process over the entire operating range of interest. Results from the analysis indicate what the complex behaviour of a process is in the face of a specific disturbance and how the changes of the design parameter values influence it. This could make it possible for adjusting the design parameter values to eliminate or avoid the undesirable complex behaviour. In this chapter an approach to modifying process designs is proposed to realise the possibility.

In principle, the proposed method is a static optimisation-based approach, combined with bifurcation analysis. The optimisation problem formulated is a NLP problem that aims at minimising the absolute values of design parameter adjustments to avoid the complex behaviour inside the range of the input, subject to the specified disturbances.

It is worth pointing out that the focus of the proposed method is on modifying an existing process design itself rather than selecting control structures.

## 4.2 Process Modification Methodology for Improved Static Controllability

In this section a process modification approach to improving controllability is proposed, based on the static feedback optimisation and combined with bifurcation analysis. It should be emphasized that this method is not a synthesis tool

for process and control system design. The method focusses on modifying an existing process design with a selected SISO control structure. The procedure and development of this method is described in the following subsections.

### 4.2.1 Economically Optimal Design

Initially, consider an existing process design, or a set of alternative flow-sheet configurations that are determined based on a process design procedure as proposed in Douglas (1988). Typically, for each process design, the optimal operating conditions and equipment sizing around a nominal operating point are determined satisfying a number of economic criteria. These criteria usually incorporate the annualized investment and operating costs. Nonlinear process models are used for the prediction of the steady-state behaviour of the plant, while a set of constraints would enforce the satisfaction of safety, environmental and operating specifications. The solution found from optimisation is economically optimal. It has been assumed that the optimal values of the state variables, manipulated variable, and design parameters obtained are  $x^*$ ,  $u^*$ , and  $p^*$ , corresponding to the nominal value  $d^N$  of disturbance.

The process design is then described by the equations:

$$\dot{x} = f(x, u, d^N, p^*) \quad (4.1)$$

where  $x \in \mathfrak{R}^n$  is the vector of state variables,  $u \in \mathfrak{R}$  is the manipulated variable,  $d^N$  is the nominal value of disturbance,  $p^*$  is the values of design variables, corresponding to the nominal value  $d^N$  of the disturbance,  $f \in \mathfrak{R}^n$  are the smooth functions.

This economically optimal process design is referred to as the “base-case” design in the ongoing discussion.

### 4.2.2 Controllability Analysis for the “Base-Case” Design

For the optimised fixed structural design with the selected SISO control scheme, the process at steady-state is described as:

$$\begin{aligned} f(u, x, p^*, d) &= 0, \\ y &= h(x). \end{aligned} \tag{4.2}$$

We choose a set of scenarios for disturbance and design parameters to analyse the properties of the steady-state solutions and the behaviour of the process gain over the entire range of the selected manipulated variable  $u$  by using the method presented in Chapter 3. Bifurcation points are identified and located in the parameter space. The bifurcation relationship between the manipulated variable, the disturbance, and the design parameters at each bifurcation point is obtained, which is functionally expressed by  $u_{bif} = f_{bif}(d, p)$ . This bifurcation relationship represents the complex behaviour that will probably cause control problems and indicates how the parameters affect it. If input multiplicity is considered, the function will represent the occurrence of the input multiplicity behaviour under changing conditions. We only consider such a bifurcation point that is close to the selected optimal operation point if there exist more than one bifurcation. It is clear that if there exists difficult control problem in such a neighbourhood around the operating point, there is no hope of control in any larger sense.

### 4.2.3 Design Modification Algorithm

An optimisation problem can be formulated and solved to modify the process design. The design parameters are adjusted to control  $y$  for a disturbance to avoid bifurcation over the operating range of the manipulated variable. The objective

function is taken to be the differences that the design parameters and manipulated variable have to move from their original optimal steady-state values. These adjustments should be kept as small as possible. A scalar cost function  $J(u, p, d)$  is defined as a quadratic function that penalises deviations of manipulated variable and design parameter variables from their nominal steady-state economic optimal values in a least squares sense,

$$J(u, p) = (p - p^*)^T \mathcal{R}(p - p^*) + (u - u^*)^T \mathcal{Q}(u - u^*), \quad (4.3)$$

where  $\mathcal{R}$  and  $\mathcal{Q}$  are appropriate cost factor matrices that have to be chosen to reflect the operating cost change in the manipulated variable and capital cost change in the design parameter variables;  $u^*$  and  $p^*$  are the values of manipulated variable and design parameters at nominal conditions, respectively. It has been assumed that all state variables have been eliminated from the cost function so that the cost function is in terms of the independent variables. Thus an optimisation problem to determine the design modification to eliminate bifurcation problems can be formulated as:

$$\min_{u, p} J = (p - p^*)^T \mathcal{R}(p - p^*) + (u - u^*)^T \mathcal{Q}(u - u^*)$$

subject to

$$f(u, x, d, p) = 0, \quad (4.4)$$

$$g(u, x, d, p) < 0,$$

$$y - y_{set} = 0,$$

$$\text{sign}(u^* - f_{bif}(p^*, d^N))(u - f_{bif}(p, d)) < 0,$$

where

- $u$  the manipulated (independent) variable
- $x$  the vector of state (dependent) variables
- $p$  the vector of design (independent) variables
- $d$  the worst case value of disturbance
- $f$  mathematic model of process, involving mass and energy balance and so forth
- $g$  process limitations, involving raw materials product qualities and so forth
- $f_{bif}$  bifurcation function
- $d^N$  the nominal value of the disturbance
- $p^*$  the economically optimal values of design variables, corresponding to the nominal values of  $d^N$
- $u^*$  the economically optimal value of the manipulated variable, corresponding to the nominal values of  $d^N$
- $y_{set}$  the set-point value of the controlled variable

For a specified disturbance  $d$  the optimisation problem ( 4.4) can be solved to have the optimal values of the manipulated variable,  $u^{**}(d)$ , design parameters,  $p^{**}(d)$ , and cost function  $J(d) = J(u, p)|_{(u^{**}, p^{**})}$ .

In physical terms, the interpretation of the optimisation problem is an attempt to achieve the required control performance using a minimum magnitude change from the existing design. Therefore, the process design modification can result in adjusting the process variables and design variables with the constraints of the controlled variable setpoint and bifurcation condition, and it effectively turns the complex optimisation problem into a simple steady-state feedback problem that

is called *feedback optimising design (FOD)*.

In this optimising design modification problem ( 4.4), we are concerned with the selected manipulated variable and the design variables as the degrees of freedom for optimisation. The optimisation takes the economically optimal solutions  $u^*$  and  $p^*$  from the standard steady-state economic optimisation as the modification base. The sign of the difference between the steady state optimal value of the manipulated variable  $u^*$  and the bifurcation value of the manipulated variable,  $u_{bif} = f_{bif}(d^N, p^*)$ , corresponding to the nominal conditions, determines the desirable operating region. The bifurcation constraint can enable the modified process to stay in the desirable operating region without encountering the bifurcation problem for the specified disturbance in a steady-state sense.

Assuming that the problem ( 4.4) has been numerically solved yielding manipulated variable  $u^{**}$  and design variables  $p^{**}$  for the specified disturbance  $d$ , the modified process is expressed as the following:

$$\begin{aligned}\dot{x} &= f(u, x, p^{**}, d^N), \\ y &= h(x),\end{aligned}\tag{4.5}$$

which is expected to be able to reject the predefined disturbance successfully in the operating region. The final operating conditions result in solving the equations in ( 4.5) at steady-state.

### 4.3 Illustrative Example: An Exothermic CSTR

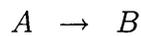
In this section we will illustrate the application of the proposed process design modification methodology to an exothermic continuous stirred tank reactor (CSTR) that exhibits input multiplicity. This example is to demonstrate how

to modify the process design to eliminate the control difficulties associated with input multiplicity for a specified disturbance in the operating range. The proposed method in Chapter 3 will be used to determine input multiplicity behaviour of the process and to analyse the effects of the parameters on it. The process modification method developed above will be applied to the process to generate process alternatives.

### 4.3.1 Process Description

Operating an exothermic reactor with cold feed can give rise to input multiplicity behaviour in temperature control problems. One specific example of this type was shown by Kravaris *et al.* (1994).

Consider a continuous stirred tank reactor with exothermic reaction where an inlet stream to the reactor consisting of pure A at concentration  $c_{A0}$  and temperature  $T_0$  enters the reactor, and an exothermic irreversible first-order reaction



takes place. A cooling jacket kept at a temperature  $T_j$  is used for the generated heat removal. The effluent stream leaves the reactor at concentrations  $c_A$ ,  $c_B$  and temperature  $T$ . The mass and energy balances describing the dynamic behaviour of the process are:

$$\dot{C}_A = \frac{F}{V}(c_{A0} - c_A) - k(T)c_A, \quad (4.6)$$

$$\dot{T} = \frac{F}{V}(T_0 - T) + \gamma k(T)c_A - \alpha(T - T_j)/V, \quad (4.7)$$

Table 4.1: Parameters and values

$k_0 = 7.2 \times 10^6$	$h^{-1}$	$E = 4.1 \times 10^4$	$kJkmol^{-1}$
$R = 8.345$	$kJkmol^{-1}K^{-1}$	$C_p = 4.2$	$kJkg^{-1}K^{-1}h^{-1}$
$-\Delta H = 7.0 \times 10^4$	$kJkmol^{-1}$	$\rho = 1000$	$kgm^{-3}$
$UA = 1680$	$kJh^{-1}K^{-1}$	$T_j = 300$	$K$
$V = 0.1$	$m^3$	$T_0 = 300$	$K$
$c_{A0} = 10$	$kmolm^{-3}$		

where

$$k(T) = k_0 \exp(E/RT),$$

$$\gamma = \frac{-\Delta H}{\rho C_p},$$

$$\alpha = \frac{UA}{\rho C_p},$$

and the values of the various process parameters and steady-state operating condition are given in Table 4.1 (Kravaris *et al.*, 1994). The control objective is to control reaction temperature  $T$  by manipulating the inlet flow rate  $F$ . The inlet temperature  $T_0$  is considered as a disturbance, and the reactor volume  $V$  as an adjustable design parameter.

### 4.3.2 Analysis for the Given Process

For the given design and control objective above, the system exhibits input multiplicity that is identified by using the method presented in Chapter 3. The steady-state solution relationship between the temperature  $T$  and the inlet feed  $F$  showing the input multiplicity condition under the variation of the inlet temperature  $T_0$  is given in Figure 4.1. The solid line shows the steady-state solution under the nominal conditions, the open square indicates the input multiplicity condition, and the dashed line shows how the inlet temperature  $T_0$  influences

the input multiplicity condition at steady state during operation. For clarity, the locus of the inlet flow rate  $F$  versus the inlet temperature  $T_0$  at the input multiplicity condition is shown in Figure 4.2.

For the process, the desired operating point under consideration is chosen on the right side of the curve in Figure 4.1 to achieve a compromise between maximising conversion and maximising product rate (Kravaris *et al.*, 1994). Assuming that the initial operating point is at the steady-state:  $c_A = 4.29 \text{ kmol/m}^3$  and  $T = 332 \text{ K}$ . The steady state value of the inlet flow rate corresponding to this operation point is  $F = 0.203 \text{ m}^3\text{h}^{-1}$ . As can be seen from Figure 4.2, the multiplicity condition is likely to be breached for this selected operating point when there is a decrease in the disturbance of the inlet temperature  $T_0$ . Figure 4.3 gives the input multiplicity condition between the temperature  $T$ , the inlet feed  $F$ , and the inlet temperature  $T_0$  at steady state. It can be seen that the operating point will move towards or through the curved plane for a decrease in the inlet temperature  $T_0$ , while keeping the reaction temperature  $T$  constant. This means that a large decrease in the inlet temperature is likely to cause the input multiplicity problem.

Now we consider the effect of the reactor volume  $V$  on the input multiplicity. Figure 4.4 shows the input multiplicity condition between the inlet flow rate  $F$ , the inlet temperature  $T_0$  and the reactor volume  $V$ . As can be seen from Figure 4.4, a decrease in the reactor volume and the inlet temperature will move the operating condition close to the multiplicity condition where the control problems associated with the input multiplicity will occur.

The results from the analysis indicate that a negative change in the inlet temperature  $T_0$  can possibly cause input multiplicity behaviour during operation.

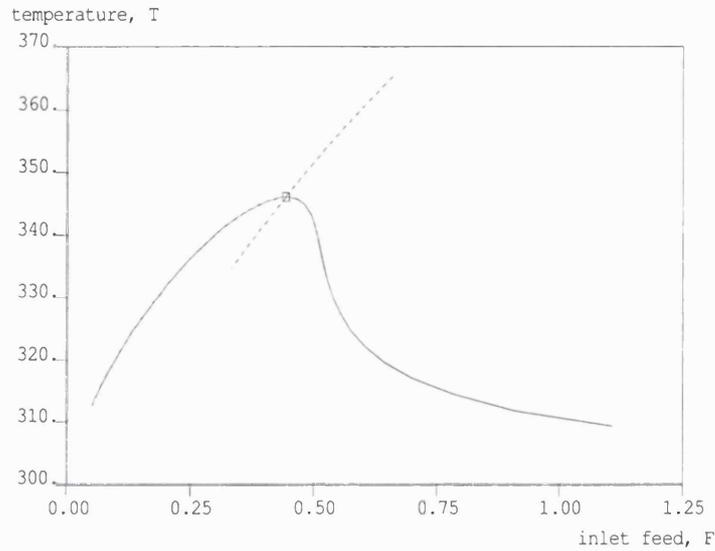


Figure 4.1: Steady-state solutions showing input multiplicity condition with variations of inlet temperature. Square: input multiplicity condition; dashed line: input multiplicity condition with variation of inlet temperature

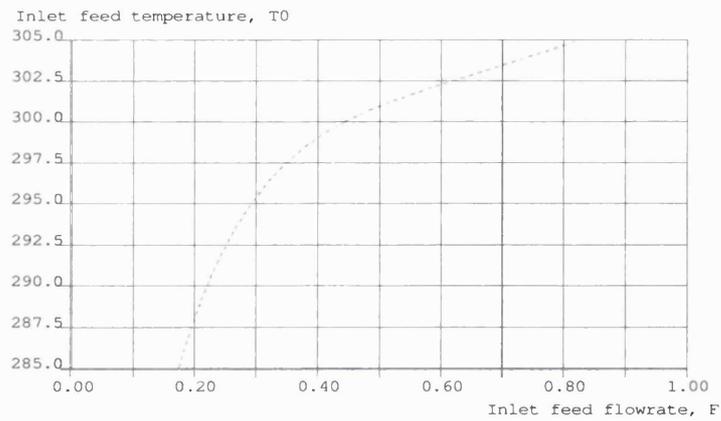


Figure 4.2: Locus of inlet flow rate versus inlet temperature at input multiplicity condition

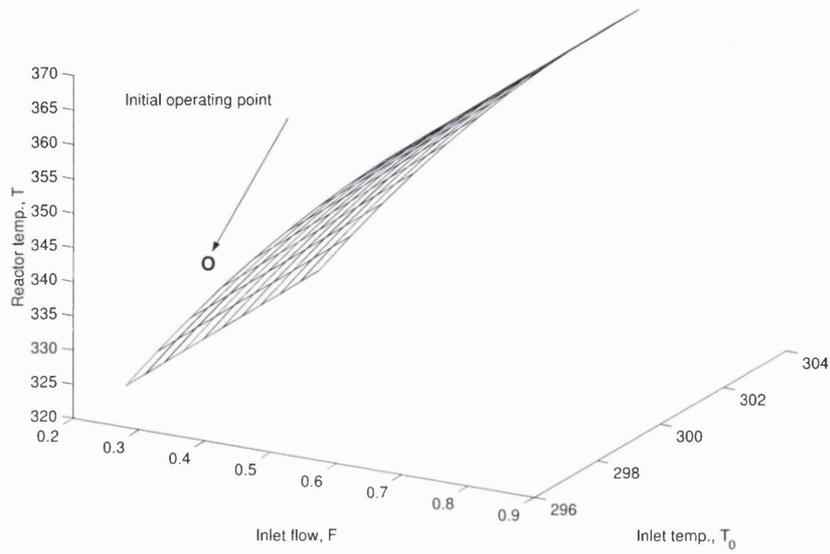


Figure 4.3: Input multiplicity condition between the reactor temperature, inlet flow rate and inlet temperature

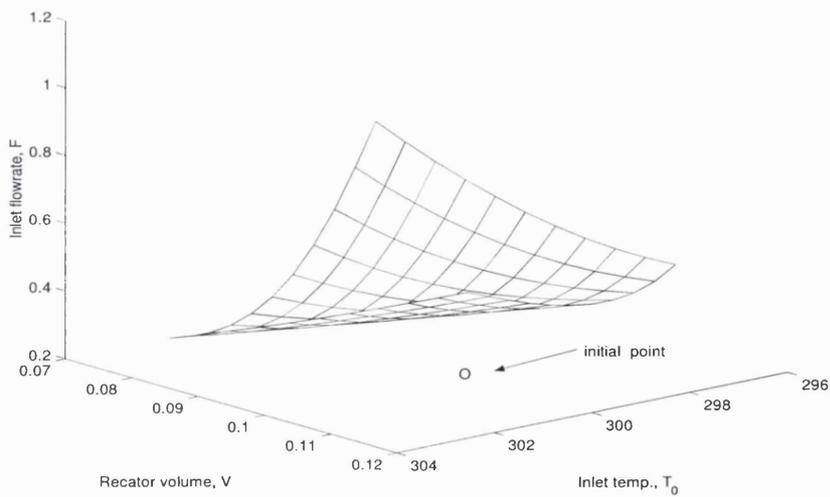


Figure 4.4: Input multiplicity condition between the inlet flow rate, inlet temperature, and reactor volume

### 4.3.3 Process Design Modifications

In this section, the process design modification method proposed is applied to the process discussed above to eliminate input multiplicity for a disturbance in the inlet temperature inside the operating range of the inlet flow rate. The condition for the existence of input multiplicity between the inlet flow rate  $F$ , the inlet temperature  $T_0$  and the reactor volume  $V$  is illustrated in Figure 4.4. The locally linearised relation of the input multiplicity condition between the inlet flow rate and inlet feed temperature and reactor volume can be obtained by using the data from the proposed bifurcation analysis method in Chapter 3, and is expressed by:

$$F_{IM} = -16.973 + 0.051T_0 + 21.195V. \quad (4.8)$$

For the chosen design variable  $V$ , the disturbance  $T_0$ , and the manipulated variable  $F$ , the feedback optimisation formula for the process design modification is described as the following:

$$\min_{F,V} \mathcal{R}(F - 2.03)^2 + \mathcal{Q}(V - 0.1)^2$$

subject to

$$\begin{aligned} \frac{F}{V}(c_{A0} - c_A) - k_0 \exp\left(\frac{E}{RT}\right)c_A &= 0, & (4.9) \\ \frac{F}{V}(T_0 - T) + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(\frac{E}{RT}\right)c_A - \frac{UA}{\rho C_p}(T - T_j)/V &= 0, \\ T - T_{set} &= 0, \\ F - F_{IM} &< 0, \end{aligned}$$

where  $\mathcal{R}$  and  $\mathcal{Q}$  are the operating and capital cost coefficients of the changes in the inlet flow rate and reactor volume, respectively, and  $F_{IM}$  is given by equation

(4.8). In this case,  $\mathcal{R}$  and  $\mathcal{Q}$  take the values of 0.001 and 100 for demonstration, respectively. The values of these weights imply that the capital cost in the change of the reactor volume is much higher than the operating cost in the change of the inlet flow rate. Therefore, keeping the adjustment of the reactor volume as little as possible is expected to compensate the effects of the specified disturbance while eliminating the input multiplicity behaviour.

For each defined value of the disturbance of the inlet temperature, we have a corresponding design modification. The design modifications resulting from solving the optimisation problem (4.9) are given in Table 4.2. For instance, in order to have the rejection capacity of a  $\Delta T_0 = -8 K$  change in the inlet temperature without possibly encountering input multiplicity, the reactor volume  $V$  is adjusted from  $0.1 m^3$  to  $0.111 m^3$ . As can be seen from Table 4.2, the reactor volume  $V$  is kept unchanged for some of the specified disturbance values. This implies that the original process design has the ability to reject these changes in the disturbance so that the process does not need modifying. The relationship between the adjusted reaction volume and the specified disturbance of the inlet temperature rejection capacity of the process is shown in Figure 4.5. It has been seen that the original process design can only reject approximately  $4 K$  negative change in the inlet temperature without encountering input multiplicity problems, which will be shown by simulations in the next section.

The steady-state operating conditions for the modified process designs showing the specified disturbance rejection ability are given in table 4.3.

The data used to obtain the functional expression equation (4.8) are from the analysis results by running AUTO with the add-in subroutine of determining input multiplicity while assigning the inlet flow rate  $F$  as the first bifurcation (freedom) parameter and the inlet feed temperature  $T_0$  or reactor volume  $V$  as the second bifurcation parameter at the input multiplicity condition which is

Table 4.2: Process design modification results for the exothermic reaction

$\Delta T_0$ (K)	-10	-8	-6	-4	0	+2	+4	+6	+8
$V$ ( $m^3$ )	0.116	0.111	0.106	0.101	0.100	0.100	0.100	0.100	0.100

Table 4.3: Parameters and operation values for the base-case and modified designs for the exothermic CSTR at steady state

	Base-case	FOD 1	FOD 2	FOD 3
$\Delta T_0$ (K)	-4	-6	-8	-10
$V$ ( $m^3$ )	0.100	0.106	0.111	0.116
$T_s$ (K)	332	"	"	"
$F_s$ ( $m^3 h^{-1}$ )	0.203	0.190	0.177	0.169
$c_{A,s}$ ( $kmol m^{-3}$ )	4.30	4.05	3.74	3.52

referred to as a bifurcation point of the augmented system.

#### 4.3.4 Closed-Loop Simulations

The initial operating point, located in the higher conversion region, is assumed to be at the steady state:  $c_A = 4.29 kmol/m^3$ , and  $T = 332K$  for the original design. A conventional PI controller was used and its tuning parameters were kept unchanged in all simulation runs for the purpose of comparison. All the simulations were done by using SIMULINK in *MATLAB*.

In the first simulation runs, the original design is considered. Figure 4.6 illustrates the closed-loop response of the reactor temperature  $T$  and the profile of the input  $F$  for the original process design,  $V = 0.1m^3$ , with respect to negative step changes in the inlet temperature  $T_0$  from  $300 K$  to  $296 K$  and from  $300K$  to  $295K$ . It can be seen that the original design,  $V = 0.1m^3$ , can successfully reject a  $-4 K$  step change in the inlet temperature, but cannot for a  $-5K$  change in the inlet temperature. This is consistent with the analysis results in the above

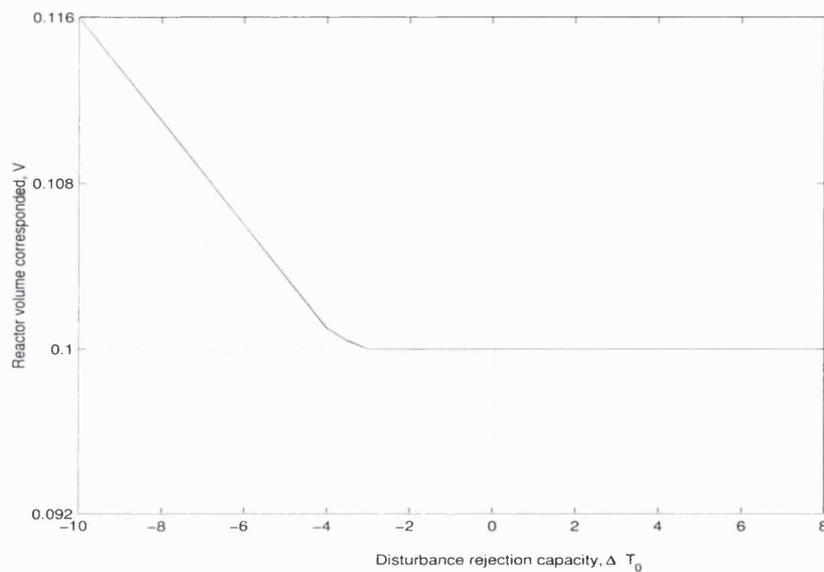


Figure 4.5: The relationship between design parameter and disturbance rejection ability

section. The control problem caused by input multiplicity is shown in Figure 4.7. For comparison, the profiles of the output  $T$  and the input  $F$  for a  $-4K$  change in the inlet temperature are given in Figure 4.8.

In the next two simulation runs, larger negative changes in the inlet temperature are imposed for the case of the modified design,  $V = 0.111m^3$ , and the rejection capability of the modified process is addressed. As can be seen from Figure 4.9, the process can come to rest at its initial point in the face of a  $-8K$  change in the inlet temperature and no control problem exists. Figure 4.10 shows that the modified process design can avoid control problems caused by input multiplicity for the disturbance.

The final set of simulation runs addresses the cases where the setpoint following ability is demonstrated. Figure 4.11 illustrates that the modification shows a slight improvement for controllability in the setpoint following ability of the reaction temperature in this case.

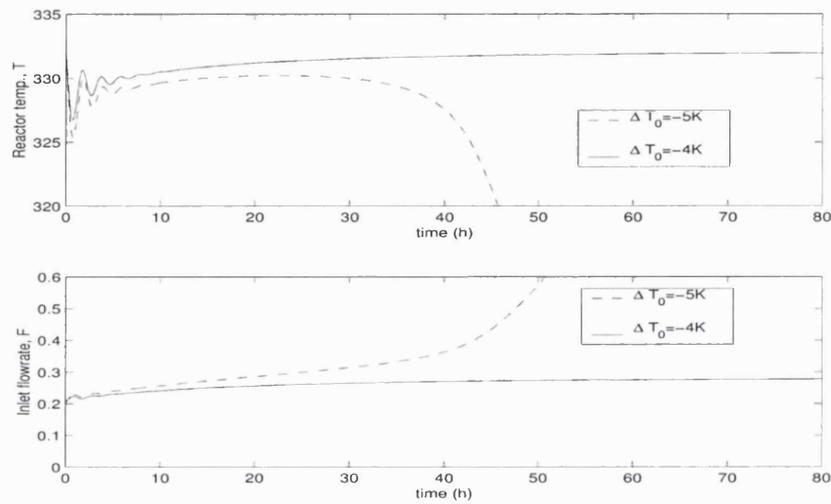


Figure 4.6: Profiles of input and output for the initial design,  $V = 0.1 m^3$ , for disturbance rejection of inlet temperature:  $-4 K$  and  $-5 K$

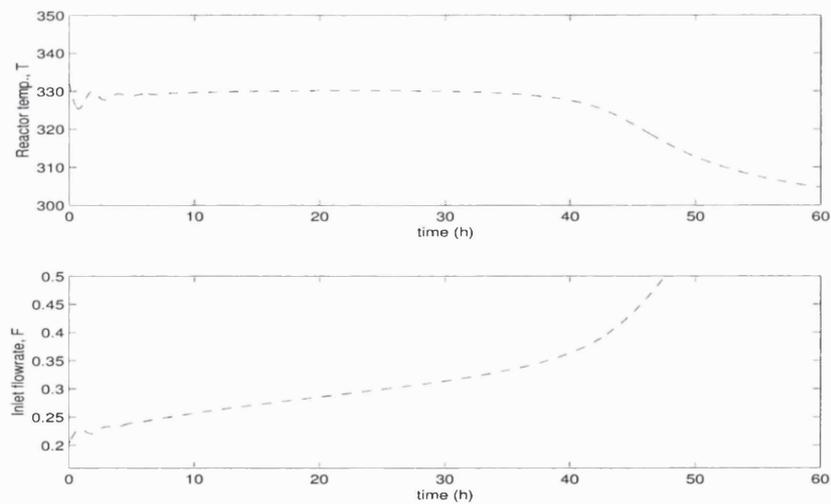


Figure 4.7: Profiles of input and output for the initial design,  $V = 0.1 m^3$ , for rejection of  $-5 K$  change in the inlet temperature

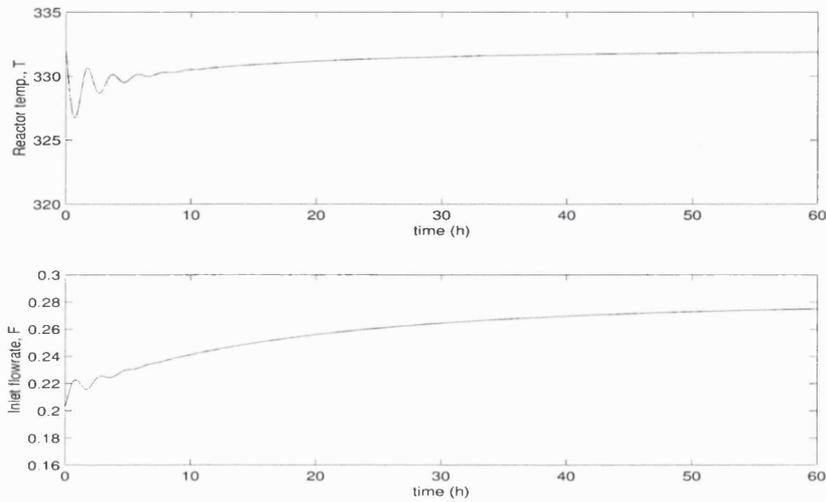


Figure 4.8: Profiles of input and output for the initial design,  $V = 0.1 m^3$ , for rejection of  $-4 K$  change in the inlet temperature

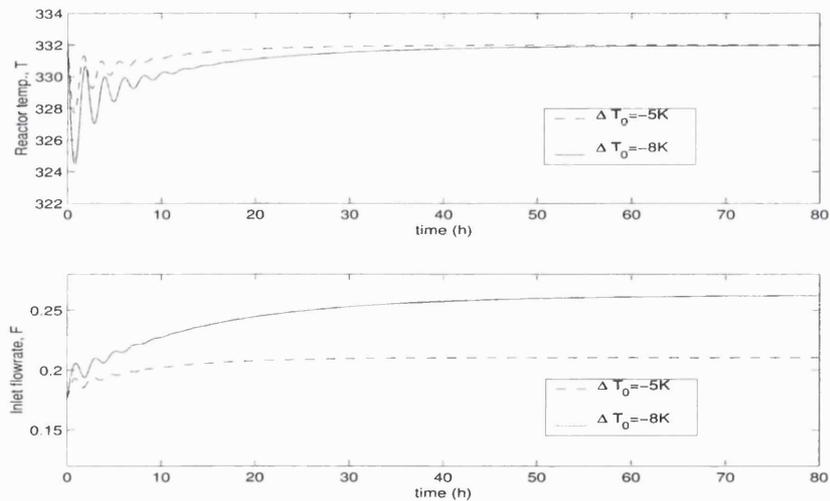


Figure 4.9: Profiles of input and output for the modified design,  $V = 0.111 m^3$ , for rejection of inlet temperature changes:  $-5 K$  and  $-8 K$

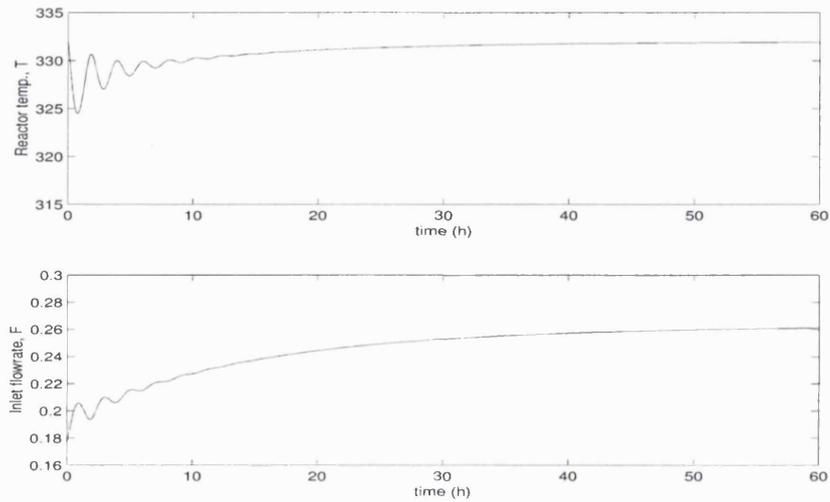


Figure 4.10: Profiles of input and output for the modified design,  $V=0.111m^3$ , for the disturbance of the inlet temperature,  $-8 K$

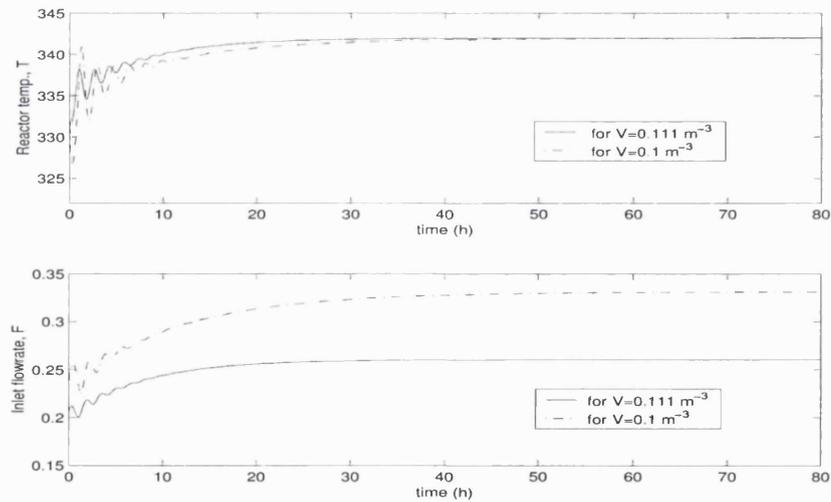


Figure 4.11: Closed-loop simulations for the original design,  $V = 0.1 m^3$ , and the modified design,  $V = 0.111 m^3$ , for a set-point change

## 4.4 Conclusions

This chapter has presented an optimisation-based approach to modifying an existing process design with a selected SISO control structure defined in terms of the controlled variable and manipulated variable. The optimisation problem solved is a NLP problem that aims at minimising the absolute values of design parameter adjustments to avoid the complex behaviour inside the range of the input, subject to the specified disturbances. The problem solved requires that the output be kept constant and the input be constrained by the undesirable behaviour conditions .

The illustrative example has shown via simulations that the modified design can avoid input multiplicity for the specified disturbance over the operating range of the input by means of slight adjustment of the reactor volume.

The process design modification approach can generate a modified design that can meet the requirement of the specified dynamic performance of the process while minimising changes to the process.

# Chapter 5

## Case Studies

---

This chapter presents the applications of the methodologies developed in Chapter 3 and Chapter 4 to two chemical process cases: a reactor-separator process including recycle; and an industrial polymerisation reaction CSTR unit. They are chosen as illustrative examples because they are typical chemical processes, and the process designs resulting from economic optimisation possess potential control problems associated with input multiplicity. The objectives of these studies presented in this chapter are: (i) to demonstrate how the bifurcation-based analysis approach presented in Chapter 3 can be used to study potential control problems of the economical optimal processes for the typical processes in the parameter space in order to achieve a better understanding of how the specific nonlinearity affect control and operability; (ii) to illustrate the applications of the static feedback optimisation design method presented in Chapter 4 to improve the static controllability.

These case studies demonstrate that the proposed methods can determine such potential control problems, and can generate process

modifications based on bifurcation analysis. The modified processes eliminate the control problems associated with input multiplicity in the operating regions for the specified disturbances. Closed-loop dynamic simulations show improved control performance for the modified designs.

The arrangement of this chapter is as follows. A reactor-separator process with recycle as recommended by Levenspiel (1972) is studied in § 5.1, and then a continuous polymerisation reactor as described by a detailed rigorous model (Daoutidis *et al.*, 1990) in § 5.2. A summary and conclusions follow in the final section of this chapter (§ 5.3).

## 5.1 Case Study I:

### A Reactor-Separator System with Recycle

#### 5.1.1 Introduction

The demand for more efficient and environmental production has resulted in chemical processes becoming more tightly integrated. Raw materials are recycled to increase the effective conversion and simultaneously reduce emissions to the environment. Material recycle may give rise to instability or complex behaviour, even the individual processing units are stable by themselves (Morud and Skogestad, 1996; Jacobsen, 1997).

The reactor-separator process shown in the following is an interesting study with respect to its multiplicity behaviour. It is a grossly simplified process model, but the characteristics of this example are suited to showing the results concerning input and output multiplicity caused by recycle. Slight design parameter modifications may change the dynamic behaviour of the process that has been studied previously by Jacobsen (1997), who analysed the process with respect steady state, i.e. with respect to controllability around a steady state. An optimal design as recommended by Levenspiel (1972) was studied and it was shown that this economically optimal design is not controllable due to the zero of the process on the imaginary axis (Jacobsen, 1997; Kuhlmann and Bogle, 1997). Two slight different designs were proposed which demonstrated improved controllability.

In this thesis, the optimal design following Levenspiel (1972) will be investigated to understand how the recycle affects on multiplicity behaviour of the process, and the process modifications required to eliminate such undesirable behaviour in the operating region of interest will be given. The design modifications

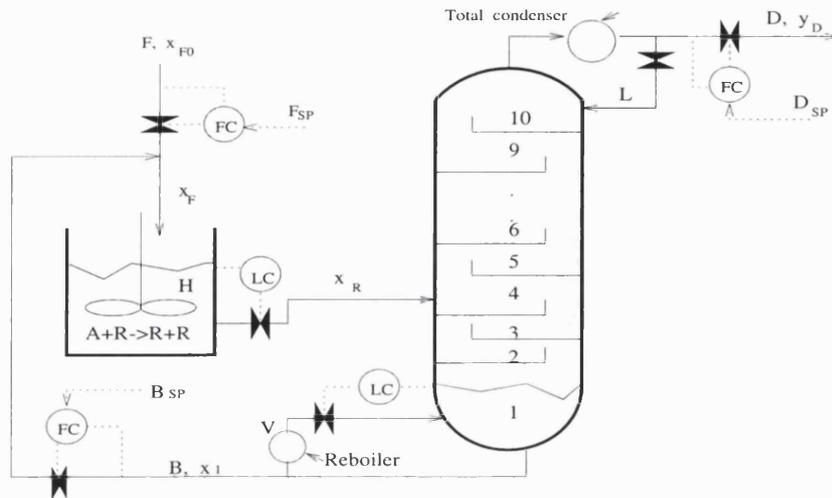


Figure 5.1: Schematic of the reactor-separator system

are determined based on the predefined setpoint following ability, rather than using an ambiguous rule of “the reactor should be operated away from the point of optimal reaction rate” suggested by Jacobsen (1997).

### 5.1.2 Process Description

A reactor-separator system, illustrated in Figure 5.1, considers the problem of converting a feed containing 100% component  $A$  into a product containing 98% component  $R$ . The conversion is made feasible by the auto-catalytic reaction:



where the reaction rate is:

$$r = kx_Ax_R = kx_R(1 - x_R). \quad (5.1)$$

The desired conversion could be achieved in a stirred tank reactor. In this case one takes particular advantage of the reaction and separator combination because auto catalytic reaction has a maximum reaction rate for some intermediate conversion (see equation 5.1). Following Levenspiel (1972) a stirred tank reactor operating at maximum conversion is combined with a distillation column to increase product purity (Jacobsen, 1997). The unconverted reactant from the distillation column is totally recycled to the reactor (see Figure 5.1). Component  $R$  is considered to be the more volatile component. The distillation column used in this case has 10 trays, including reboiler and condenser. The feed tray is at tray no.4 from the bottom. The main objective is to control the product purity  $y_D$  at a desired level.

### 5.1.3 Process Model Equations

The reactor-separator system is modelled by the following set of equations (material balances).

#### Reactor dynamics

$$\dot{x}_R = \frac{F+B}{H}(x_F - x_R) + kx_R(1 - x_R), \quad (5.2)$$

$$x_F = \frac{Fx_{F0} + Bx_1}{F+B}, \quad (5.3)$$

where  $x_F$  and  $x_R$  are the concentrations of the product  $R$  in the inlet and outlet of the reactor, respectively,  $H$  is the volume of the reactor,  $F$  is the flow rate of the reactant into the reactor,  $B$  is the flow rate recycled from the column to the reactor, and  $x_1$  is the concentration of the product  $R$  in the recycled  $B$ . The reactor is assumed to be perfectly mixed.

There are simplifying assumptions for the distillation column model:

- constant molar overflow (no energy balance),
- well-mixed liquid and vapour phases,
- constant relative volatility,
- constant holdup on all trays plus reboiler and reactor (perfect level control).

The relationship between liquid and vapour concentrations inside the column is defined as:

$$y_i = \frac{vx_i}{1 + (v - 1)x_i} \quad (5.4)$$

with a constant relative volatility  $v$ , and  $y_i$  are the vapour concentrations corresponding to the liquid concentrations  $x_i$ .

### Reboiler dynamics

The reboiler has a liquid inlet from tray 1 of the column which is partially vaporised by using an external heat input. Vapour is returned to tray 1 while the remain liquid from the column is totally recycle to the reactor (see Figure 5.2).

The reboiler effectively acts as a tray and is modelled as:

$$\dot{x}_1 = (L + F + B)x_2 - Bx_1 - Vy_1, \quad (5.5)$$

where  $L$  is the flow rate of the liquid reflux inside the distillation column,  $V$  is the vapour flow that is equal to  $L + D$  at steady state (see Figure 5.6),  $y_1$  is the concentration of product  $R$  in vapour in the reboiler.

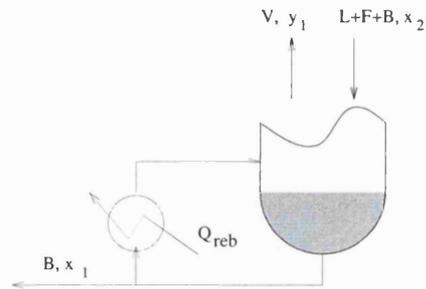


Figure 5.2: Schematic of a distillation bottom reboiler

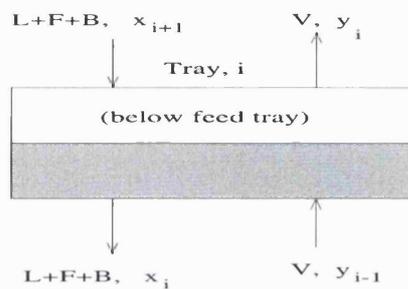


Figure 5.3: Schematic of a distillation below feed tray

### Tray below feed tray

A schematic of the  $i$ th tray below feed tray is shown in Figure 5.3. Molar balances are:

$$\dot{x}_2 = (L + F + B)(x_3 - x_2) + V(y_1 - y_2), \quad (5.6)$$

$$\dot{x}_3 = (L + F + B)(x_4 - x_3) + V(y_2 - y_3). \quad (5.7)$$

### Feed tray

A schematic of the feed tray is shown in Figure 5.4, Molar balances are:

$$\dot{x}_4 = (F + B)x_R + Lx_5 - (L + F + B)x_4 + V(y_3 - y_4). \quad (5.8)$$

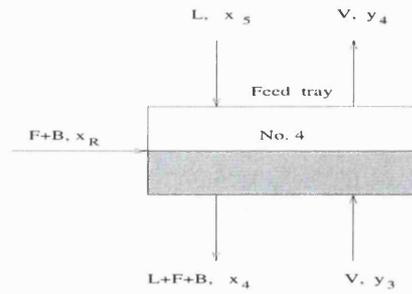


Figure 5.4: Schematic of a distillation feed tray

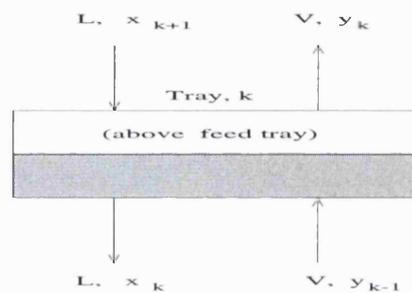


Figure 5.5: Schematic of a distillation above feed tray

### Tray above feed tray

A schematic of the  $k$ th tray above feed tray is shown in Figure 5.5. Molar balances are:

$$\dot{x}_5 = L(x_6 - x_5) + V(y_4 - y_5), \quad (5.9)$$

$$\dot{x}_6 = L(x_7 - x_6) + V(y_5 - y_6), \quad (5.10)$$

$$\dot{x}_7 = L(x_8 - x_7) + V(y_6 - y_7), \quad (5.11)$$

$$\dot{x}_8 = L(x_9 - x_8) + V(y_7 - y_8), \quad (5.12)$$

$$\dot{x}_9 = L(x_{10} - x_9) + V(y_8 - y_9). \quad (5.13)$$

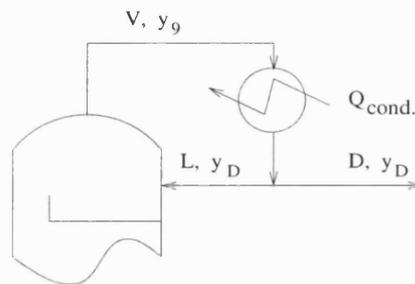


Figure 5.6: Schematic of a distillation overhead total condenser

### Condenser

The condenser for the top part of the distillation column is shown in Figure 5.6. It receives vapour inlet from the top tray, which is totally condensed by means of a coolant such as cooling water flowing through a coil.  $R$  and  $D$  denote the flow rates of reflux and distillate. Dynamic equation for the condenser is given:

$$\dot{y}_D = -(L + D)y_D + Vy_9. \quad (5.14)$$

The optimal design parameters recommended by Levenspiel (1972), where the stirred tank reactor was designed to operate at the maximum reaction rate while the distillation column was designed to increase the product purity to the desired level, are given in Table 5.1 (taken from Jacobsen, 1997). The main control objective is to keep the product purity  $y_D$  at a desired level, 98%. The possible manipulated variables are the reflux  $L$ , the recycle  $B$  or vapour flow  $V$ .

In this example, the  $y_D - L$  control configuration scheme:  $y_D$  is controlled by manipulating  $L$ , is chosen. Alternative to this control configuration such as  $y_D - B$  or  $y_D - V$  is possible, which will result in the same control problem when considering control of  $y_D$  alone (Jacobsen, 1997). Attention here focusses on determining potential control problems existing for the given process design with the selected control, analysing how the design parameters influence them, and

Table 5.1: Parameters and values for the optimal design

$x_{F0}$	=	0.0	$F$	=	1.0 kmol/min
$k$	=	0.06	$H$	=	65.33 kmol
$N$	=	9	$L$	=	1.704 kmol/min
$N_F$	=	4	$B$	=	1.2 kmol/min
$v$	=	3.0	$y_D$	=	0.98 kmol/kmol
			$x_R$	=	0.5 kmol/kmol

then modifying the process design itself to be controllable for the selected control structure in the operating region. In the following process analysis, this optimal design with the  $y_D - L$  control structure is referred to as the “base case” design.

#### 5.1.4 Controllable Analysis for the Base Case Design

In this section, the proposed analysis method in Chapter 3 is applied to this base case design to study multiplicity for the “base case” design. The control problems of the product purity  $y_D$  associated with input multiplicity and effects of the reflux  $L$ , recycle  $B$ , and reactor volume  $H$  on the behaviour of the process are investigated.

##### Steady-state multiplicity and control problems

For the base case design with the assigned  $y_D - L$  control configuration, Figure 5.7 shows its steady-state solutions under the variation of the reflux  $L$ . It is seen that the process exhibits input multiplicity for the given parameter values and selected operating conditions.

The input multiplicity condition as indicated by the square in Figure 5.7 is at the selected operating point, at which  $L = 1.702 \text{ kmol/min}$  and  $y_D = 0.98$ . Thus, the process is essential uncontrollable with the chosen control structure for the selected operating point (Jacobsen, 1997).

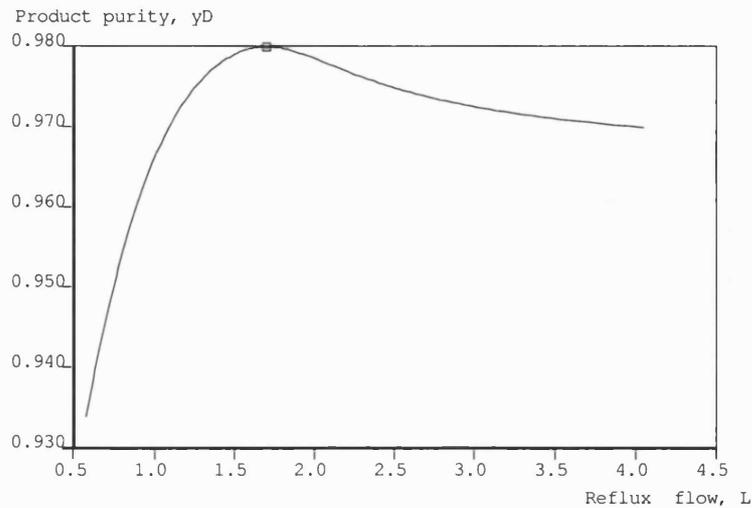


Figure 5.7: Steady-state solutions showing input multiplicity condition for the variation of the reflux  $L$  for the base case design. Open square: input multiplicity condition.

### Design parameter effects

The presence of recycle implies that the bottom composition  $x_1$  affects the reactor feed composition  $x_F$ , and then the reactor feed composition  $x_F$  affects  $x_1$ , which seems like a feedback (see Figure 5.1). Jacobsen (1997) stated that the presence of the recycle “may move the poles towards, and possibly the zeros, across the imaginary axis”, resulting in input and/or output multiplicity. In other words, the recycle  $B$  will affect the multiplicity behaviour of the process. Figure 5.8 indicates that the system exhibits both input multiplicity and output multiplicity for a larger value of  $1.8 \text{ kmol/min}$  of the recycle  $B$ . The locus in Figure 5.9 indicates the output multiplicity conditions between the reflux and recycle, where the behaviour of the process is divided into open-loop stable and unstable regions. It can be seen that an increase in the recycle  $B$  will cause an output multiplicity problem. Therefore, output multiplicity may occur if the value of the recycle  $B$  is above  $1.68 \text{ kmol/min}$  for the base case design.

The input multiplicity condition between the reflux  $L$  and the recycle  $B$  is

shown in Figure 5.10. As can be seen from Figure 5.10, there will exist no input multiplicity problem if the recycle  $B$  is below the value of about  $0.97 \text{ kmol}/\text{min}$ .

As a result of this analysis, a decrease in the recycle will possibly eliminate the output and input multiplicity behaviour.

Similarly, we study the effects of the design parameters on the multiplicity behaviour. The reactor volume  $H$  is chosen as an adjustable design parameter and only input multiplicity is considered since it will impose control difficulty on the system (Dash and Koppel, 1989). Figure 5.11 illustrates how the reactor volume  $H$  influences the input multiplicity behaviour for the variations of the recycle  $B$  and reflux  $L$ . The curved plane indicates the possible occurrence of the input multiplicity. The relationship can be expressed as  $L_{IM}(B, H) = f_{im}(B, H)$ .

The locally linearised expression of  $f_{im}(B, H)$  is given by:

$$L_{IM}(B, H) = -31.855 - 1.868B + 0.5479H, \quad (5.15)$$

which will be used as a constraint on the input in the modification optimisation problem to eliminate such an input multiplicity behaviour.

### 5.1.5 Process Design Modifications

As a result of the analysis above, the changes in the recycle and the reactor volume could eliminate the control problem associated with input multiplicity behaviour in the operating region of the reflux.

Jacobsen (1997) proposed design alternatives, based on the rule that “the reactor should be operated far away from the point of optimal reactor rate”. As a result of this, the reactor holdup  $H$  was adjusted from  $H = 65.33 \text{ kmol}$  (base case design in Table 5.2 where reactor rate is  $r = 0.015$ ) to  $H = 65.36 \text{ kmol}$  (same as the case FOD 3 in Table 5.2 where the reactor rate  $r = 0.01499$ ), which

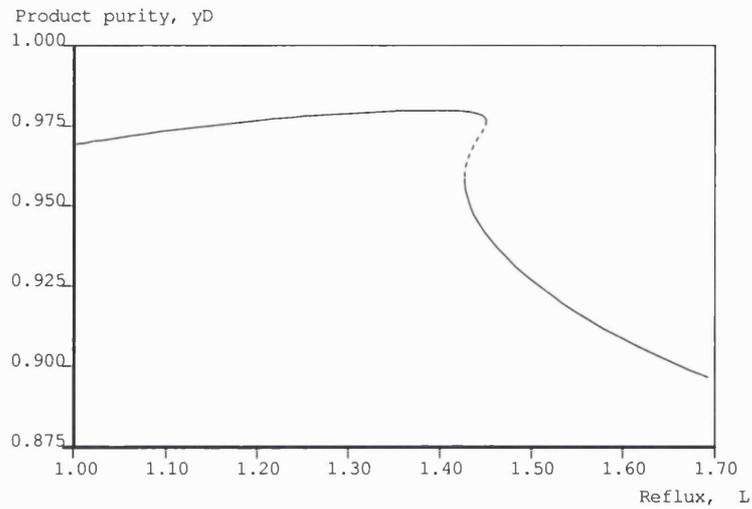


Figure 5.8: Input multiplicity and output multiplicity for the base case with a larger recycle:  $B=1.8$  kmol/min. Dashed line: unstable state

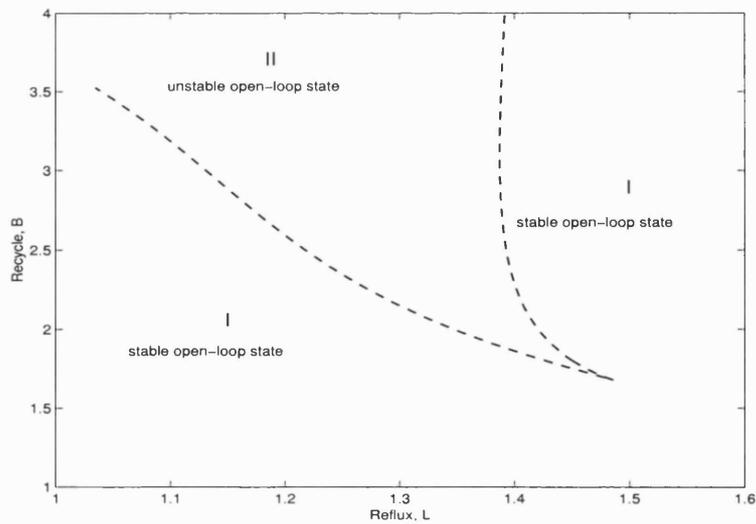


Figure 5.9: Locus of output multiplicity conditions between reflux and recycle for the base case

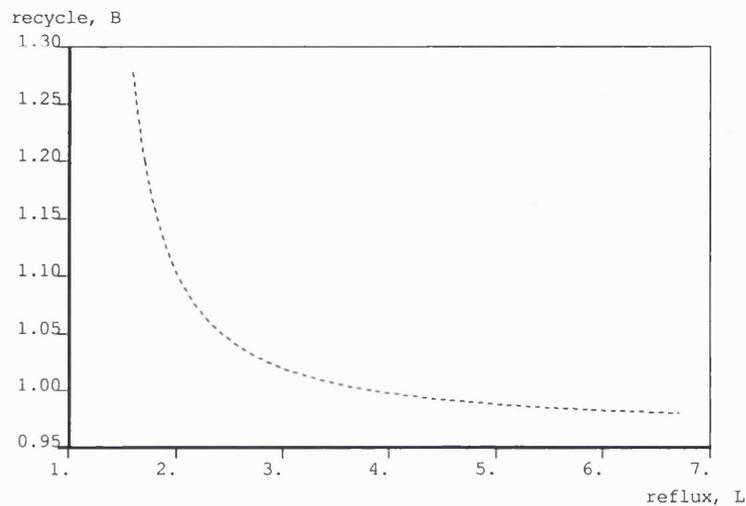


Figure 5.10: Locus of input multiplicity condition between reflux and recycle for the base case

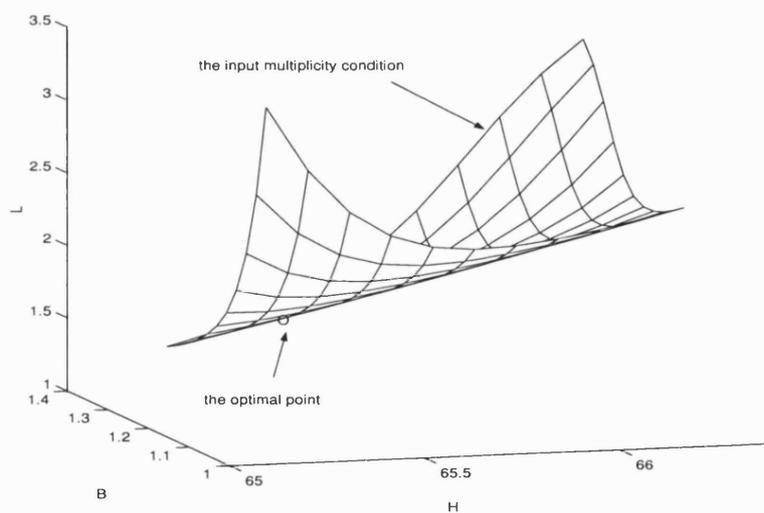


Figure 5.11: Relationship between reflux  $L$ , recycle  $B$ , and reactor volume  $H$  at input multiplicity condition for the base case design

shows improved controllability.

For the purpose of comparison with ones presented by Jacobsen (1997), the reactor holdup  $H$  and recycle  $B$  are also considered as the adjustable design parameters and the reflux  $L$  as the manipulated variable for the following process modification problem. The effect of these parameters on the input multiplicity have been analysed in the last subsection, as expressed by the equation (5.15).

The aim of the process design modification is to have the desired setpoint following ability in the operating range of the reflux  $L$ , i.e. a setpoint change will not encounter control problems associated with the input multiplicity, while maintaining the process modification as small as possible. Thus, the design modification optimisation formula for improved setpoint following ability is expressed as:

$$\min_{L,B,H} \{ \mathcal{R}(L - 1.703)^2 + \mathcal{Q}(B - 1.2)^2 + \mathcal{W}(H - 65.33)^2 \},$$

subject to

$$\begin{aligned} f(x) &= 0, & (5.16) \\ y_D - y_{D,exp} &= 0, \\ L - L_{IM}(B, H) &< 0, \end{aligned}$$

where  $f(x)$  represent the reactor-separator system model equations at steady-state,  $y_{D,exp}$  is the value of the output set-point to be followed,  $L_{IM}(B, H)$  is the input multiplicity condition given by the equation (5.15),  $\mathcal{R}$ ,  $\mathcal{Q}$ , and  $\mathcal{W}$  represent the appropriate operating cost factors in the change of the reflux  $L$  and recycle  $B$  operation, and the capital cost of the reactor volume change, respectively. For instance, the factors are selected to reflect the importance of the reactor

volume change, which are  $\mathcal{R} = 1$ ,  $\mathcal{Q} = 5$ , and  $\mathcal{W} = 10$ . In the optimisation problem (5.16), there are three degrees of freedom, i.e. the reflux  $L$ , recycle  $B$ , and reactor volume  $H$ , and the constraint on the reflux  $L$  forces the process to stay inside of the lower operating region of the reflux flow rate while eliminating the input multiplicity.

The optimal solutions from solving the optimisation problem (5.16), corresponding to the required setpoint following ability of the product purity  $y_D$ , are given in Table 5.2. If it is required that the process is able to follow a 0.1% change in the setpoint of the product purity  $y_D$ , i.e.  $\Delta y_{D,set} = 0.1\%$  of  $y_{D,set}$ , for example for case FOD 4 in Table 5.2, the reactor volume  $H$  has to be adjusted from  $H = 65.33 \text{ kmol}$  to  $H = 65.40 \text{ kmol}$ .

As can be seen in Table 5.2, the slight increase in the reactor volume  $H$  and decrease in the recycle can improve the setpoint following ability of the reactor-separator system. In other words, the control problems associated with input multiplicity can be avoided by adjustment of the reactor volume and recycle  $B$  to meet the specified setpoint following ability in the operating range of the reflux. For clarity and comparison, the steady state solutions for the base case design and modifications are shown in Figure 5.12. It is seen that the modified designs move the input multiplicity condition away from the operating point and thus enable the setpoint of the product purity  $y_D$  to have larger changeable margin. Simulations in the next subsection will demonstrate the improved setpoint following ability for the modified designs.

**Remark 5.1** *The data used to obtain the functional expression equation (5.15) of input multiplicity are from the analysis results by running AUTO with the add-in subroutine to determine the input multiplicity. The reflux  $L$  was defined initially as the first bifurcation (freedom) parameter to identify input multiplicity*

Table 5.2: Modification results of the reactor-separator system for cost weights:  $\mathcal{R} = 1$ ,  $\mathcal{Q} = 5$ , and  $\mathcal{W} = 10$

	Base case	FOD 1	FOD 2	FOD 3	FOD 4	FOD 5	FOD 6
$\Delta y_{D,set}$ (%)	0.0	0.01	0.03	0.05	0.1	0.2	0.5
$F$	1.0	"	"	"	"	"	"
$x_{F0}$	0.0	"	"	"	"	"	"
$k$	0.06	"	"	"	"	"	"
H	65.33	65.34	65.35	65.37	65.40	65.47	65.67
$N$	9	11	"	"	"	"	"
$N_F$	4	"	"	"	"	"	"
$v$	3.0	"	"	"	"	"	"
L	1.704	1.663	1.632	1.611	1.571	1.515	1.409
B	1.2	1.186	1.177	1.171	1.163	1.155	1.152
$y_{D,set}$	0.98	"	"	"	"	"	"
$x_1$	0.10	0.105	0.108	0.111	0.117	0.127	0.150
$x_R$	0.5	0.505	0.509	0.511	0.516	0.523	0.536

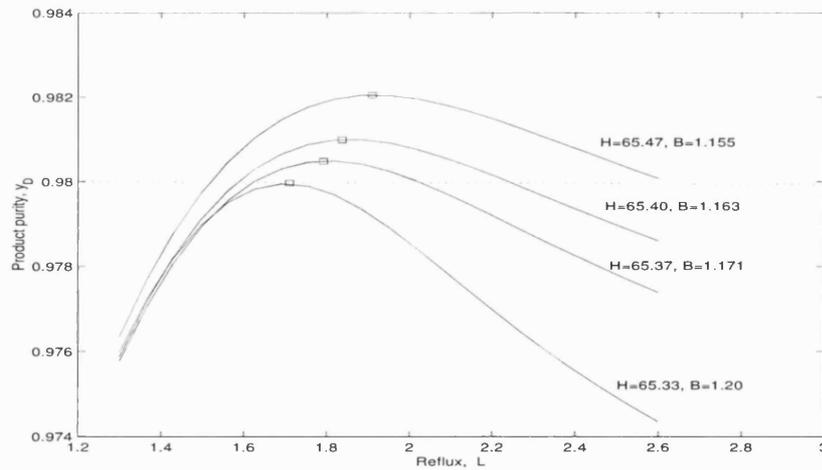


Figure 5.12: Steady states of the design modifications for the reactor-separator system. Square: input multiplicity condition

Table 5.3: Modification results of the reactor-separator system for cost weights:  $\mathcal{R} = 0.15$ ,  $\mathcal{Q} = 0.55$ , and  $\mathcal{W} = 1000$

	Base case	FOD 1	FOD 2	FOD 3	FOD 4	FOD 5
$\Delta y_{D,set}$ (%)	0.0	0.01	0.03	0.05	0.1	0.2
$F$	1.0	"	"	"	"	"
$x_{F0}$	0.0	"	"	"	"	"
$k$	0.06	"	"	"	"	"
$H$	65.33	65.34	65.35	65.37	65.40	65.47
$N$	9	11	"	"	"	"
$N_F$	4	"	"	"	"	"
$v$	3.0	"	"	"	"	"
$L$	1.704	1.668	1.642	1.623	1.585	1.522
$B$	1.2	1.183	1.171	1.164	1.153	1.150
$y_{D,set}$	0.98	"	"	"	"	"
$x_B$	0.10	0.104	0.106	0.109	0.114	0.125
$z_F$	0.5	0.505	0.509	0.511	0.516	0.523

in the reflux space, referred to as a bifurcation point, and then the recycle  $B$  or reactor volume  $H$  was assigned as the second bifurcation parameter starting at this bifurcation point.

To include a nonlinear expression for the bifurcation locus in the optimisation problem would require repeated automatic calls of the AUTO software.

**Remark 5.2** The results for the design modification optimisation problem (5.16) depend on the values of the cost weights selected. For comparison, results for a different set of the values of the cost weights were given as shown in Table 5.3. For this case, there is not a big difference.

### 5.1.6 Simulations

In this section, closed-loop dynamic simulations for the product purity set point control of the modified designs are given to demonstrate that the modified processes have the set point rejection ability as required. A conventional PI controller

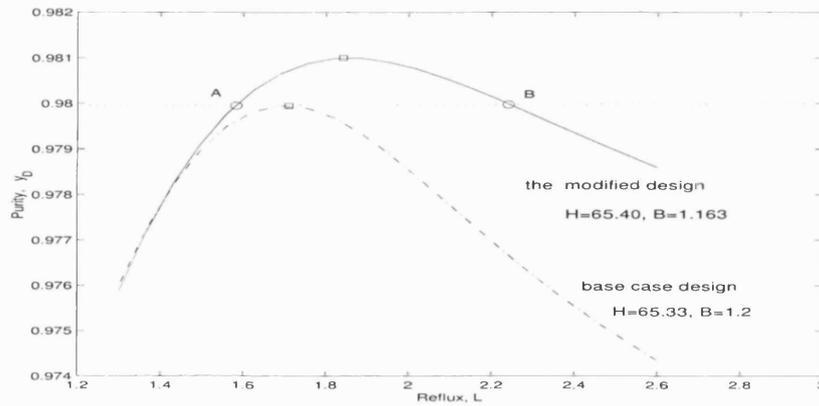


Figure 5.13: Steady states for the modified design,  $H=65.40$  and  $B=1.163$ , and the base case design. Open square: input multiplicity condition

(whose parameters were tuned following the Ziegler and Nichols' rule for quarter decay ratio (Ziegler and Nichols, 1942)) was utilised in the simulation runs. One of the modified designs resulting from the feedback optimal design, the example case FOD 4 in Table 5.2, in which the reactor volume was adjusted from  $65.33 \text{ kmol}$  to  $65.40 \text{ kmol}$  to have the required rejection ability of a 0.1% change in the set point of the product purity  $y_D$ , was chosen as demonstration.

As shown in Figure 5.13, there are two different stable operating points for  $y_D = 0.98$ : one operation point (A) with a lower reflux  $L = 1.567 \text{ kmol/min}$ , located on the left side of the peak point of the steady-state solution curve, and another operation point (B) with a higher value of  $2.217 \text{ kmol/min}$  of the reflux  $L$ , located on the right side of the peak. The operating point (B) with a lower conversion ( $x_R = 0.4842$ ) has unstable zero dynamics that will cause an inverse response in the product purity  $y_D$  to a change in the reflux  $L$  (Jacobsen, 1997).

Figure 5.14 illustrates that the modified process has the ability to reject the required set point in  $y_{D,set}$ , 0.1% of  $y_{D,set}$ , and fails for a slight increase over the required set point change, 0.12% of  $y_{D,set}$ , while initially operating at point (A).

At time zero, a 0.1% positive change in  $y_{D,set}$  is acting on the process. It is

seen that the system comes to rest very quickly at the desired set point following such a set point change. Then a negative disturbance identical to the magnitude above in set point change in  $y_{D,set}$  is applied to the process at about time  $4 \times 10^4$  and the system returns to its initial set point. When a similar set point change of magnitude of 0.12% in  $y_{D,set}$  is applied to the system at about time  $6 \times 10^4$ , the system becomes destabilised eventually. Figure 5.15 gives the details of the response of the  $y_D$  of Figure 5.14 for time from 0 to 500 minutes.

Similarly, Figure 5.16 shows that a sudden destabilisation occurs for the modified design initially operating at (B), if the change in  $y_{D,set}$  exceeds the value as required in the process modification. Figure 5.16 also indicates the inverse response in  $y_D$  due to unstable zero dynamics in this operating region (Jacobsen, 1997).

All other modifications can be proved by simulations that they have the required set point rejection ability in  $y_{D,set}$ . The simulations for the modified design of the case FOD 5 in Table 5.2 ( $H = 65.47 \text{ kmol}$  and  $B = 1.155 \text{ kmol/min}$ , corresponding to meet the requirement of a 0.2% change in  $y_{D,set}$ ) is shown in Figure 5.17. As can be seen, the modified design rejects the set point change as required, 0.2% change in  $y_{D,set}$ , but failed for the set point change over this value, a 0.21% change in  $y_{D,set}$ .

The simulations have demonstrated that the modifications resulting from the proposed feedback optimal design methodology have the set point rejection ability as required and the input multiplicity that could cause a sudden destabilisation problem in the control system is moved away from the operating range of the reflux.

All the simulations were done by using SIMULINK in *MATLAB*.

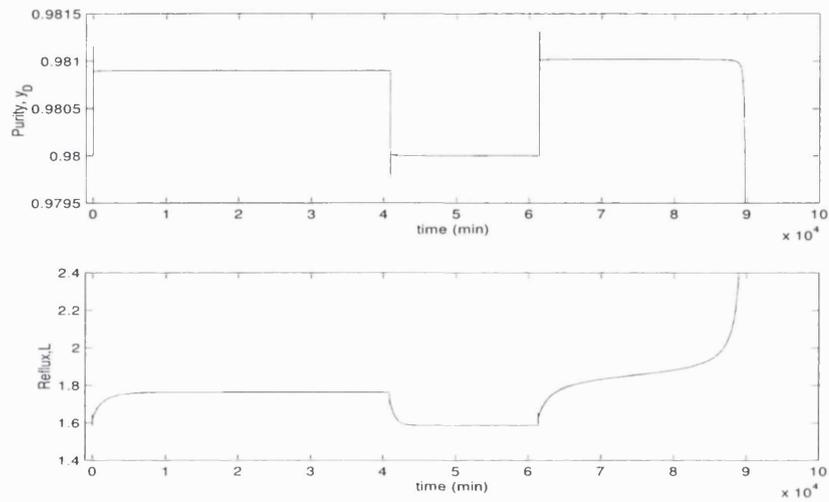


Figure 5.14: Step responses to 0.1% ( $t = 0$ ) and 0.12% ( $t \approx 6 \times 10^4$ ) changes in  $y_{D,set}$  for the modified design  $H = 65.40$  and  $B = 1.163$  initially operating at (A)

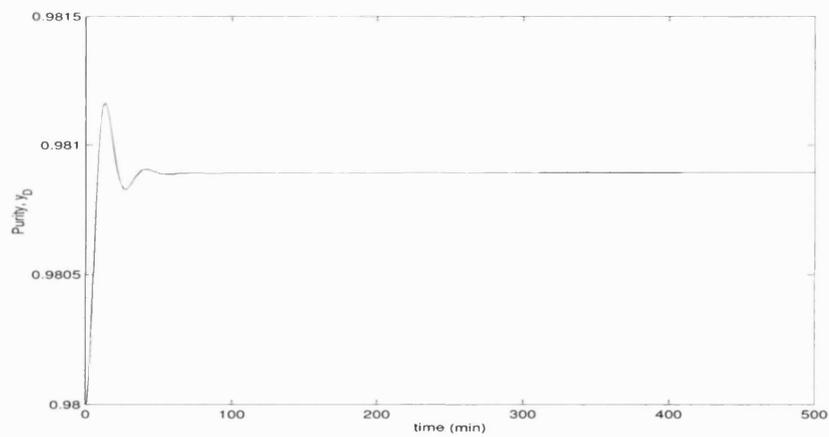


Figure 5.15: Details of output  $y_D$  for time from 0 to 100 minutes of Figure 5.14

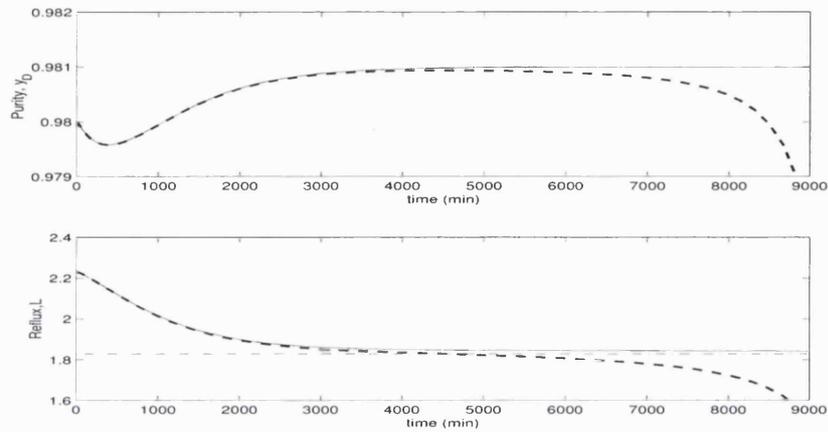


Figure 5.16: Step response to set point changes in  $y_{D,set}$  for the modified design  $H = 65.40$  and  $B = 1.163$  initially operating at (B). Solid line: 0.1% change in  $y_{D,set}$ ; dashed line: 0.12% change in  $y_{D,set}$

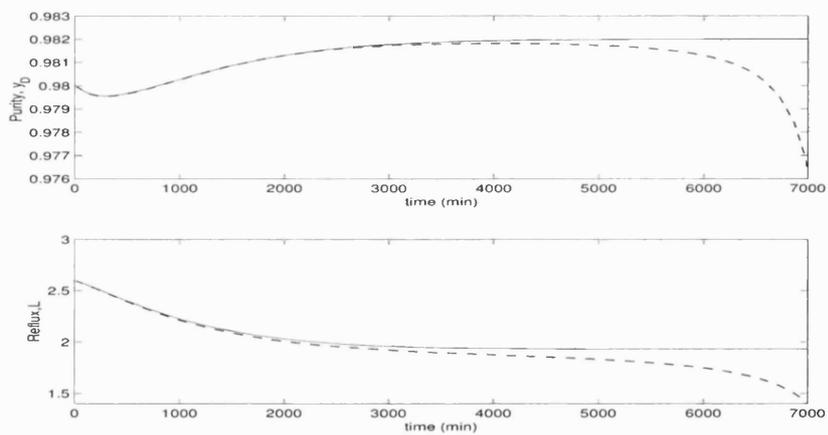


Figure 5.17: Step response to set point changes in  $y_{D,set}$  for the modified design  $H = 65.47$  and  $B = 1.155$  initially operating at point (B). Solid line: 0.2% change in  $y_{D,set}$ ; dashed line: 0.21% change in  $y_{D,set}$

### 5.1.7 Summary

The approach to controllability analysis and process modification presented in Chapter 3 and Chapter 4 was demonstrated with the reactor-separator process with recycle. It showed that multiplicity behaviour of the process affected by the recycle is easily evaluated in the parameter space by using the bifurcation based approach. When the value of the recycle is larger, both input multiplicity and output multiplicity are found, but for the smaller value of the recycle, the process only has input multiplicity and possibly no multiplicity exists. The optimal operating point resulting from the design according to Levenspiel (1972) is fundamentally uncontrollable (Jacobsen, 1997) because input multiplicity occurs exactly at the operating condition. Slight modifications to the optimal design by means of the proposed feedback optimal design methodology move the input multiplicity behaviour away outside of the operating range of difficulty to obtain the required set point rejection ability.

The case study employed a specific set of design parameters, but the lessons can apply to a wider set of conditions. As already stated by Jacobsen (1997), the control problem discussed here is not caused by some specific choice of parameters, but the problem is generic in the sense that it applies to all reactor-separator systems with recycle, with an autocatalytic reaction of type (Skogestad *et al.*, 1996) and designed according to Levenspiel (1972), at the nominal operating conditions. The results derived in this thesis also apply to any intermediate reaction scheme without side reaction if the process has only one maximum in the steady state locus (Kulhmann and Bogle, 1997).

## 5.2 Case Study II:

### An Industrial Polymerization Reaction

#### 5.2.1 Introduction

A variety of industrially relevant polymerisation reactions are highly exothermic, and thus have very interesting and troublesome nonlinear dynamics that make these systems difficult to operate and control. Complex nonlinear dynamics found in polymerisation processes have been presented by Ray and Villa (2000) in their comprehensive review work, who analysed phenomena such as multiplicity, oscillatory behaviour in continuous stirred tank reactors (CSTRs), and these and other phenomena in other types of reactors for polymerisation. The particular nonlinear behaviour depends on the polymer produced, the type of polymerisation kinetics, the reactor type, the phase behaviour, the heat removal system, etc. Multiplicity and sustained oscillation phenomena are common ones that arise routinely in industrial practice.

Previous researchers showed poor single-input-single-output control performance due to multiplicity behaviour for a given set of polymerisation CSTR design parameters (Hidalgo *et al.*, 1990; Daoutidis *et al.*, 1990; Russo and Bequette, 1995; Lewin and Bogle, 1996). The poor heat transfer from the reactor to the cooling water jacketed in polymerisation systems is one of the major causes for strong process nonlinearity, and the effects of the cooling system on the polymerisation process should be considered in the control system design. Neglecting the cooling energy balance in the control system design is a poor assumption (Russo and Bequette, 1998).

In this case, a continuous polymerisation reactor including the cooling energy balance, as described by a detailed rigorous model (Daoutidis *et al.*, 1990),

is employed. The specific control objective is to maintain the molecular weight distribution of the polymer at a desired level by manipulating the coolant flow rate for a disturbance. The potential control problems of the process with the assigned SISO control configuration scheme will be analysed to identify that input multiplicity behaviour in the jacket outlet temperature is a cause of sudden destabilisation in the process behaviour and to show how the design parameters influence it, leading to process modifications. It will be shown that the modified process designs by using the proposed methodologies in this thesis can successfully eliminate such potential control problems associated with the input multiplicity inside the operating region for a defined disturbance.

The outline of this section is as follows. The process model equations and optimal operation design resulting from the economical optimisation are presented in § 5.2.2, followed by controllability analysis on the optimal design. In § 5.2.5, the modifications to the process design are given, corresponding to the required disturbance rejection ability. Dynamic simulations are shown in § 5.2.6. A brief summary follows in the final subsection (§ 5.2.7) of this case study.

## 5.2.2 Process Model and Optimal Operation Design

A free-radical polymerisation of MMA (methyl methacrylate) with AIBN (azo-bis-isobutyronide) as initiator and toluene as solvent takes place in a jacketed CSTR. A model for the process, which is given by Daoutidis *et al.* (1990), describes the dynamics of the monomer and initiator concentrations ( $C_m$  and  $C_I$ ), the reactor and jacket temperature ( $T$  and  $T_j$ ), and the zeroth and first bulk moments of the molecular weight distribution of the polymer ( $D_0$  and  $D_1$ ). The following assumptions in the modelling are made:

- Perfect mixing in the reactor

- Constant density of the reacting mixture (no volume shrinkage)
- Constant heat capacity of the reacting mixture
- Uniform coolant temperature in the jacket
- Insulated reactor and cooling system
- Constant density and heat capacity of the coolant
- No polymer in the inlet stream
- No gel effect (because of low monomer conversion)
- Constant reactor volume
- Standard mechanism of free-radical polymerisation

The dynamic equations of the system are given as:

$$\dot{C}_m = -(R_p + R_{fm})C_m P_0(C_I, T) + \frac{F}{V}(C_{m,in} - C_m), \quad (5.17)$$

$$\dot{C}_I = -(R_I + C_I) + \frac{1}{V}(F_I C_{I,in} - F C_I), \quad (5.18)$$

$$\dot{T} = R_p C_m (-\delta H_p / \rho C_p) P_0(C_I, T) - \frac{UA}{\rho C_p V}(T - T_j) + \frac{F}{V}(T_{in} - T), \quad (5.19)$$

$$\dot{D}_0 = (0.5R_{Tc} + R_{Td})P_0^2(C_I, T) + R_{fm}C_m P_0(C_I, T) - \frac{FD_0}{V}, \quad (5.20)$$

$$\dot{D}_1 = M_m(R_p + R_{fm})C_m P_0(C_I, T) + \frac{FD_1}{V}, \quad (5.21)$$

$$\dot{T}_j = \frac{T_{w0} - T_j}{V_0} F_{cw} + \frac{UA}{\rho_w C_w V_0}(T - T_j), \quad (5.22)$$

where

$$P_0(C_I, T) = \left[ \frac{2f^* C_I R_I}{R_{Tc} + R_{Td}} \right]^{0.5}. \quad (5.23)$$

The kinetic expressions,  $R_i$ , are expressed in the Arrhenius form:

$$R_i = K_i \exp(-E_i/RT). \quad (5.24)$$

The kinetic parameters are given in Table 5.4, and the design and operation parameter values in Table 5.5 from the study by Daoutidis *et al.* (1990). The typical outputs to be controlled are the molecular weight number  $MW_{av}$ , given as the ratio  $D_1/D_0$ , and the reaction temperature  $T$ . The possible manipulated variables are the initiator flow rate  $F_I$  and the jacketed cooling flow rate  $F_{cw}$ . The main disturbances are the inlet monomer concentration  $C_{m,in}$  and the inlet reactor temperature  $T_{in}$ .

The operation objectives for this basic design are to ensure safe, steady operation of the reactor and to maintain the  $MW_{av}$  constant despite disturbances in the monomer feed concentration and the temperature of the inlet feed. Furthermore, it is desired to operate the reactor with the minimum initiator flow rate possible because the initiator is expensive. An optimal operation condition of the reactor was sought in such a way, presented by Lewin & Bogle (1996), that the molecular weight number was maintained at  $MW_{av} = 25,000$  while minimising the consumption of the expensive initiator. The conversion,  $\Delta C = C_{min} - C_m$ , is to be kept relatively low on purpose to avoid the gel effect.

Thus the operating optimisation formula is given by:

$$\min F_I,$$

subject to

$$f(x) = 0, \quad (5.25)$$

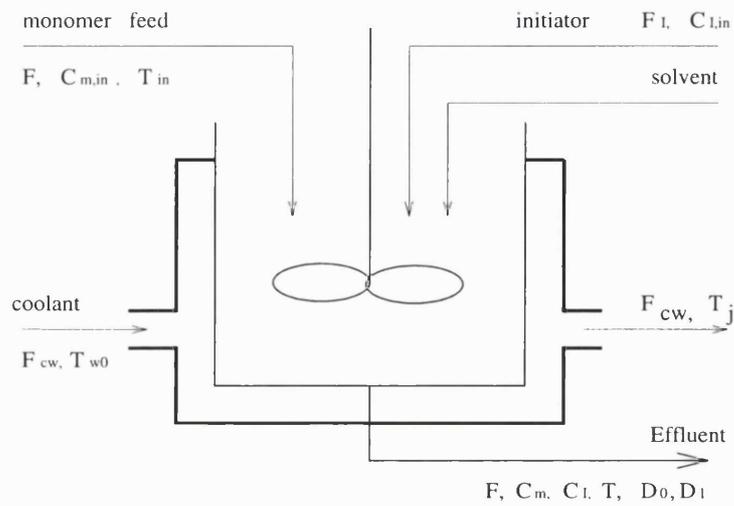


Figure 5.18: Process flow diagram for the jacketed polymerisation CSTR

$$D_1/D_0 = 25000,$$

$$T_{in} = 350, \text{ (nominal value)}$$

$$\Delta C = C_{min} - C_m,$$

where  $f(x)$  represents six state equations (equation 5.17 to equation 5.22) of the process at steady state. The optimal operating point resulting in solving the optimisation problem ( 5.25) is  $F_I = 0.00354$ , corresponding to  $\Delta C = 0.5$ . The relevant inputs at the optimal operation are :  $[F_{cw}, C_{m,in}] = [0.1673, 6.438]$ , respectively. The process with the optimal operating condition is referred to as the “base case” design in the ongoing discussion.

### 5.2.3 Analysis for the Base Case Design

#### Steady-State Multiplicity

The steady state solution diagrams for the controlled molecular weight number  $MW_{av}$  and the six states versus the cooling water flow rate  $F_{cw}$  are shown in

Table 5.4: Kinetic parameters

$i_j$	$R_{i_j}$	$E_{i_j}$
$T_c$	$3.8223e10^{10} \text{ kmol}/\text{m}^3.\text{h}$	$2.9442e10^3 \text{ kJ}/\text{kmol}$
$T_d$	$3.1457e10^{11} \text{ kmol}/\text{m}^3.\text{h}$	$2.9442e10^3 \text{ kJ}/\text{kmol}$
$I$	$3.7920e10^{18} \text{ kmol}/\text{m}^3.\text{h}$	$1.2877e10^5 \text{ kJ}/\text{kmol}$
$P$	$1.7700e10^9 \text{ kmol}/\text{m}^3.\text{h}$	$1.8283e10^4 \text{ kJ}/\text{kmol}$
$f_m$	$1.0067e10^{15} \text{ kmol}/\text{m}^3.\text{h}$	$7.4478e10^4 \text{ kJ}/\text{kmol}$
$f^* = 0.58$		

Table 5.5: Process design and operation parameter values

$C_p = 2.0$	$\text{kJkg}^{-1}\text{K}^{-1}\text{h}^{-1}$	$C_w = 4.2$	$\text{kJkg}^{-1}\text{K}^{-1}\text{h}^{-1}$
$-\Delta H_p = 57,800$	$\text{kJkmol}^{-1}$	$T_{in} = 350$	$\text{K}$
$V = 0.1$	$\text{m}^3$	$V_0 = 0.02$	$\text{m}^3$
$\rho_w = 1000$	$\text{kgm}^{-3}$	$\rho = 866$	$\text{kgm}^{-3}$
$U = 720$	$\text{kJh}^{-1}\text{K}^{-1}.\text{m}^{-2}$	$A = 0.1$	$\text{m}^2$
$M_m = 100.12$	$\text{kg.kmol}^{-1}$	$C_{I,in} = 6.0$	$\text{kmol.m}^{-3}$
$T_{w_0} = 293.2$	$\text{K}$	$R = 8.314$	$\text{kJkmol}^{-1}\text{K}^{-1}$
$F = 1.0$	$\text{m}^3\text{h}^{-1}$		

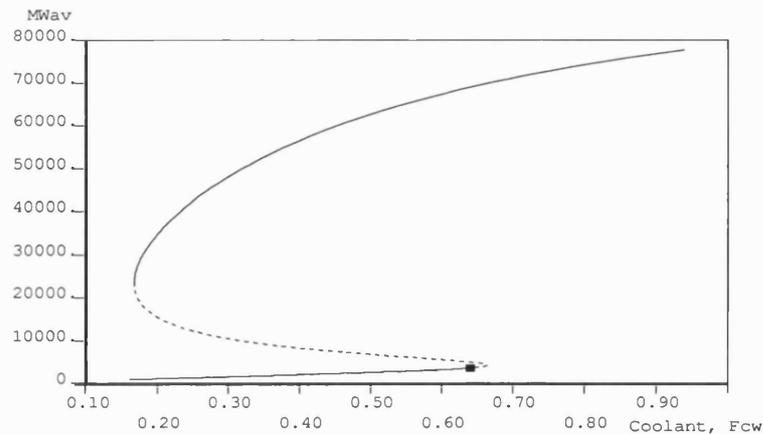


Figure 5.19: Steady states of molecular weight number versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

Figure 5.19 to Figure 5.25. As can be seen from these figures, the process exhibits multiplicity and Hopf bifurcation behaviour in the space of the flow rate of the cooling water  $F_{cw}$ . The molecular weight number  $MW_{av}$  and the reaction temperature  $T$  exhibit output multiplicity; the jacket temperature  $T_j$  exhibits both input and output multiplicity; and the other states show output multiplicity characteristics. One Hopf bifurcation point, indicated by the solid square in the diagrams, is found which is located in the upper reaction temperature steady state region. The middle steady states are unstable because a small increase in steady state temperature results in heat generation exceeding heat removal, which causes the reactor to operate at the upper steady state. Likewise, if there is a small decrease in steady state temperature at the middle operating point, heat removal dominates heat generation, causing the reactor to operate at the lower temperature steady states (Hidalgo *et al.*, 1990).

We here focus on the following SISO control scheme: the molecular weight number  $MW_{av}$  is controlled by the cooling water flow rate  $F_{cw}$ , while the initiator  $F_I$  is fixed at its optimal operation value of 0.00354, and then study what the potential control problems caused by multiplicity and bifurcation are and how

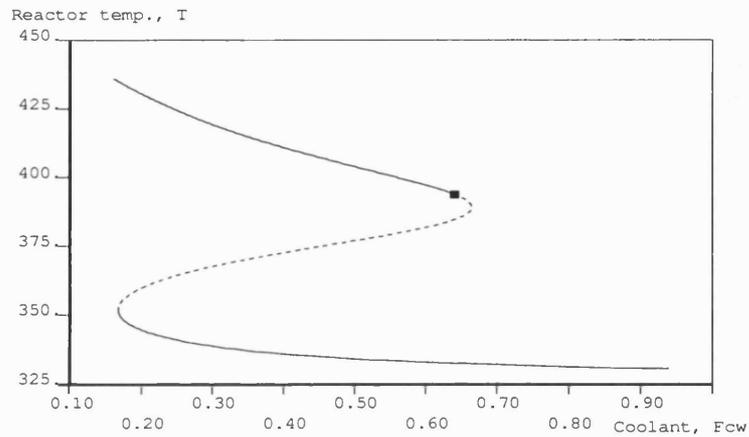


Figure 5.20: Steady states of reaction temperature versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

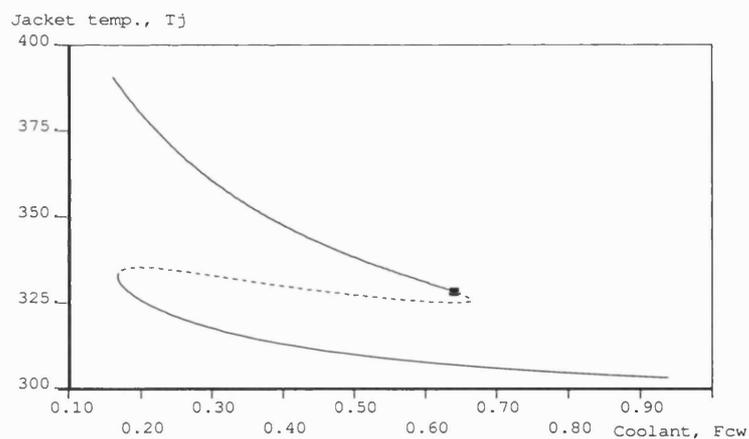


Figure 5.21: Steady states of jacket temperature versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

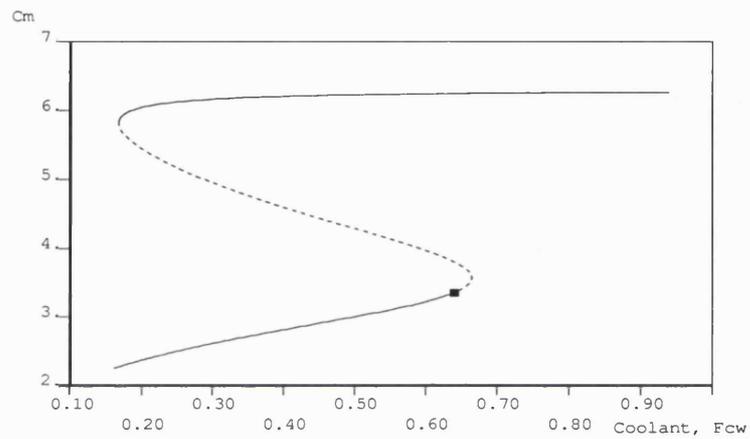


Figure 5.22: Steady states of monomer concentration versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

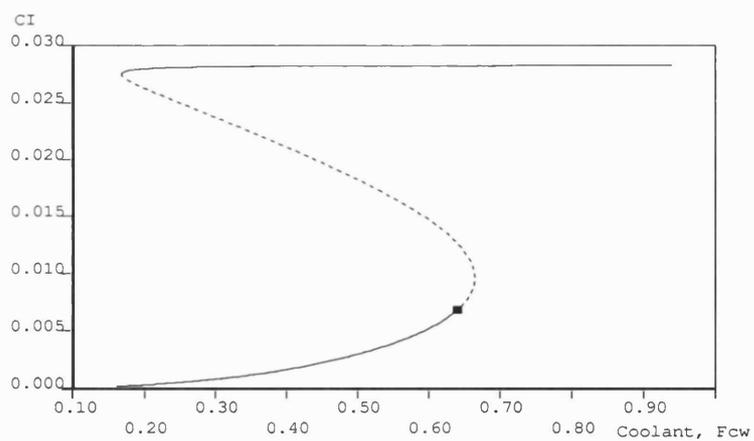


Figure 5.23: Steady states of initiator concentration versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

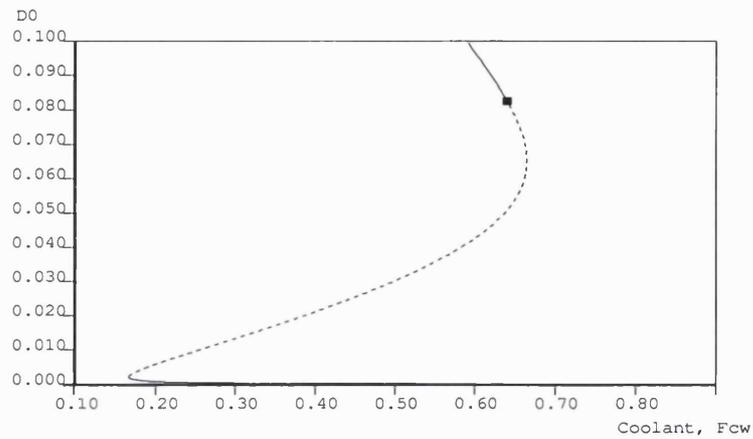


Figure 5.24: Steady states of zeroth moment of molecular weight distribution versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

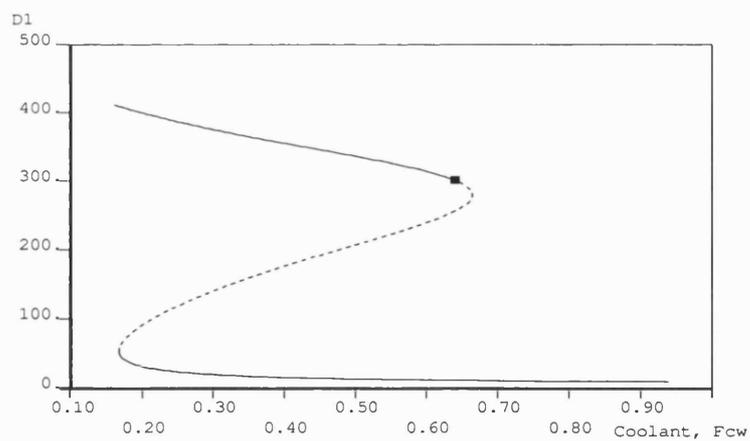


Figure 5.25: Steady states of the first moment of molecular weight distribution versus coolant. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point

the design and operation parameters affect them.

By using the proposed methodology presented in Chapter 3, input multiplicity conditions were identified as indicated by open squares in Figure 5.26 and Figure 5.27. The selected optimal operation point for the “base case” design at steady state is:  $MW_{av,s} = 25,000$  and  $F_{cw,s} = 0.1673m^3/h$ . The steady-states of the six states at the operating point are:  $[C_m, C_I, T, D_0, D_1, T_j] = [5.8667, 0.0276, 350.89, 0.002, 49.98, 331.97]$ , respectively. This operating point is close to one of the limit points ( $MW_{av} = 23,516$  and  $F_{cw} = 0.1666m^3/h$ ) at which the open-loop steady states change their stability and one of the input multiplicity conditions ( $MW_{av} = 15,765$  and  $F_{cw} = 0.1977m^3/h$ ) at which the jacket temperature gain changes its sign (see Figure 5.26 and Figure 5.27).

It can be seen that only output multiplicity exists in the controlled  $MW_{av}$  -  $F_{cw}$  loop. It would seem that no potential control problems exist using feedback control with integral action since the steady state corresponding to the specified set point value of  $MW_{av}$  will be maintained and no other steady state will be allowed (Koppel, 1985). In this case however input multiplicity in the jacket outlet temperature  $T_j$ - $F_{cw}$  (Figure 5.27) may cause a sudden destabilisation of the controlled system. This case differs from one presented by Dash and Koppel (1989) in that input multiplicity exists in another internal state rather than in the controlled variable. To illustrate potential sudden destabilisation problems associated with the input multiplicity, closed loop dynamic simulations are given for the  $MW_{av}$  controlled by a conventional PI controller (whose parameters were tuned following the Ziegler and Nichols’ rule (Ziegler and Nichols, 1942)) for a disturbance of the inlet temperature  $T_{in}$ , initially operating at the selected optimal point ( $MW_{av} = 25000$  and  $F_{cw} = 0.1673$ ). Figure 5.28 shows the transients of the controlled variable,  $MW_{av}$ , manipulated variable,  $F_{cw}$ , and the internal state,  $T_j$ , for a  $3K$  positive step change in the inlet temperature,  $T_{in}$ , ( $\Delta T_{in} = +3K$ ).

As can be seen, the system comes to rest at the initial point following such a disturbance. When a similar disturbance of  $\Delta T_{in} = +4K$  is applied to the process, it experiences a “sudden destabilisation” and finally comes to rest at its initial point, as shown in Figure 5.29. Such a sudden destabilisation in this example can be possibly explained as follows by using a pseudo-steady-state path followed by the process during such a destabilisation, depicted in Figure 5.30.

As shown in Figure 5.30, when the  $MW_{av}$  is initially at the selected optimal operation point  $a$ , indicated by the solid circle, and an increase in the disturbance of the inlet temperature  $T_{in}$  is acting on the process, the  $MW_{av}$  goes along the curve  $ab1$  towards point  $1$  (input multiplicity condition indicated by the open square), and the coolant flow rate  $F_{cw}$  subject to the controller:  $F_{cw} = k_p(MW_{av,set} - MW_{av}) + k_c \int_0^t (MW_{av,set} - MW_{av})dt + F_{cw,s}$  ( $k_p$  and  $k_c$  are proportional and integral gains of the controller, respectively) is increased slowly to compensate for the offset of the  $MW_{av}$  imposed by the disturbance. The internal state  $T_j$  goes along the curve  $a'b'1'$  towards point  $1'$  (input multiplicity condition indicated by the open square), following the increase in  $F_{cw}$ . At point  $1'$ , the steady state path followed by the reaction depends on how the coolant is manipulated. If the manipulated variable  $F_{cw}$  is reduced before reaching the point, i.e. the input multiplicity condition is not breached, the process comes to rest at its initial point without a sudden destabilisation problem, as shown in Figure 5.28. If the input multiplicity condition is breached and any further increase of coolant flow rate  $F_{cw}$  changes the internal state  $T_j$  behaviour and the  $T_j$  will go vertically to the upper stable curve  $c'd'$  so that the  $MW_{av}$  goes to the lower stable curve  $cd$ , directly below point  $1$ .

At this point, the  $MW_{av}$  is increased along the section  $cd$  towards the point  $d$  indicated by solid square (Hopf bifurcation point at which  $MW_{av} = 3639$  and  $F_{cw} = 0.6405$ ) as the coolant flow rate  $F_{cw}$  is continuously increased due to the still

existing offset in the controlled  $MW_{av}$ . This continues until the point  $d$  is reached at which point oscillatory behaviour of the process occurs. But, this oscillation does not last once the second input multiplicity condition  $\mathcal{Q}$  ( $MW_{av} = 5000$  and  $F_{cw} = 0.6425$ ) indicated by an open square is breached, since the point  $d$  is very close to the second turning point  $e$  ( $MW_{av} = 4286$  and  $F_{cw} = 0.665$ ) and the second input multiplicity condition point  $\mathcal{Q}$ . At this instant, the jacket outlet temperature  $T_j$  changes its behaviour again as happened at the first input multiplicity condition, and the  $T_j$  goes to the lower stable curve  $f'a'$  and the  $MW_{av}$  goes to the upper stable curve  $fa$ . Thus the coolant flow rate  $F_{cw}$  is decreased dramatically due to larger negative offset between  $MW_{av,set}$  and  $MW_{av}$ . Along the stable curve  $fa$  the process can reach the desired set point value of 25,000 of  $MW_{va}$  by proper manipulation of the coolant flow rate  $F_{cw}$ .

This pseudo steady state analysis possibly explains the sudden destabilisation in the controlled  $MW_{av}$  because of the presence of input multiplicity in the internal state  $T_j$ . As a result of this analysis, one can conclude that input multiplicity that existed in the jacket outlet temperature  $T_j$  is the likely cause of sudden destabilisation during operation of the polymerisation reaction. Such a characteristic is an inherent property of the process itself. Therefore, input multiplicity behaviour should be eliminated or avoided by modifying the process design itself. The following subsections will approach this problem.

#### 5.2.4 Effects of Design and Operation Parameters

In order to eliminate input multiplicity by means of process modification, the effects of the design and operation parameters on the input multiplicity behaviour of the polymerisation reaction is explored in this subsection.

In the last subsection, the behaviour of the process under variation of the

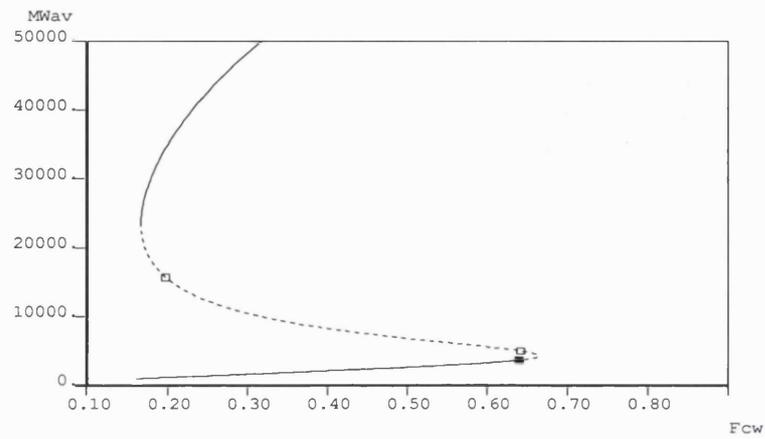


Figure 5.26: Steady states of  $MW_{av}$  showing input multiplicity condition. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point; open square: input multiplicity condition

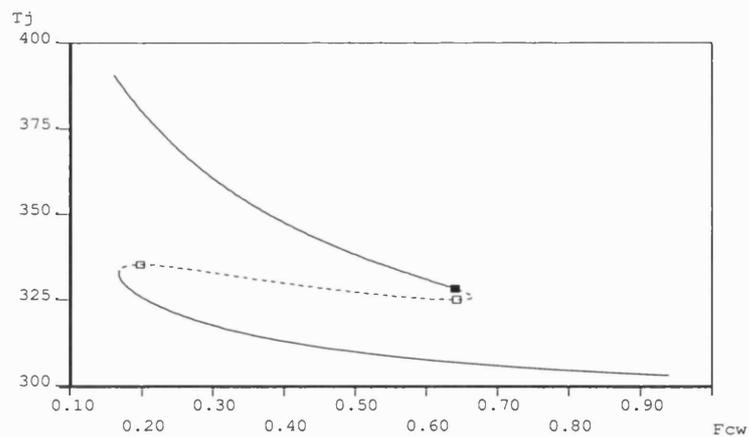


Figure 5.27: Steady states of the jacket temperature showing input multiplicity condition. Solid line: stable state; dashed line: unstable state; solid square: Hopf bifurcation point; open square: input multiplicity condition

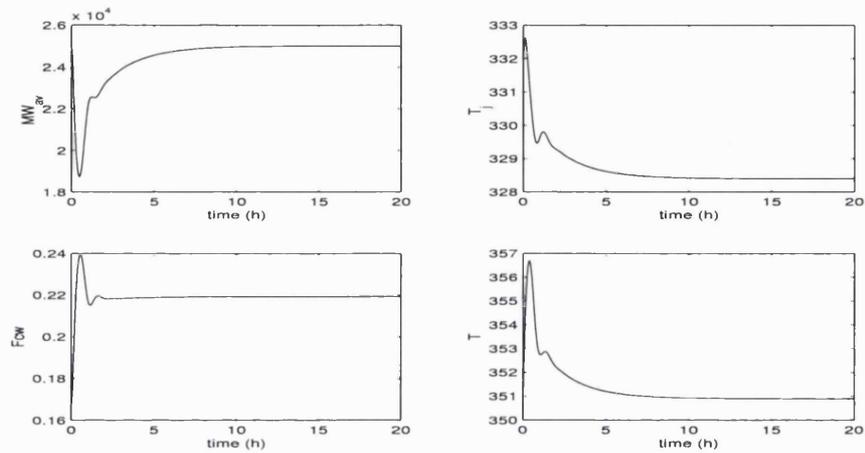


Figure 5.28: Trajectories of the output, input, and profile of the internal state for a step change in inlet temperature:  $\Delta T_{in} = +3K$

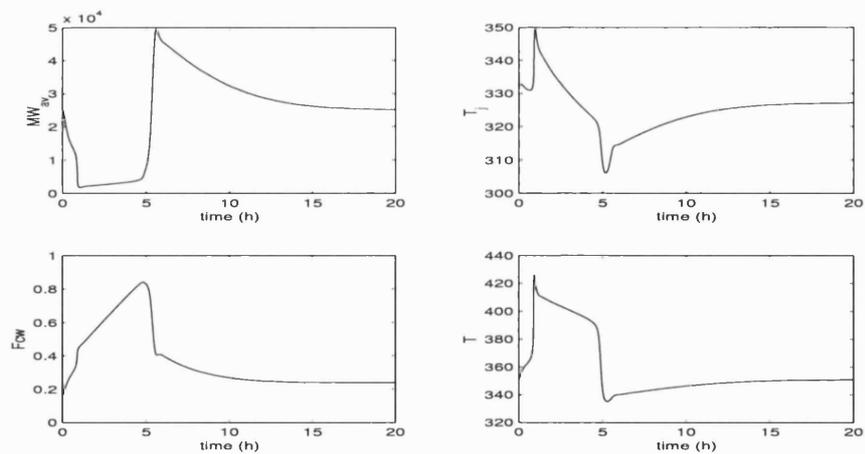


Figure 5.29: Trajectories of the output, input, and profile of the internal state for a step change in inlet temperature:  $\Delta T_{in} = +4K$



a neighbourhood, there is no hope of control in any large sense.

### Effects of Disturbance

In § 5.2.3, the simulations (Fig. 5.28 and Fig. 5.29) have shown the effects of the specific values of the disturbance of the inlet feed temperature  $T_{in}$  on the process behaviour. In this subsection, more generally, the effect of a disturbance of the inlet feed temperature  $T_{in}$  on the input multiplicity behaviour of the process is discussed. The locus of the first input multiplicity condition between the cooling flow rate  $F_{cw}$  and the inlet feed temperature  $T_{in}$  is shown in Figure 5.31. It can be seen that an increase in the cooling water flow rate will possibly move the initial operation condition ( $T_{in} = 350K$  and  $F_{cw} = 0.1673 m^3/h$ ) to breach the first input multiplicity condition where the value of the  $F_{cw}$  is  $F_{cw} \approx 0.1977 m^3/h$  (not the same as the values from simulations in § 5.2.3 because of the dependence of the input multiplicity condition on the operation conditions, i.e. different values of  $T_{in}$  in this example). For clarity, the relationship between the jacket temperature  $T_j$ , the cooling flow rate  $F_{cw}$ , and the inlet feed temperature  $T_{in}$  for the first input multiplicity condition is illustrated in Figure 5.32. It indicates that the input multiplicity is more likely to occur if there are both increases in the  $F_{cw}$  and  $T_{in}$ .

In this particular system, an increase in the inlet feed temperature will cause an increase in the cooling water flow rate to maintain the process at its initial condition since the reaction temperature will increase due to the increase in the feed temperature, and thus more cooling water is needed. Hence, an increase in the inlet temperature will be the worst disturbance to cause control problems.

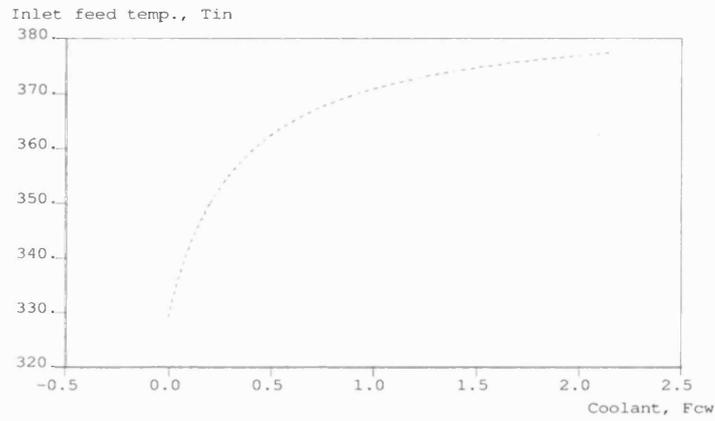


Figure 5.31: Locus of input multiplicity condition for the cooling water versus the inlet feed temperature

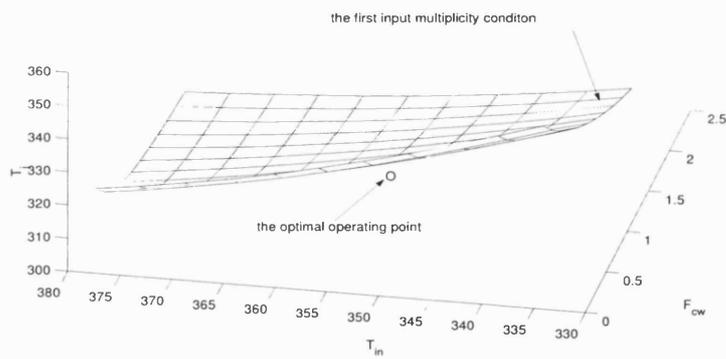


Figure 5.32: Input multiplicity condition between jacket temperature, cooling water, and inlet feed temperature

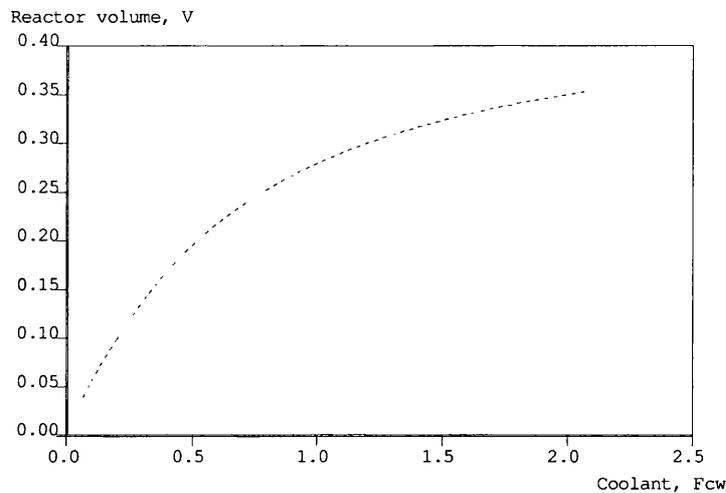


Figure 5.33: Locus of input multiplicity condition for the cooling water flow rate versus the reactor volume

### Effects of Reactor Volume

Similarly, the effect of the reactor volume on the first input multiplicity behaviour of the process is analysed. The locus of the input multiplicity condition between the cooling water flow rate and the reactor volume is shown in Figure 5.33. Figure 5.34 illustrates the relationship of the first input multiplicity condition between the jacket temperature, the reactor volume, and the cooling water flow rate. Clearly, a slight decrease in the reactor volume will significantly move the input multiplicity condition away from the operating point. Therefore, a decrease in the reactor volume may improve the controllability of the process since the modified operating point will be further away from the input multiplicity condition allowing a large margin to reject the disturbance.

The effects of the reactor volume and the inlet feed temperature on the steady-state characteristics of the process have been studied separately with respect to the cooling water flow rate  $F_{cw}$ . Figure 5.35 illustrates the simultaneous effects of the reactor volume  $V$ , the inlet feed temperature  $T_{in}$ , and cooling water flow rate

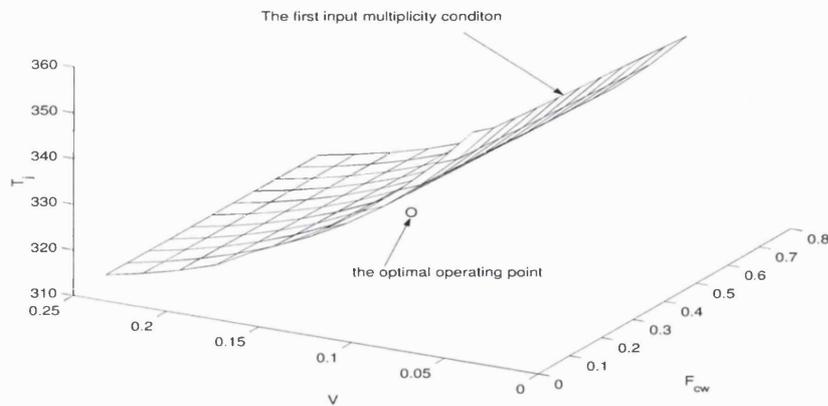


Figure 5.34: Input multiplicity condition between the jacket temperature, the cooling water flow rate, and the reactor volume.

$F_{cw}$  on the process, which is obtained by using a set of data from the bifurcation analysis. The relationship can be functionally expressed as  $F_{cw,IM} = f_{im}(V, T_{in})$ .

The locally linearised expression of  $f_{im}(V, T_{in})$  is given as:

$$F_{cw,IM} = -6.3383 + 2.7V + 0.01795T_{in}, \quad (5.26)$$

which will be used as a constraint on the input to avoid the input multiplicity in the process optimisation problem that will be discussed next.

### 5.2.5 Process Design Modifications

As discussed in § 5.2.3, the base case (optimal) design will face control problems subject to changes in the disturbance  $T_{in}$  when it is operated at the selected optimal point ( $MW_{av} = 25,000$  and  $F_{cw} = 0.1673 \text{ m}^3/\text{h}$ ). In order to have the desired disturbance rejection ability, the base case design needs modifying. As pointed out earlier (see § 5.2.3), the control problem is associated with the input multiplicity behaviour. The modification is to enable the process to eliminate the

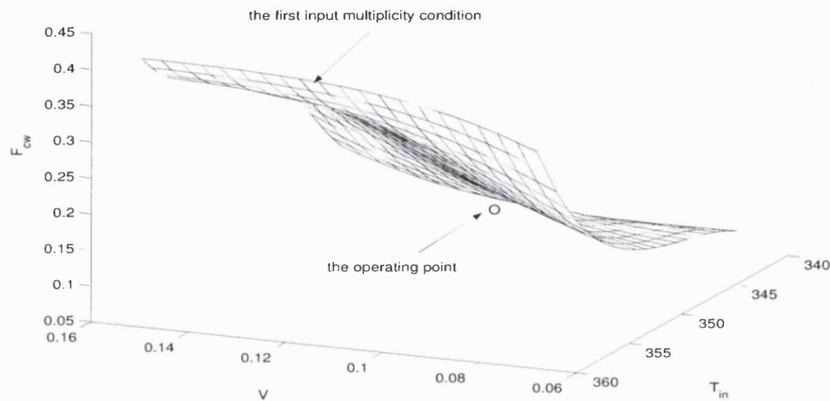


Figure 5.35: Relationship between the cooling water flow rate  $F_{cw}$ , inlet feed temperature  $T_{in}$ , and reactor volume  $V$  for the first input multiplicity condition

potential control problem associated with the input multiplicity for a specified disturbance of the inlet feed temperature  $T_{in}$  in the operating region by adjusting the design parameter, while keeping the modification cost at a minimum.

We here choose the reactor volume  $V$  as an adjustable design parameter in process modifications. The input multiplicity condition for the process subject to variations in the operating variables  $F_{cw}$ , the disturbances,  $T_{in}$ , and the design parameter  $V$  have been studied in the last subsection and is functionally expressed by equation 5.26.

The modified design optimisation formula is expressed by:

$$\min \{ \mathcal{R}(V - V_{opt})^2 + \mathcal{Q}(F_{cw} - F_{cw,opt}^2) \}$$

subject to

$$f(x) = 0, \quad (5.27)$$

$$D_1/D_0 = 25000,$$

Table 5.6: Process design modification results

$\Delta T_{in} (K)$	-5	-3	-1	0	+1	+2	+3	+4	+5
$V (m^3)$	0.102	0.101	0.1	0.1	0.1	0.099	0.098	0.097	0.095

$$F_I = 0.00354,$$

$$F_{cw} < F_{cw,IM},$$

$$T_{in} = 350 + \Delta T_{in},$$

where  $f(x)$  represents the six state equations of the process at steady state;  $F_{cw,IM}$  is the value at the input multiplicity condition;  $V_{opt}$  and  $F_{cw,opt}$  are the nominal design parameter value of  $0.1 m^3$  and optimal operation value of  $0.1673 m^3/h$ , respectively;  $\Delta T_{in}$  is the disturbance value to be defined;  $\mathcal{R}$  and  $\mathcal{Q}$  represent the cost factors in the changes of the reactor volume and cooling water flowrate, respectively ( $\mathcal{R} = 60$  and  $\mathcal{Q} = 1$ , for instance). The degrees of freedom in the optimisation problem are the reactor volume  $V$  and the cooling water flow rate  $F_{cw}$ .

The solutions for the reactor volume resulting in solving the design optimisation formula ( 5.27), corresponding to the required disturbance rejection ability defined by the values of  $\Delta T_{in}$ , are given in Table 5.6. The optimisation problems were solved using GAMS/MINOS.

The results from the feedback optimal process design modifications indicate that a decrease in the reactor volume will improve the disturbance rejection ability of the process. This is consistent with the previous analysis results. The improved control performance will be illustrated by simulations in the next subsection.

## 5.2.6 Closed-Loop Simulations

In this section closed-loop simulations are given to demonstrate the improved controllability of the modifications resulting from the feedback optimal design methodology. The process is initially at the selected operating point from the base case design, i.e.  $MW_{av,s} = 25,000$  and  $F_{cw,s} = 0.1673 m^3/h$ .

Figure 5.36 and Figure 5.37 illustrate the closed-loop (using a conventional PI controller whose parameters were tuned following the Ziegler and Nichols' rule and were kept constant in all simulation runs for the purpose of comparison) responses of  $MW_{av}$  for the base case (optimal) process to a positive step in the inlet feed temperature  $T_{in}$  from  $350K$  to  $353K$  ( $\Delta T_{in} = +3K$ ) and from  $350K$  to  $354K$  ( $\Delta T_{in} = +4K$ ), respectively. The base case design has the ability to reject a  $+3K$  step change in  $T_{in}$  but fails for a  $+4K$  step change in  $T_{in}$ . But, the output  $MW_{av}$  comes to rest eventually at its set point by the feedback control.

Figure 5.38 shows that the modified design of the case of  $V = 0.097m^3/h$  has the ability to reject a  $+4$  step change in  $T_{in}$  as required. The modified process fails to reject a step change in  $T_{in}$  over the specified value of  $\Delta T_{in} = +4K$ , for example  $\Delta T_{in} = +5K$  as shown in Figure 5.39. However, as shown in Figure 5.40, the modified process design for the case of  $V = 0.95m^3/h$  can reject the  $+5K$  step change in  $T_{in}$  that is expected in the process design modification.

The simulations indicate that the modifications have the ability to reject larger disturbances in the inlet temperature  $T_{in}$  than the base case design does. It is worth noticing that both the base case and the modifications can be eventually stabilised by the feedback control since there only exists output multiplicity in the  $MW_{av} - F_{cw}$  loop. But, a "sudden" change in the output could happen for a large disturbance during operation.

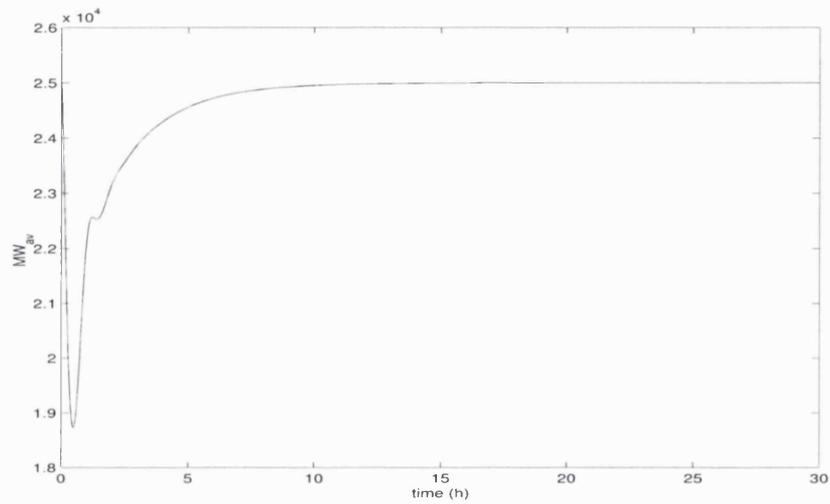


Figure 5.36: Simulation for the base case design:  $V = 0.1m^3$  and disturbance  $\Delta T_{in} = +3K$

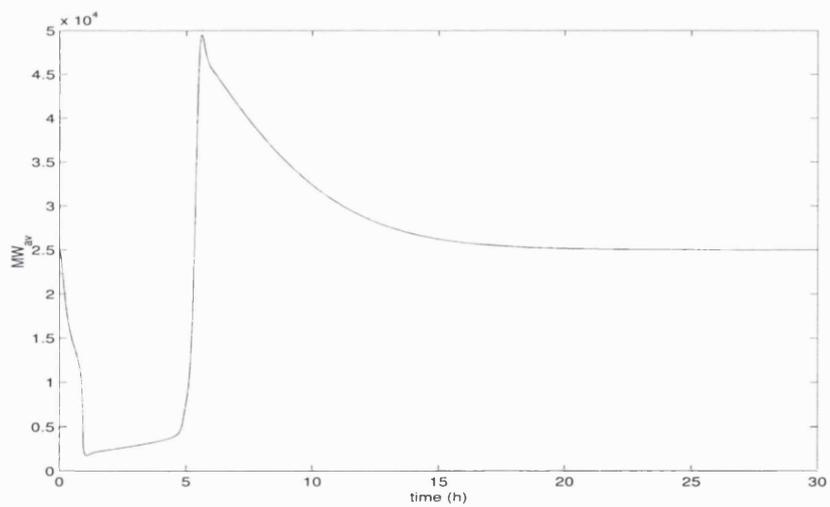


Figure 5.37: Simulation for the base case:  $V = 0.1m^3$  and  $\Delta T_{in} = +4K$

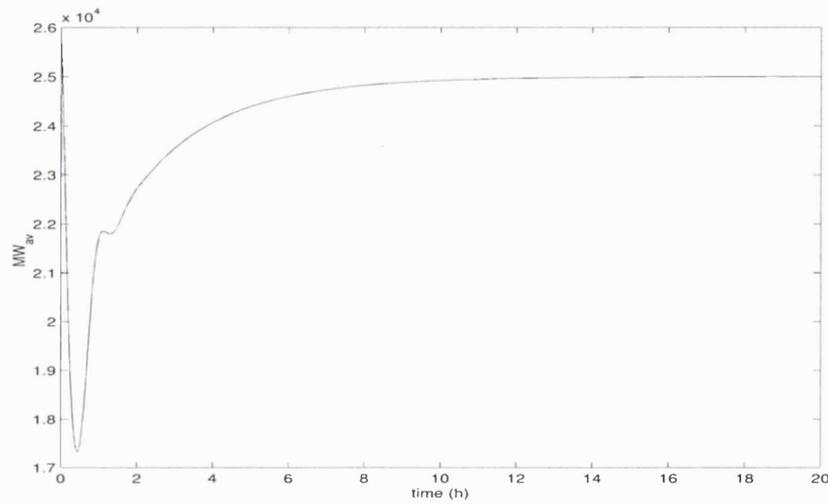


Figure 5.38: Simulation for the design modification:  $V = 0.097m^3$  and disturbance  $\Delta T_{in} = +4K$

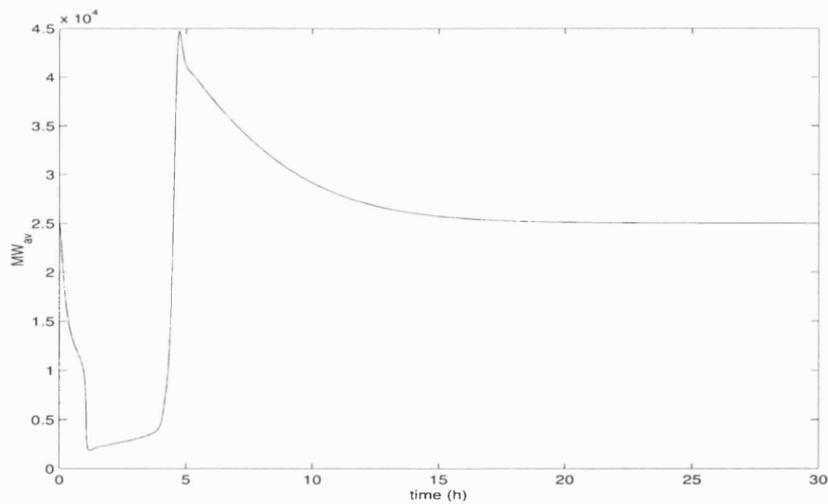


Figure 5.39: Simulation for the design modification:  $V = 0.097m^3$  and disturbance  $\Delta T_{in} = +5K$

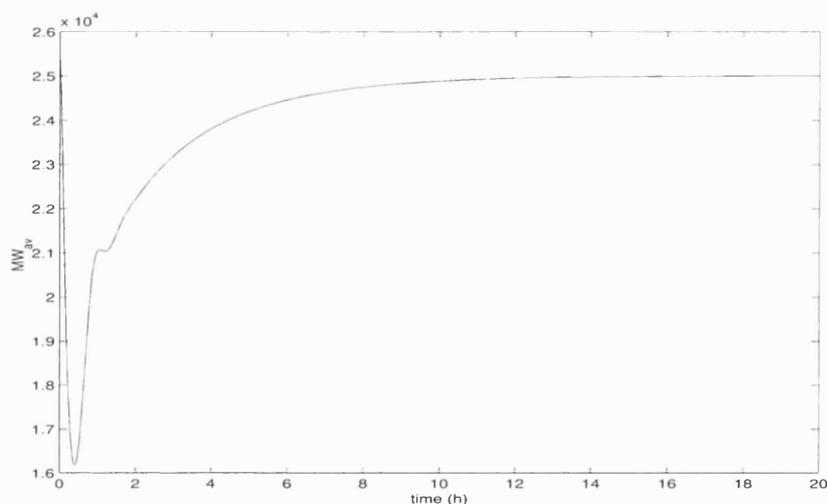


Figure 5.40: Simulation for the design modification:  $V = 0.095m^3$  and disturbance  $\Delta T_{in} = +5K$

### 5.2.7 Summary

It has been shown via simulations that the proposed process modification method can be applied to modify the design of an industrial polymerisation reaction. The method generated a modified process which has good dynamic behaviour and good economic performance as defined by the objective function, and it was able to extend the range of control and permit safe operation following a sizeable disturbance.

The case study utilised a specific polymerisation reaction taking place in a continuous stirred tank reactor, but the lessons can apply to a variety of the polymerisation reactions for which multiplicities arise routinely in industrial practice (Ray and Villa, 2000).

### 5.3 Conclusions

In this chapter, the reactor-separator system with recycle and the industrial polymerisation reaction have been studied. The control problems associated with input multiplicity of the processes themselves were identified in the parameter space and the modified designs have improved control performance. These two case studies demonstrate that the bifurcation-based analysis method can identify the control problems associated with input multiplicity in the parameter space, and the proposed feedback optimising design modification methodology can generate a “near optimal” design, which has good controllability. The undesired behaviour of the processes can be avoided by adjusting the values of the design parameters. The feedback optimisation with output and input constraints effectively turns the complex optimisation problem for controllability into a simple feedback control problem, which results in a design modification that can eliminate potential control problems associated with input multiplicity for a disturbance in the operating region, while minimising changes to the process.

# Chapter 6

## Conclusions and Future Work

---

This chapter summaries the main findings and contributions of the work presented in this thesis. A number of suggestions are also given for future developments to build on this work.

### 6.1 Summary of Findings

#### 6.1.1 New Method for Analysis

The first part of this thesis focussed on the development of a new method for the controllability analysis of nonlinear systems. In Chapter 2, the aspects of controllability and limitations imposed by the inherent characteristics of a process with respect to the inversion of the process were presented, the existing approaches to controllability analysis were reviewed and a number of limitations were identified. These include the facts that: (i) Input multiplicity behaviour is a main cause of a sudden destabilisation of a controlled process with integral action and proves the need for and complexity of control system design. (ii) For a SISO process any combination is possible of input multiplicity and unstable zero dynamics. The

presence of such behaviour forbids the implementation of any controller from the class of nonlinear inversion based controller since such a controller is unstable. (iii) A process having input multiplicity will pose inherent limitations on the control performance in the perfect control and optimal ISE sense. (iv) No linear-based controllability analysis methods could be extended to nonlinear systems in a large scale sense. (v) Bifurcation analysis is recognised as a powerful tool to carry out nonlinear system analysis that is widely used in chemical process analysis. Defined by the mathematics of bifurcation theory, the necessary condition for the existence of input multiplicity has significance and can be referred to as a bifurcation condition in bifurcation analysis since that when the condition is true one cannot be confident of the unique behaviour (exchange of stability) of the inverse of the system.

In response to this, a bifurcation-based analysis method was presented for identifying input multiplicity behaviour and analysing the parameter effects on it. The foundation of this approach is to augment the necessary condition of input multiplicity with the open-loop dynamic system to set up a new dynamic system. The algorithm developed incorporates the necessary condition for the existence of input multiplicity at a variety of steady states as an add-in subroutine to an available bifurcation analysis package, AUTO. This allows one to straight away determine input multiplicity along with the open-loop characteristics of the system and to analyse the parameter effects on them. The results of this analysis provides guidance to modify the process to eliminate the control problems associated with the input multiplicity. Using bifurcation analysis to conduct controllability analysis has one significant advantage, that it can capture nonlinearity by only using open-loop data at steady-state. The qualitative behaviour of a control system can be evaluated being independent of the detailed controller design. The results and conclusions are reliable over large operating

ranges compared to current static measures. Moreover, by employing numerical techniques, the size of the problems to be solved is significantly increased compared to analytical methods. It is evident that the benefits offered by the bifurcation-based approach increase as the number of the considered parameter increases for large and complex nonlinear processes.

All of the features described above have been demonstrated through a number of typical chemical process examples.

### **6.1.2 Process Design Modifications for Improved Controllability**

The second part of this thesis aimed at the development of a methodology for process design modifications for improved static controllability. An overview of the existing design methods for controllability was given in § 2.5.3. These methods were divided into the classes of problems that they are able to deal with and a number of limitations were highlighted. These include the facts that: (i) Although optimisation-based approaches are able to handle most aspects of controllability with respect to simultaneous effects of disturbances, uncertainties, and changing operation conditions, the results and conclusions resulting from the steady-state based approaches are only reliable around the specified conditions and the controller-dependent dynamic measures are strongly dependent on the controller tuning parameters. (ii) Bifurcation analysis is recognised as a powerful tool for nonlinear system analysis, but mainly used for analysis purpose, and few applications to process design have been reported.

Chapter 4 presented an optimisation-based approach, combined with bifurcation analysis results, to modifying process design for improved static controllability. The feedback optimal control concept was utilised to process design

modifications. The control and economic objectives were incorporated within a static feedback optimisation framework that evaluates the required contribution of the selected input variables and process design parameters to eliminate undesirable behaviour in the operating regions for a disturbance. This optimisation to be solved is a NLP problem that aims at minimising the absolute values of design parameter adjustments to avoid the undesirable behaviour inside the operating regions. This gives a simpler static optimisation problem in process design for controllability.

The work in this thesis concentrated on a SISO control system to eliminate input multiplicity behaviour in the range of input for a specified disturbance by adjusting the values of design parameters. But, undesirable characteristics can be the other types of bifurcations such as Hopf bifurcation, depending on what are specified in the optimisation problem.

There are some limitations of using this method: (i) NLPs are not guaranteed to have solutions, particularly for systems with high degrees of nonlinearity; (ii) It is assumed that the function for input multiplicity condition is monotonic and the local linearisation of the function limits the accuracy of the modification solutions.

## 6.2 Key Contributions

The contributions of the work presented in this thesis can be summarised as follows:

- A new bifurcation-based method is proposed and verified for directly determining input multiplicity along with the open-loop characteristics of nonlinear processes in the parameter space. The algorithm developed incorporates the necessary condition for the existence of input multiplicity at a variety

of steady states as an add-in subroutine to an available bifurcation analysis package. This allows one to effectively analyse the effects of the parameters, such as inputs, disturbances and design variables, on the input multiplicity behaviour. The results of the analysis provides guidance to adjust the design and operation parameters to eliminate such behaviour in the operating regions for the disturbances.

- A formulation developed for static feedback optimisation for process modifications is of significance since it is independent of the detailed controller designs while considering the dynamic performance of process designs subject to changing conditions. The results from bifurcation analysis are directly embedded in a process design modification formulation as a trade-off between economics and controllability.
- Two typical chemical processes a polymerisation reactor and a reactor-separator process with recycle, employed in the case studies, clearly demonstrated: (i) how the input multiplicities can be detected and the processes can be modified while preserving minimum economic loss and avoiding the control difficulties associated with input multiplicity over the operating regions in the presence of the disturbances and setpoint changes; (ii) and that it is now possible to solve a simple static feedback optimisation problem in process design for desirable qualitative dynamic behaviour being independent of detailed controller design.

### 6.3 Recommendations for Further Work

The work in this thesis raises a number of issues that could be directions for further work.

- **Improved methods for multivariable nonlinear control systems**

This work has mainly concentrated on the aspects of controllability (the ability to cope with setpoint following and disturbance rejection) with respect to input multiplicity on one particular system- a SISO control system. Naturally one would like to consider more general, multivariable types of control systems in order to form a readily applicable method for controllability analysis and process design modifications at process design stage for multivariable control systems. Future work in this project should contribute to the development of a framework for multivariable control systems in a practically meaningful sense when manipulated variables change simultaneously in the presence of disturbances. In other words, the interaction between parameters for multivariable control system should be further studied.

- **Incorporation of bifurcation models**

In the feedback process modification optimisation method, input multiplicity constraint expression on the input is a locally approximated function between the input, design variables and disturbances. If a precise bifurcation model is embedded in the optimisation problem, the accuracy could be improved. It may be possible to utilise neural network techniques to obtain the bifurcation model with a set of data from the proposed bifurcation-based analysis method, and to interface the bifurcation model onto the optimisation. But, one should be aware of the possible problems arising from the bifurcation model itself such as nonmonotonicity.

- **Process Synthesis Issues**

The process design modification case studies presented in Chapter 5, based on the existing structural process designs and control strategies, did not

explore process alternative issues such as whether it might be preferable to use two or more reactors or more separator columns. However, the consideration of alternative process structure may not straightforward from a modelling and analysis perspective since bifurcation constraints on inputs depend on each individual structure.

# Bibliography

- [1] R. Aris. Chemical reactors and some bifurcation phenomena. In Okan Gurel and Otto E. Rössler, editors, *Bifurcation theory and applications in scientific disciplines*, volume 316, pages 314–331. Annals of the New York Academy of Sciences, New York, **1979**.
- [2] R. Aris. *Mathematical Modeling— A Chemical Engineer’s Perspective*, volume 1 of *Process Systems Engineering*. Academic Press, London, **1999**.
- [3] R. Aris and N. R. Amundson. An analysis of chemical reactor stability and control-i. the possibility of local, with perfect or imperfect control mechanisms. *Chem. Eng. Sci.*, 7(3):121–131, **1958**.
- [4] P. A. Bahri, J. A. Bandoni, and J. A. Romagnoli. Effect of disturbances in optimizing control: Steady-state open-loop backoff problem. *AIChE J.*, 42(4):983–994, **1996**.
- [5] P. A. Bahri, J. A. Bandoni, and J. A. Romagnoli. Integrated flexibility and controllability analysis in design of chemical processes. *AIChE J.*, 43(4):997–1015, **1997**.
- [6] V. Balakotaiah and D. Luss. Analysis of multiplicity pattern of a CSTR. *Chem. Eng. Commun.*, 13:111–132, **1981**.

- [7] V. Bansal, J. D. Perkins, E. N. Pistikopoulos, R. Ross, and J. M. G. van Schijndel. Simultaneous design and control optimisation under uncertainty. *Computers chem. Engng.*, 24(2-7):261–266, **2000a**.
- [8] V. Bansal, R. Ross, J.D. Perkins, and E. N. Pistikopoulos. The interactions of design and control: Double-effect distillation. *J. Pro. Cont.*, 10:219–227, **2000b**.
- [9] N. Bekiaris, T. E. Güttinger, and M. Morari. Multiple steady states in distillation: Effect of vl(l)e inaccuracies. *AIChE J.*, 46(5):955–979, **2000**.
- [10] P. W. Belanger and W. L. Luyben. Plantwide design and control of processes with inerts. 1. light inerts. *Industrial & Engineering Chemistry Research*, 37(2):516–527, **1998a**.
- [11] P. W. Belanger and W. L. Luyben. Plantwide design and control of processes with inerts. 2. heavy inerts. *Industrial & Engineering Chemistry Research*, 37(2):528–534, **1998b**.
- [12] A. Bemporad, F. D. Torrisi, and M. Morari. Performance analysis of piecewise linear systems and model predictive control systems. *Proceedings of the 39<sup>th</sup> IEEE Conference on Decision and Control, Sydney, Australia*, pages 4957–4962, December, **2000**.
- [13] B. S. Bennett. *Simulation fundamentals*. Prentice Hall, New Jersey, **1995**.
- [14] B. Wayne Bequette. Nonlinear control of chemical processes: A review. *Ind. Eng. Chem. Res.*, 30:1391–1413, **1991**.
- [15] C. S. Bildea and Alexandrew C. Dimian. Multiplicity and stability approach to the design of heat integrated multibed pfr. *Computers chem. Engng.*, Suppl.:S171–S174, **1999**.

- [16] G. L. Blankenship, R. Ghanadan, H. G. Kwatny, C. LaVigna, and V. Polyakov. Tools for integrated modelling, design, and nonlinear control. *IEEE Control Systems*, pages 65–77, April, **1995**.
- [17] I. David. L. Bogle and M. Rashid. An assessment of dynamic operability measures. *Computers chem. Engng.*, 13(11-12):1277–1282, **1989**.
- [18] E. H. Bristol. A new measure of interaction for multivariable process control. *IEEE Trans. Auto. Cont.*, AC-II 13:133–134, **1966**.
- [19] R. W. Brockett and R. S. Millman. Differential geometric control theory. *Proceedings of the conference held at Michigan Technological University*, June 28-July 2, **1982**.
- [20] A. E. Jr. Bryson and Yu-Chi Ho. *Applied Optimal Control: Optimization, Estimation, and Control*. Hemisphere Publishing Co., Washington D.C., **1975**.
- [21] C. I. Byrnes and Xiaoming Hu. The zero dynamics algorithm for general nonlinear systems and its application in exact output tracking. *Journal of Mathematical Systems, Estimation, and Control*, 3(1):51–72, **1993**.
- [22] Y. Cao, D. Biss, and J.D. Perkins. Assessment of input-output controllability in the presence of control constraints. *Computers chem. Engng.*, 20(4):337–346, **1996**.
- [23] Y. Cao and D. Rossiter. An input prescreening technique for control structure selection. *Computers chem. Engng.*, 21(6):563–569, **1997**.
- [24] Y. Cao and D. Rossiter. Input selection and localized disturbance rejection. *J. Pro. Cont.*, 8(3):175–198, **1998**.

- [25] H. Chang and L. Chen. Bifurcation characteristics of nonlinear systems under conventional PID control. *Chem. Eng. Sci.*, 39:1127–1142, **1984**.
- [26] Hsueh-Chia Chang and Joseph M. Calo. Exact criteria for uniqueness and multiplicity of an nth order chemical reaction via a catastrophe theory approach. *Chem. Eng. Sci.*, 34(3):285–299, **1979**.
- [27] J. W. Chang and C. C. Yu. Relative disturbance gain array. *AIChE J.*, 38(4):521–534, **1992**.
- [28] H. Chen and F. Allgöwer. A quasi-infinite horizon nonlinear model predictive control scheme with guaranteed stability. *Automatica*, 34(10):1205–1217, **1998**.
- [29] S. D. Chenery and S. P. Walsh. Process controllability analysis using linear programming. *J. Pro. Cont.*, 8(3):165–174, **1998**.
- [30] M. Chidambaram and G. P. Reddy. Short note: Nonlinear control of systems with input multiplicities. *Computers chem. Engng*, 19(2):249–252, **1995**.
- [31] B. D’Andrea and L. Praly. About finite nonlinear zeros in decouplable systems. *Systems and Control Letters*, 10:103–109, **1988**.
- [32] P. Daoutidis and C. Kravaris. Inversion and zero dynamics in nonlinear multivariable control. *AIChE J.*, 37(4):527–538, **1991**.
- [33] P. Daoutidis, M. Soroush, and C. Kravaris. Feedforward/feedback control of multivariable nonlinear processes. *AIChE J.*, 36(10):1471–1484, **1990**.
- [34] S. K. Dash and L. B. Koppel. Sudden destabilisation of controlled chemical processes. *Chem. Eng. Comm*, 84:129–157, **1989**.

- [35] V. Dimitriadis and E. Pistikopoulos. Flexibility analysis of dynamic systems. *Ind. Chem. Eng. Res.*, 34:4451–4462, **1995**.
- [36] E. Doedel, H. B. Keller, and J. P. Kernevez. Numerical analysis and control of bifurcation problems. (I) bifurcation in finite dimensions. *International Journal of Bifurcation and Chaos*, 1(3):493–520, **1991a**.
- [37] E. Doedel, H. B. Keller, and J. P. Kernevez. Numerical analysis and control of bifurcation problems. (II) bifurcation in infinite dimensions. *International Journal of Bifurcation and Chaos*, 1(4):745–772, **1991b**.
- [38] E. J. Doedel, A. R. Champneys, T. F. Fairgrieve, Y. A. Kuznetsov, B. Sandstede, and Xianjun Wang. *AUTO 97: Continuation and Bifurcation Software for Ordinary Differential Equations (with HomCont)*. Concordia University, Montreal, Canada, **1998**.
- [39] C. Dorn, Moonyong Lee, and M. Morari. Stability and transient behaviour of homogeneous azeotropic distillation. *Computers chem. Engng.*, Suppl.:S191–S194, **1999**.
- [40] J. M. Douglas. *Conceptual design of chemical processes*. McGraw-Hill, New York, **1988**.
- [41] F. J. Doyle and M. A. Henson. *Nonlinear System Theory, in Nonlinear process Control*. Prentice Hall, New Jersey, **1997**.
- [42] F. J. Doyle, B. A. Ogunnaike, and R. K. Pearson. Nonlinear model based control using second order volterra models. *Automatica*, 31(5):697–714, **1995**.

- [43] N. Dragan and Iven M. Y. Mareels. Dead beat controllability of polynomial systems: Symbolic computation approach. *IEEE Transactions on Automatic control*, 43(2), February, 1998.
- [44] T. R. Elliot and W. L. Luyben. Capacity-based economic approach for the quantitative assessment of process controllability during the conceptual design. *Ind. Eng. Chem. Res.*, 34:3907–3915, 1995.
- [45] W. Findeisen, F. N. Bailey, M. Brdys, K. Malinowski, P. Tatjewski, and A. Woźniak. *Control and coordination in hierarchical systems*. John Wiley & Sons, New York, 1980.
- [46] W. R. Fisher, M. F. Doherty, and J. M. Douglas. The interface between design and control. 1. process controllability. *Ind. Eng. Chem. Res.*, 27:597–605, 1988.
- [47] C. A. Floudas. *Non-linear and mixed-integer optimization fundamentals and application*. Oxford University press, 1995.
- [48] J. M. Fox, Jr. W. J. Schmidt, and J. C. Kantor. Comparison sensitivity and feedback control for optimized chemical reactors. *Proceedings of the American Control Conference, San Diego, CA*, pages 1621–1627, 1984.
- [49] I. P. Gal, J. B. Varga, and K. M. Hangos. Integrated structure design of a process and its control system. *J. Pro. Cont.*, 8(4):251–263, 1998.
- [50] GAMS. *A user's guide*. GAMS Development Corporation, 1998.
- [51] R. Gani and S.T. Jørgensen. Multiplicity in numerical solution of non-linear models: Separation processes. *Computers chem. Engng.*, 18:S55–S61, 1994.
- [52] C. E. García and M. Morari. Model predictive control: Theory and practice - A survey. *Automatica*, 25:335, 1989.

- [53] E. R. Gilliland, L.A. Gould, and T. J. Boyle. Dynamic effects of material recycle. *Preprint JACC, Stanford, California, USA*, pages 140–146, **1964**.
- [54] M. Giona and O. Paladino. Bifurcation analysis and stability of a controlled CSTR. *Computers. chem. Engng.*, 18(9):877–887, **1994**.
- [55] I. E. Grossmann, K. P. Haleman, and R. E. Swaney. Optimisation strategies for flexible chemical processes. *Computers chem. Engng.*, 7:439–462, **1983**.
- [56] K. Havre and S. Skogestad. Effect of RHP zeros and poles on the sensitivity functions in multivariable systems. *J. Pro. Cont.*, 8(3):155–164, **1998**.
- [57] M. A. Henson and D. E. Seborg. Nonlinear control strategies for continuous fermenters. *Chem. Eng. Sci.*, 47(4):821–835, **1992**.
- [58] M. A. Henson and D. E. Seborg. *Nonlinear Process Control*. Prentice-Hall, New Jersey, **1997**.
- [59] P. M. Hidalgo and C. B. Brosilow. Nonlinear model predictive control of styrene polymerization at unstable operating points. *Computers chem. Engng.*, 20(Suppl.):S871–S876, **1990**.
- [60] R. C. Hilborn. *Chaos and Nonlinear Dynamics: Introduction for scientists and engineers*. Oxford University Press, Inc., New York, **1994**.
- [61] R. M. Hirschorn. Invertibility of nonlinear control systems. *SIAM J Control and Optimization*, 17:289–297, **1979**.
- [62] R. M. Hirschorn. Invertability of nonlinear control systems. *SIAM J. Control and Optimization*, 17:289–297, **1979**.

- [63] B. R. Holt and M. Morari. Design of resilient processing plants-V. the effect of deadtime on dynamic resilience. *Chem. Eng. Sci.*, 40(7):1229–1237, **1985**.
- [64] B. R. Holt and M. Morari. Design of resilient processing plants-VI. the effect of right-half plane zeros on dynamic resilience. *Chem. Eng. Sci.*, 40(1):(59–74, **1985**.
- [65] M. Hovd and S. Skogestad. Controllability analysis for unstable process. *Interactions between process design and process control, IFAC Workshop, London, UK*, pages 49–54, 7-8 September, **1992**.
- [66] I. Huq, M. Morari, and R. C. Sorensen. Modifications to model iv fluid catalytic cracking unit to improve dynamic performance. *AIChE J.*, 41:1481–1496, **1995**.
- [67] G. Iooss and D. D. Joseph. *Elementary stability and bifurcation theory*. Springer-Verlag New York Inc., New York, 2nd edition, **1990**.
- [68] A. Isidori. *Nonlinear control system, An introduction*. Springer-Verlag, Berlin, 3rd edition, **1995**.
- [69] E. W. Jacobsen. *Studies on Dynamics and Control of Distillation Columns*. PhD thesis, University of Trondheim, the Norwegian Institute of Technology Trondheim, December, **1991**.
- [70] E. W. Jacobsen. Effect of recycle on the plant zero dynamics. *Computers chem. Engng.*, 21(Suppl.):S279–S284, **1997**.
- [71] H. B. Keller. Applications of bifurcation theory: Numerical solution of bifurcation and nonlinear eigenvalue problems. *Proceedings of An advanced Seminar, Academic Press, Inc., New York*, pages 359–384, **1977**.

- [72] H. B. Keller. *Lectures on numerical methods in bifurcation problems*. In A. K. Nandakumaran and M. Ramaswamy (editors), Indian Institute of Science, Bangalore (Springer-Verlag), **1987**.
- [73] J. Khinast, D. Luss, M. P. Harold, J. J. Ostermaier, and R. McGill. Continuously stirred decanting reactor: Operability and stability. *AIChE J.*, 44(2):372–387, **1998**.
- [74] Y. Kim, B. Lee, S. Eo, and En Sup Yoon. A study on the evaluation and improvement of structural controllability of chemical processes. *Computers chem. Engng.*, 24:931–936, **2000**.
- [75] I.K. Kookos and J.D. Perkins. An algorithmic method for the selection of multivariable process control structures. *J. Pro. Cont.*, 12(1):85–99, **2002**.
- [76] L. B. Koppel. Input multiplicities in nonlinear multivariable control system. *AIChE. J.*, 28(6):935–945, **1982**.
- [77] C. Kravaris, P. Daoutidis, and R. A. Wright. Output feedback control of nonminimum phase nonlinear processes. *Chem. Eng. Sci.*, 49(13):2107–2122, **1994**.
- [78] C. Kravaris and J. C. Kantor. Reviews: Geometric methods for nonlinear process control. 1. background. *Ind. Eng. Chem. Res.*, 29:2295–2310, **1990a**.
- [79] C. Kravaris and J. C. Kantor. Reviews: Geometric methods for nonlinear process control. 2. controller. *Ind. Eng. Chem. Res.*, 29:2310–2323, **1990b**.
- [80] M. Kubíček and M. Marek. *Computational methods in bifurcation theory and dissipative structures*. Springer-Verlag New York Inc., New York, **1983**.

- [81] A. Kuhlmann. *Studies on controllability evaluation of nonminimum phase processes*. PhD thesis, Department of Chemical Engineering, University College London, United Kingdom, **1998**.
- [82] A. Kuhlmann and D. Bogle. Study on nonminimum phase behaviour and optimal operation. *Computers chem. Engng.*, 21(Suppl.):S397–S402, 1997.
- [83] A. Kuhlmann and D. Bogle. Controllability evaluation for nonminimum phase-processes with multiplicity. *AIChE J.*, 47(11):2627–2632, **2001**.
- [84] O. Levenspiel. *Chemical Reaction Engineering*. Wiley & Sons, New York, 2nd edition, **1972**.
- [85] D. R. Lewin. A simple tool for disturbance resiliency diagnosis and feed-forward control design. *Computers chem. Engng.*, 20(1):13–25, **1996**.
- [86] D. R. Lewin and D. Bogle. Controllability analysis of an industrial polymerization reactor. *Computers chem. Engng.*, 14(4/5):481–494, **1996**.
- [87] F. L. Lewis. *Applied optimal control & estimation : Digital design & implementation*. Prentice Hall, New Jersey, **1992**.
- [88] L. C. Limqueco and J. C. Kantor. Nonlinear output feedback control of an exothermic reactor. *Computers. chem. Engng.*, 14:427–437, **1990**.
- [89] M. L. Luyben and C. A. Floudas. A multiobjective approach for analyzing the interaction of design and control, interactions between process design and process control. *IFAC Workshop, London, UK*, pages 101–106, 7-8 September, **1992**.
- [90] M. L. Luyben and C. A. Floudas. Analyzing the interaction of design and control. Part 1: A multiobjective framework and application to binary distillation synthesis. *Computers chem. Engng.*, 18(10):933–969, **1994a**.

- [91] M. L. Luyben and C. A. Floudas. Analyzing the interaction of design and control. Part 2: Reactor-separator-recycle system. *Computers chem. Engng.*, 18(10):971–994, **1994b**.
- [92] M. L. Luyben and W. L. Luyben. *Essentials of Process Control*. McGraw-Hill, Singapore, international edition, **1997**.
- [93] W. L. Luyben. *Process Modelling, Simulation, and Control for Chemical Engineering*. McGraw-Hill, New York, 2nd edition, **1990**.
- [94] W. L. Luyben. Dynamics and control of recycle systems: 1. Simple open-loop and closed-loop systems. *Ind. Eng. Chem. Res.*, 32:466–475, **1993a**.
- [95] W. L. Luyben. Dynamics and control of recycle systems: 2. Comparison of alternative process designs. *Ind. Eng. Chem. Res.*, 32:476–486, **1993b**.
- [96] W. L. Luyben. Dynamics and control of recycle systems: 3. Alternative process designs in a ternary system. *Ind. Eng. Chem. Res.*, 32:1142–1153, **1993c**.
- [97] K. Ma and David Bogle. An approach to controllability and economic design of nonlinear systems with multiplicity. European Symposium on Computer Aided Process Engineering-11, 34<sup>th</sup> European Symposium of the Working Party on Computer Aided Process Engineering, ESCAPE-11, 27-30 May, **2001**, Kolding, Denmark.
- [98] K. Ma and David Bogle. Analysing the interaction of open-loop multiplicity and control pairing of nonlinear systems. Pre-prints, 6th IFAC Symposium on Dynamic and Control of Process Systems, Jeju Island, Korea, June 4-6, **2001**.

- [99] A. G. J. MacFarlane and N. Karcanias. Poles and zeros of linear multivariable systems: A survey of algebraic, geometric and complex variable theory. *International J. of Control*, 24:33–74, **1976**.
- [100] V. Manousiouthakis and M. Nikolaou. Analysis of decentralized control structures for nonlinear systems. *AIChE J.*, 35(4):549–559, **1989**.
- [101] MATLAB. *User's guide*. The Mathworks, Inc., 1992.
- [102] R. Maya-Yescas, D. Bogle, and Felipe López-Isunza. Approach to the analysis of the dynamics of industrial FCC units. *J. Pro. Cont.*, 8(2):89–100, **1998**.
- [103] D. Q. Mayne, J. B. Rawlings, C. V. Rao, and P. O. M. Scokaert. Constrained model predictive control: Stability and optimality. *Automatica*, 36:789–814, **2000**.
- [104] T. J. McAvoy. Synthesis of plantwide control systems using optimization. *Ind. Eng. Chem. Res.*, 38:2984–2994, **1999**.
- [105] M. A. McKarnin, R. Aris, and L. D. Schmidt. Autonomous bifurcations of a simple bimolecular surface-reaction model. *Proceeding of the Royal Society, London, A Volume 415*, pages 363–387, **1988**.
- [106] M. J. Mohideen, J. D. Perkins, and E. N. Pistikopoulos. Optimal design of dynamic systems under uncertainty. *AIChE J.*, 42(8):2251–2272, **1996**.
- [107] M. Morari. Plenary address, effect of design on the controllability of chemical plants, interactions between process design and process control. *IFAC Workshop, London, UK*, pages 3–16, 7-8 September, **1992**.

- [108] M. Morari. Design of resilient processing plants-III. a general framework for the assessment of dynamic resilience. *Chem. Eng. Sci.*, 38(11):1881–1891, **1983a**.
- [109] M. Morari. Robust stability of system with integral control. *Proceedings of the IEEE, 22nd CDC*, pages 865–869, **1983b**.
- [110] M. Morari, Y. Arkun, and G. Stephanopoulos. Studies in the synthesis of control structures of chemical processes. Part I: Formulation of the problem. process decomposition and the classification of the control task. analysis of the optimizing control structures. *AIChE J.*, 26(2):220–232, **1980**.
- [111] M. Morari and E. Zafriou. *Robust process control*. Prentice Hall International, Inc., New Jersey, **1989**.
- [112] J. Morud and S. Skogestad. Dynamic behaviour of integrated plants. *J. Proc. Cont.*, 6(2/3):145–156, **1996**.
- [113] D. Nagrath, V. Prasad, and B. W. Bequette. Model predictive control of open-loop unstable cascade systems. *Proceedings of the American Control Conference, Chicago, Illinois, USA*, pages 3747–3752, June, **2000**.
- [114] L. T. Narraway and J. D. Perkins. Selection of process control structures based on linear dynamic economics. *Ind. Eng. Chem. Res.*, 32(11):2681–2692, **1993**.
- [115] L. T. Narraway, J. D. Perkins, and G. W. Barton. Interaction between process design and process control: economic analysis of process dynamics. *J. Pro. Cont.*, 1:243–250, **1991**.

- [116] T.C. Nguyen, G.W. Barton, J.D. Perkins, and R.D. Johnston. A condition number scaling policy for stability robustness analysis. *AIChE J.*, 34(7):1200–1206, **1988**.
- [117] B. Noble and J. W. Danidenel. *Applied linear algebra*. Prentice Hall Inc., New Jersey, 2nd edition, **1977**.
- [118] B. A. Ogunnaike and W. Harmon Ray. *Process dynamics, modeling, and control*. Oxford University Press, Oxford, 1994.
- [119] A. Palazoglu, B. Manousiouthakis, and Y. Arkun. Design of chemical plants with improved dynamic operability in an environment of uncertainty. *Ind. Eng. Chem. Proc. Des. Dev.*, 24(3):802–813, **1985**.
- [120] J. D. Perkins. Interactions between process design and process control. *preprints IFAC Symposium DYCORN+ '89, Maastricht, Netherlands*, pages 349–357, August, **1989**.
- [121] J. D. Perkins and S. P. K. Walsh. Optimization as a tool for design/control integration. *Proc. of the IFAC Workshop on Integration of Process Design and Control*, E. Zafiriou Ed.(1), **1994**.
- [122] J. D. Perkins and S. P. K. Walsh. Optimization as a tool for design/control integration. *Computers chem. Engng.*, 20(4):315–323, **1996**.
- [123] J. C. Pinto. The dynamic behaviour of continuous solution polymerization reactors- a full bifurcation analysis of a full scale copolymerization reactor. *Chem. Eng. Sci.*, 50(21):3455–3475, **1995**.
- [124] S. Pushpavanam and A. Kienle. Nonlinear behavior of an ideal reactor separator network with mass recycle. *Chem. Eng. Sci.*, 56:2837–2849, **2001**.

- [125] L. Qiu and E. J. Davison. Performance limitations of non-minimum phase systems in the servomechanism problem. *Automatica*, 29(2):337–349, **1993**.
- [126] W. H. Ray. *Applications of Bifurcation Theory Edited by Paul H. Rabinowitz: Bifurcation Phenomena in Chemically Reacting Systems*. Proceedings of An advanced Seminar, Academic Press, Inc., New York, **1977**.
- [127] W. H. Ray and C. M. Villa. Nonlinear dynamics found in polymerization processes— A review. *Chem. Eng. Sci.*, 55:275–290, **2000**.
- [128] N. K. Read and W. Harmon Ray. Applications of nonlinear dynamic analysis in the identification and control of nonlinear systems - I. Simple dynamics. *J. Pro. cont.*, 8(1):1–15, **1998**.
- [129] H. H. Rosenbrock. *State space and multivariable theory*. Thomas Nelson and Sons Ltd, London, **1970**.
- [130] L. W. Russell and J. D. Perkins. Towards a method for diagnosis of controllability and operability problems in chemical plants. *Chem. Eng. Res. Des.*, 65(6):453–461, **1987**.
- [131] L. P. Russo and B. W. Bequette. Effects of process design on the open-loop behaviour of a jacketed exothermic CSTR. *Computers chem. Engng.*, 20(4):417–426, **1996**.
- [132] L. P. Russo and B. W. Bequette. Operability of chemical reactors: Multiplicity behaviour of a jacketed styrene polymerization reaction. *Chem. Eng. Sci.*, 53(1):27–45, **1998**.
- [133] L. P. Russo and B. Wayne Bequette. Process design for operability: A styrene polymerization application. *Computers chem. Engng.*, 21(Suppl.):S571–S576, **1997**.

- [134] D. E. Seborg, T. F. Edgar, and D. A. Mellichamp. *Process Dynamics and Control*. John Wiley & Sons, New York, **1989**.
- [135] W. D. Seider, D. D. Brengel, A. M. Provost, and S. Widagdo. Nonlinear analysis in process design. Why overdesign to avoid complex nonlinearities? *Ind. Eng. Chem. Res.*, 29(5):805–818, **1990**.
- [136] W. D. Seider, D. D. Brengel, and S. Widagdo. Nonlinear analysis in process design. *AIChE J.*, 37(1):1–38, **1991**.
- [137] H. Seki and M. Morari. Receding horizon implementation of optimal servo problem: Application to a nonlinear process with input multiplicities. *Proceedings of the American Control Conference, Philadelphia, Pennsylvania, USA*, pages 791–795, June, **1998**.
- [138] M. M. Seron, J. H. Braslavsky, P.V. Kokotović, and D. Q. Mayne. Feedback limitations in nonlinear systems: From bode integrals to cheap control. *Proceedings of the 36th Conference on Decision & Control, San Diego, California, USA*, pages 2067–2072, December, **1997**.
- [139] F. G. Shinskey. *Process Control Systems. Application/Design/Adjustment*. McGraw-Hill, New York, 2nd edition, **1979**.
- [140] SIMULINK. *User's guide*. The Mathworks, Inc., 1992.
- [141] P. B. Sistu and B. W. Bequette. Nonlinear predictive control of uncertain processes: Application to a CSTR. *AIChE J.*, 37(11):1711–1723, **1991**.
- [142] P. B. Sistu and B. W. Bequette. Model predictive control of process with input multiplicities. *Chem. Eng. Sci.*, 50(6):921–936, **1995**.
- [143] S. Skogestad. Plantwide control: the search for the self-optimising control structure. *J. Pro. Cont.*, 10:487–507, **2000**.

- [144] S. Skogestad, M. Hovd, and P. Lundstrom. Simple frequency-dependent tools for analysis of inherent control limitations. *Model Ident. Control*, 12(4):159–177, **1991**.
- [145] S. Skogestad and M. Morari. Design of resilient processing plants - IX. The effect of model uncertainty on dynamic resilience. *Chem. Eng. Sci.*, 42(7):1765–1780, **1987**.
- [146] S. Skogestad and Ian Postlethwaite. *Multivariable Feedback control analysis and design*. John Wiley & Sons Ltd, Chichester, England, **1996**.
- [147] S. Skogestad and E. A. Wolff. Controllability measures for disturbance rejection , interactions between process design and process control. *IFAC Workshop, London, UK*, pages 23–30, 7-8 September, **1992**.
- [148] J.-J. E. Slotine and Weiping Li. *Applied Nonlinear Control*. Prentice-Hall, New Jersey, **1991**.
- [149] M. Soroush. Evaluation of achievable control quality in nonlinear processes. *Computers chem. Engng.*, 20(4):357–363, **1996**.
- [150] M. Soroush. Evaluation of achievable control quality in nonlinear processes. *Computers chem. Engng.*, 20(4):357–364, **1996**.
- [151] G. Stephanopoulos. *Chemical process control*. Prentice-Hall International, Englewood Cliffs, New Jersey, **1984**.
- [152] G. Stephanopoulos and C. Ng. Perspective on the synthesis of plant-wide control structure. *J. Pro. Cont.*, 10:97–111, **2000**.
- [153] S. Subramanian and C. Georgakis. Steady-state operability characteristics of reactors. *Computers chem. Engng.*, 24(2-7):1563–1568, **2000**.

- [154] S. Subramanian and C. Georgakis. Steady-state operability characteristics of reactors. *Computers chem Engng.*, 24:1563–1568, **2000**.
- [155] S. Subramanian, D. Uztürk, and C. Georgakis. An optimization-based approach for the operability analysis of continuously stirred tank reactors. *Ind. Eng. Chem. Res.*, 40:4238–4252, **2001**.
- [156] R. E. Swaney and I. E. Grossmann. An index for operational flexibility in chemical process design. Part I: Formulation and theory. *AIChE J.*, 31(4):621–630, **1985**.
- [157] R. E. Swaney and I. E. Grossmann. An index for operational flexibility in chemical process design. Part II: computational algorithm. *AIChE J.*, 31(4):631–641, **1985**.
- [158] F. Teymour and W. H. Ray. The dynamic behaviour of continuous solution polymerization reactor-IV: Dynamic stability and bifurcation analysis of an experimental reactor. *Chem. Eng. Sci.*, 44:1967–1982, **1989**.
- [159] J. M. T. Thompson and H. B. Stewart. *Nonlinear Dynamics and Chaos*. John Wiley & Sons Ltd., New York, **1987**.
- [160] B. D. Tyreus and W. L. Luyben. Dynamics and control of recycle systems: 4. ternary systems with one or two recycle streams. *Ind. Eng. Chem. Res.*, 32:1154–1162, **1993**.
- [161] A. Uppal, W. H. Ray, and A. B. Poore. On the dynamic behaviour of continuous stirred tank reactors. *Chem. Eng. Sci.*, 29:967–985, **1974**.
- [162] J. G. van de Vusse. Plug flow type reactor versus tank reactor. *Chem. Eng. Sci.*, 19:994–997, **1964**.

- [163] D. R. Vinson and C. Georgakis. A new measure of process output controllability. *J. Pro. Cont.*, 10:185–194, **2000**.
- [164] P. Wang and T. McAvoy. Synthesis of plantwide control system using a dynamic model and optimization. *Ind. Eng. Chem. Res.*, 40(24):5732–5742, **2001**.
- [165] O. Weitz and D. R. Lewin. Dynamic controllability and resiliency diagnosis using steady state process flowsheet data. *Computers chem. Engng.*, 20(4):325–335, **1996**.
- [166] V. White, J. D. Perkins, and D. M. Espie. Switchability analysis. *Computers chem. Engng.*, 20(4):469–474, **1996**.
- [167] S. Wiggins. *Introduction to applied nonlinear dynamical systems and chaos*. Springer-Verlag, New York, **1990**.
- [168] M. P. F. Wong. Assessing controllability of chemical plants. *Chem. Eng. Res. Des.*, 63(6):358–362, **1985**.
- [169] J. C. C. Young, C. L. E. Swartz, and R. Ross. On the effects of constraints, economics and uncertain disturbances on dynamic operability assessment. *Computers chem. Engng.*, 20(Suppl.):S677–S682, **1996**.
- [170] E. Zafriou and H.W. Chiou. On the dynamic resiliency of constrained processes. *Computers chem. Engng.*, 20(4):347–355, **1996**.
- [171] E. Zafriou, B.R. Holt, and M. Morari. Design of resilient processing plants- new characterization of the effect of RHP zeros. *Chem. Eng. Sci.*, 42(10):(2425–2428, **1987**.
- [172] Y. Zhang and Michael A. Henson. Bifurcation analysis of continuous biochemical reactor models. *Biotechnol. Prog.*, 17:647–660, **2001**.

- 
- [173] A. Zheng and R. V. Mahajanam. A quantitative controllability index. *Industrial & Engineering Chemistry Research*, 38(3):999–1006, **1999**.
- [174] J. G. Ziegler and N. B. Nichols. Process lags in automatic control circuits. *Trans. ASME*, 65:433–444, **1943**.
- [175] J. G. Ziegler and N. B. Nichols. Optimum setting for automatic controller. *Trans. ASME*, 64:759, 1942.

# Appendix A

## Acronyms

---

Acronyms	Meanings
BP	Bifurcation (or Branching) Point
CLDG	Closed Loop Disturbance Gain
CN	Condition Number
CSTR	Continuous Stirred Tank Reactor
FOD	Feedback Optimising Design
GUI	Graphical User Interface
HP	Hopf bifurcation Point
IM	Input Multiplicity
IMC	Internal Model Control
ISE	Integral Square Error
LD	Linear Dynamics
LHP	Left Hand Plane
MIMO	Multiple Input Multiple Output
MP	Minimum Phase
MPC	Model Predictive Controller
NLD	Non-Linear Dynamics

---

NLP	Non-Linear Programming
NMP	Non-Minimum Phase
NMPC	Nonlinear Model Predictive Control
OM	Output Multiplicity
PID	Integral Proportional Derivative
RGA	Relative Gain Array
RHP	Right Hand Plane
SISO	Single Input Single Output

# Appendix B

## Zero Dynamics

---

This chapter presents the concept of the zero dynamics of a nonlinear system and how to obtain them. The necessary mathematical background from differential geometry that is used in obtaining the zero dynamics is given.

### B.1 Introduction

Analogous to the RHP zeros of linear systems, the concept of zero dynamics of nonlinear systems is introduced. The zero dynamics for a nonlinear system is defined to be the internal dynamics of the system (Isidori, 1995). The zero dynamics of a system represent the characteristic behaviour of its inverse. The study on the dynamics of the inverse can be carried out by employing the zero dynamics.

## B.2 Mathematical Preliminaries

### B.2.1 Lie Derivatives

The Lie derivative  $L_f h(x)$  is the directional derivative of a scalar field  $h(x)$  in the direction of a vector field  $f(x)$ , defined as

$$\begin{aligned} L_f h(x) &= f_1(x) \frac{\partial h(x)}{\partial x_1} + \dots + f_n(x) \frac{\partial h(x)}{\partial x_n}, \\ &= \sum_{i=1}^n f_i(x) \frac{\partial h(x)}{\partial x_i}. \end{aligned} \quad (\text{B.1})$$

Repeated Lie derivatives are defined as the following:

$$L_g L_f h(x) = \sum_{i=1}^n g_i(x) \frac{\partial L_f h(x)}{\partial x_i}. \quad (\text{B.2})$$

If the scalar field is repeatedly differentiated in the direction of the same vector field, the following notion is used

$$\begin{aligned} L_f^2 &= L_f L_f \\ L_f^3 &= L_f L_f^2 \\ &\vdots \\ L_f^k &= L_f L_f^{k-1} \end{aligned} \quad (\text{B.3})$$

### B.2.2 Lie Brackets

The Lie brackets  $[f, g]$  of the vector fields  $f(x)$  and  $g(x)$  are defined as

$$[f, g](x) = ad_f g(x),$$

$$= \frac{\partial g(x)}{\partial x} f(x) - \frac{\partial f(x)}{\partial x} g(x), \quad (\text{B.4})$$

where  $\frac{\partial f(x)}{\partial x}$  and  $\frac{\partial g(x)}{\partial x}$  are the Jacobian of  $f(x)$  and  $g(x)$ , respectively.

If the Lie brackets are used repeatedly the standard notion is

$$\begin{aligned} ad_f^0 g &= g, \\ ad_f^1 g &= [f, g], \\ ad_f^2 g &= [f, [f, g]], \\ &\vdots \\ ad_f^k g &= [f, ad_f^{k-1} g]. \end{aligned} \quad (\text{B.5})$$

### B.3 Nonlinear Inversion: Zero Dynamics

For a linear system, the zeros are the roots of the polynomial numerator of the system. In other words, the zeros are the poles of the inverse of its transfer function. The zeros of a linear system are completely determined by the dynamics of its inverse. A transfer function, on which linear system zeros are based, can not be defined for nonlinear systems and therefore can not have zeros as a set of numbers. For nonlinear systems the analogue to the linear system, the notion of *zero dynamics* is imported. It is defined as the dynamics of the minimal order realisation of the inverse of a nonlinear system.

### B.3.1 Relative Order

Consider an SISO affine control nonlinear system with form:

$$\begin{aligned}\dot{x} &= f(x) + g(x)u, \\ y &= h(x).\end{aligned}\tag{B.6}$$

It is assumed that  $f(x)$  and  $g(x)$  are  $C^\infty$  vector field on  $\mathfrak{R}^n$  and  $h(x)$  is a  $C^\infty$  scalar field on  $\mathfrak{R}$ . The relative order has been defined by Hirschorn (1979) as following:

**Definition B.1** *The relative order of the system of the form ( B.6) is the smallest integer  $r$  for which*

$$L_g L_f^{r-1} h(x) \neq 0,\tag{B.7}$$

where  $L_g L_f^{r-1}$  are Lie derivatives.

The relative order, in other words, represents the number of times that the system output  $y$  has to be differentiated with respect to time in order to have the input  $u$  explicitly appearing. This definition is consistent with the relative order of the linear system, where one considers the difference in the degree of the denominator and the numerator polynomials. It is important to note that there may exist some points  $x_0$ , at which  $L_g L_f^{r-1} h(x) = 0$ , but nonzero at points arbitrarily close to them. If this is the case, the relative order is said to be not well defined. Such points are called as singular points (Slotine, 1991; Doyle and Henson, 1997).

### B.3.2 Normal Forms

The normal form of a system is of interest since it gives the system equations a structure convenient to extract the zero dynamics. It is obtained by means of a

change of coordinates in the state space.

A new coordinate transformation from  $\mathfrak{R}^n$  to  $\mathfrak{R}^n$  is given by the form:

$$\begin{aligned}\xi_1 &= \Xi_1(x_1, x_2, \dots, x_n), \\ \xi_2 &= \Xi_2(x_1, x_2, \dots, x_n), \\ &\vdots \\ \xi_n &= \Xi_n(x_1, x_2, \dots, x_n),\end{aligned}\tag{B.8}$$

where  $\Xi_1, \Xi_2, \dots, \Xi_n$  are  $C^1$  scalar fields on  $\mathfrak{R}^n$ , or in a more compact form:

$$\xi_i = \Xi_i(x).\tag{B.9}$$

The transformation ( B.8) is invertible if and only if  $\Xi_1, \Xi_2, \dots, \Xi_n$  are linearly independent. An invertible transformation  $x \in \mathfrak{R}^n \Rightarrow \xi_i = \Xi_i(x) x \in \mathfrak{R}^n$  define a new coordinate system. To transform a dynamic system in new coordinates means transforming the vector fields  $f(x)$  and  $g(x)$  and the scalar field  $h(x)$  in new coordinates (Kravaris and Kantor, 1990a). Under such a transformation, the nonlinear system ( B.6) will become

$$\begin{aligned}\dot{\xi} &= \left[ \frac{\partial \Xi}{\partial x}(x) f(x) \right]_{x=\Xi^{-1}} + \left[ \frac{\partial \Xi}{\partial x}(x) g(x) \right]_{x=\Xi^{-1}} u, \\ y &= [h(x)]_{x=\Xi^{-1}}.\end{aligned}\tag{B.10}$$

or, in a more explicit form,

$$\begin{aligned}\dot{\xi}_1 &= [ \langle d\Xi_1, f(x) \rangle ]_{x=\Xi^{-1}} + [ \langle d\Xi_1, g(x) \rangle ]_{x=\Xi^{-1}} u, \\ \dot{\xi}_2 &= [ \langle d\Xi_2, f(x) \rangle ]_{x=\Xi^{-1}} + [ \langle d\Xi_2, g(x) \rangle ]_{x=\Xi^{-1}} u, \\ &\vdots\end{aligned}\tag{B.11}$$

$$\begin{aligned}\dot{\xi}_n &= [\langle d\xi_n, f(x) \rangle]_{x=\Xi^{-1}} + [\langle d\xi_n, g(x) \rangle]_{x=\Xi^{-1}}u, \\ y &= [h(x)]_{x=\Xi^{-1}}.\end{aligned}$$

When the relative order  $r$  is defined and  $r < n$ , a nonlinear system can be transformed, using  $y, \dot{y}, \ddot{y}, \dots, y^r$  as part of the new state components, into the so called "normal form", which will give a more formal look at the notions of internal dynamics and zero dynamics that will be introduced.

Applying the following transformation:

$$\xi = \Xi(x) = \begin{pmatrix} t_1 \\ \vdots \\ t_{n-r} \\ y \\ \dot{y} \\ \vdots \\ y^r \end{pmatrix}$$

where  $t_1, t_2, \dots, t_{n-r}$  are linearly independent to  $y, \dot{y}, \ddot{y}, \dots, y^r$ , leads to a system in normal form.

If  $t_1, t_2, \dots, t_{n-r}$  are chosen to be solution for the  $\omega(x)$  of the partial differential equation

$$\langle d\omega(x), g(x) \rangle = 0$$

The transformation transforms the system to Byrnes-Isidori normal form (Isidori, 1995, Kravaris and Kantor, 1990a)

$$\begin{aligned}
\dot{\xi}_1 &= F_1(\xi), \\
\dot{\xi}_2 &= F_2(\xi), \\
&\vdots \\
\dot{\xi}_{n-r} &= F_{n-r}(\xi), \\
\dot{\xi}_{n-r+1} &= \xi_{n-r+2}, \\
&\vdots \\
\dot{\xi}_{n-1} &= \xi_n, \\
\dot{\xi}_n &= y^{(r)}, \\
y &= \xi_n, \\
u &= \frac{y^r - \Phi(\xi)}{G(\xi)},
\end{aligned} \tag{B.12}$$

where

$$\begin{aligned}
F_i(\xi) &= [\langle dt_i(x), f(x) \rangle]_{x=\Xi^{-1}}, \quad i = 1, \dots, n-r, \\
\Phi(\xi) &= [L_f^r h(x)]_{x=\Xi^{-1}}, \\
G(\xi) &= [L_g L_f^{r-1} h(x)]_{x=\Xi^{-1}}.
\end{aligned}$$

The normal form is useful to obtain a minimal realisation of the inverse of a nonlinear system with form ( B.6), as shown in the next.

### B.3.3 Nonlinear Inversion

**Definition B.2** (*Hirschorn Inversion*). Consider a dynamic system of the form ( B.6) whose relative order is  $r$ . Then the inverse of the system ( B.6) can be

calculated via

$$\begin{aligned}\dot{Z} &= f(Z) + g(Z) \frac{y^{(r)} - L_f^r h(Z)}{L_g L_f^{r-1} h(Z)}, \\ u &= \frac{y^{(r)} - L_f^r h(Z)}{L_g L_f^{r-1} h(Z)}.\end{aligned}\tag{B.13}$$

It has been pointed out by Kravaris and Kantor (1990a) that the inverse thus obtained is not the realisation of non-minimal order since there are  $r$  zero pole cancellations at the origin. The following method is suggested by Kravaris and Kantor (1990a) to have the minimal order realisation of the inverse. Since the input and output behaviour of a dynamic system is coordinate-independent, one can first transform the system in normal form and then apply the Hirschorn Inversion to obtain the inverse. Therefore, the minimal order realisation of the inverse is as the following:

$$\begin{aligned}\dot{Z}_1 &= F_1(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r}), \\ &\vdots \\ \dot{Z}_{n-r} &= F_{n-r}(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r}), \\ u &= \frac{y^r - \Phi(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r})}{G(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r})}.\end{aligned}\tag{B.14}$$

### B.3.4 Zero Dynamics

The zero dynamics can be extracted from the normal form. The zero dynamics are characterised as the remaining dynamics of the nonlinear system if the outputs are required to be 0 (constant) for all time (Isidori, 1995).

The zero dynamics are defined as the dynamics of the minimal order realisation

of the inverse of a nonlinear system, which are governed by:

$$\begin{aligned}\dot{Z}_1 &= F_1(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r}), \\ &\vdots \\ \dot{Z}_{n-r} &= F_{n-r}(Z_1, \dots, Z_{n-r}, y, \dot{y}, \dots, y^{n-r}).\end{aligned}\tag{B.15}$$

The minimal order inverse given by equation B.15 is called the *forced zero dynamics* because it is the system driven by the inputs and its derivatives ( $y, \dot{y}, \ddot{y}, \dots, y^r$ ). As discussed above, this contains more information than the system zeros. In order to have the same information as the linear zeros, the steady state is required. Then the dynamic system become

$$\begin{aligned}\dot{Z}_1 &= F_1(Z_1, \dots, Z_{n-r}, 0, \dots, 0), \\ &\vdots \\ \dot{Z}_{n-r} &= F_{n-r}(Z_1, \dots, Z_{n-r}, 0, \dots, 0).\end{aligned}\tag{B.16}$$

called the *unforced zero dynamics*, namely the *zero dynamics*.

The eigenvalues of this expression for a particular steady state are equal to the zeros of the linearised system at this steady state ( D'Andrea and Praly, 1988).

Doyle and Henson (1997) indicate that in the case where the system output is constrained to a constant set point, which can be assumed to be zero without loss of generality, the stability of the closed -loop system in which the inverse is employed as the controller is completely determined by the stability of the zero dynamics. In the case where the output must follow a trajectory, the inverse dynamics are driven by the output and its derivatives. In this case, the stability of the forced zero dynamics must be assessed to determined closed loop stability.

---

**Remark B.1** *See the papers by Kravaris and Kantor (1990a, b), Doyle and Henson (1997) and Daoutidis and Kravaris (1991) and the books by Isidori (1995) and Slotine et al. (1991) for more details.*

# Appendix C

## Numerical Techniques in Bifurcation Problems

---

This appendix describes the basic numerical techniques of continuation and bifurcation, which were used in the software package AUTO. Throughout, the fundamental tool is pseudo-arclength continuation. Much of the chapter was derived from the Tata Institute Lecture Notes of Keller (1987) and the Doedel's papers (1991a, b).

### C.1 Introduction

We consider here the problems for nonlinear equations in the form:

$$\dot{x} = f(x, \alpha), \tag{C.1}$$

where  $x, f \in \mathfrak{R}^n$  and  $\alpha \in \mathfrak{R}$ . Throughout, it is assumed that the function  $f$  is sufficiently smooth.

## C.2 Continuation of Solutions

A first step in the bifurcation analysis of the system ( C.1) consists of determining the steady state solution branches (or solution path). These solutions are  $(x(s), \alpha(s))$  of the nonlinear system of equations at steady state:

$$0 = f(x(s), \alpha(s)), \quad x, f \in \mathfrak{R}^n, \alpha \in \mathfrak{R}, \quad (\text{C.2})$$

where  $s$  denotes a parameter. Let  $X = (x, \alpha)$ . Then the equations of ( C.2) are written as:

$$0 = f(X), \quad f : \mathfrak{R}^{n+1} \rightarrow \mathfrak{R}^n. \quad (\text{C.3})$$

In the formulation ( C.3), it is not distinguished between parameter and state. A solution path to ( C.3) is denoted as  $X(s)$ .

### C.2.1 Regular Solution Paths

A solution  $X_0 = X(s_0)$  is called regular if  $f_X^0 = f_X(X_0)$  has rank  $n$ . A segment of a solution path is regular if  $X(s)$  is regular along the segment. In the parameter formulation ( C.2), we have  $\text{Rank} [f_X(X_0)] = \text{Rank} [f_x^0 | f_\alpha^0] = n$  iff either (i)  $f_x^0$  is nonsingular, or (ii)  $\dim N(f_x^0) = 1$  and  $f_\alpha^0 \notin R(f_x^0)$ . If a solution  $X_0$  is regular, then the path  $X(s)$  will also be regular nearby  $X_0$ .

**Remark C.1** *If  $\text{Rank} [f_x^0 | f_\alpha^0] = n$ , then either  $f_x^0$  is nonsingular and, from the Implicit Function Theorem, we obtain  $x = x(\alpha)$  near  $X_0 = (x_0, \alpha_0)$ , or we can interchange columns in  $f_X^0$  to see that the solution can be locally parametrised by one of the components of  $x$ .*

*Thus it can be seen that a unique branch of the solutions passes through a regular solution. It has been assumed that  $f$  is sufficiently smooth so that the Implicit Function Theorem holds and the resulting solution branch is smooth.*

### C.2.2 Folds

A solution is called a simple fold (or simple limit point ) if

$$\dim N(f_x^0) = 1, \quad \text{and } f_\alpha^0 \notin R(f_x^0). \quad (\text{C.4})$$

Differentiating the equations ( C.2) gives

$$f_x \dot{x}(s) + f_\alpha \dot{\alpha}(s) = 0. \quad (\text{C.5})$$

Note that at a fold point  $(x_0, \alpha_0)$ ,  $\dot{\alpha}_0 = 0$  because  $f_\alpha^0 \notin R(f_x^0)$ . Thus  $f_x \dot{x} = 0$ , and since  $\dim N(f_x^0) = 1$  we have  $N(f_x^0) = \text{span}\{\dot{x}\}$ . Differentiating ( C.5) give

$$f_x^0 \ddot{x}_0 + f_\alpha^0 \ddot{\alpha}_0 + f_{xx}^0 \dot{x}_0 \dot{x}_0 + 2f_{x\alpha}^0 \dot{x}_0 \dot{\alpha}_0 + f_{\alpha\alpha}^0 \dot{\alpha}_0 \dot{\alpha}_0 = 0. \quad (\text{C.6})$$

At a simple fold point  $(x_0, \alpha_0)$ , we can take

$$\begin{aligned} N(f_x^0) &= \text{span}\{\phi\}, \\ N((f_x^0)^T) &= \text{span}\{\psi\}. \end{aligned}$$

Multiplying ( C.6) on the left by  $\psi^T$  and using  $\dot{\alpha}_0 = 0$  and the fact that  $\psi \perp R(f_x^0)$  gets

$$\psi^T f_\alpha^0 \ddot{\alpha}_0 + \psi^T f_{xx}^0 \dot{x}_0 \dot{x}_0 = 0. \quad (\text{C.7})$$

Since  $f_\alpha^0 \notin R(f_x^0)$ , we obtain  $\psi^T f_\alpha^0 \neq 0$ , and so

$$\ddot{\alpha}_0 = \frac{\psi^T f_{xx}^0 \dot{x}_0 \dot{x}_0}{\psi^T f_\alpha^0}. \quad (\text{C.8})$$

But  $\dot{x}_0 = \beta\phi$  for some scalar  $\beta$ , thus

$$\ddot{\alpha}_0 = -\beta^2 \frac{\psi^T f_{xx}^0 \phi \phi}{\psi^T f_\alpha^0}. \quad (\text{C.9})$$

If  $\frac{\psi^T f_{xx}^0 \phi \phi}{\psi^T f_\alpha^0} \neq 0$ , then the point  $(x_0, \alpha_0)$  is called a simple quadratic fold. Similarly, we can define a “fold of order  $m$ ” if  $\alpha^{(k)}(s_0) = 0$  for all  $k = 1, \dots, m - 1$  and  $\alpha^{(m)}(s_0) \neq 0$ .

### C.2.3 Natural Parameter Continuation

We here take the  $\alpha$  as the continuation parameter. Suppose we have a solution  $(x_0, \alpha_0)$  of (C.2) as well as the direction vector  $\dot{x}_0$ . To find the solution  $x_1$  at a fixed, nearby value of  $\alpha$ , say,  $\alpha_1 = \alpha_0 + \Delta\alpha$ , we use Newton’s method:

$$\begin{aligned} f_x(x_1^k, \alpha_1) \Delta x_1^k &= -f(x_1^k, \alpha_1), \\ x_1^{k+1} &= x_1^k + \Delta x_1^k, \end{aligned} \quad (\text{C.10})$$

where  $k = 0, 1, 2, \dots$ .  $x_1^0 = x_0 + \Delta\alpha \dot{x}_0$  can be taken as an initial approximation. If  $f_x(x_1, \alpha_1)$  is nonsingular and  $\Delta\alpha$  is small enough, the iteration will converge. After convergence of the Newton iterations the new direction  $\dot{x}_1$  can be obtained from differentiating  $f(x(\alpha), \alpha) = 0$  with respect to  $\alpha$ :

$$f_x(x_1, \alpha_1) \dot{x}_1 = -f_\alpha^1. \quad (\text{C.11})$$

This clearly indicates that natural parameter continuation fails at a simple fold point.

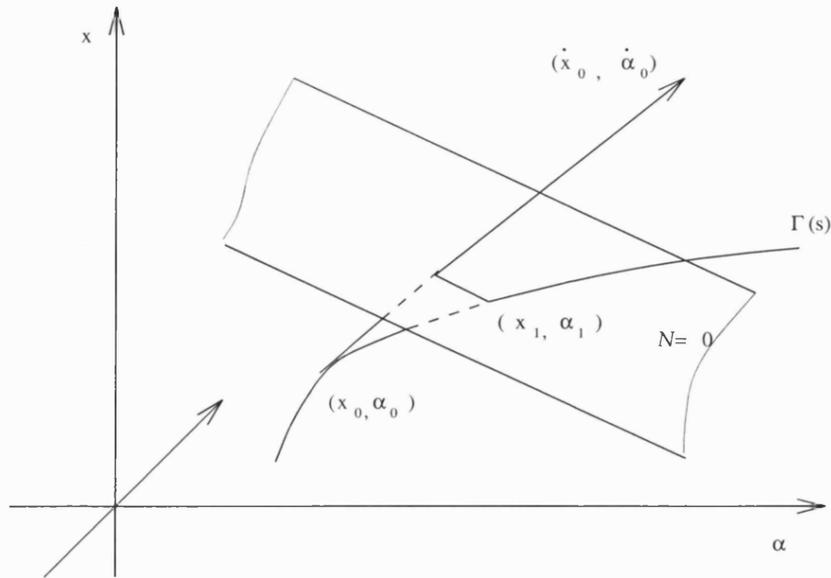


Figure C.1: Schematics for pseudo-arclength continuation

### C.2.4 Pseudo-arclength Continuation

It has been already mentioned above that Newton's method fails at fold points on a regular path during natural parameter continuation. A pseudo-arclength continuation was proposed by Keller (1977), which is the fundamental tool in the software package AUTO. The main idea of this method is to drop the natural parameterisation by  $\alpha$  and use some other parameterisation.

Consider the system with the form of ( C.2):

$$f(x(s), \alpha(s)) = 0, \quad x, f \in \mathfrak{R}^n, \alpha \in \mathfrak{R}. \quad (\text{C.12})$$

If  $(x_0, \alpha_0)$  is any point on a regular path and  $(\dot{x}_0, \dot{\alpha}_0)$  is the unit tangent to the path, then we adjoin to ( C.2) to have the scalar parameterisation:

$$(x_1 - x_0)^T \dot{x}_0 + (\alpha_1 - \alpha_0) \dot{\alpha}_0 - \Delta s = 0. \quad (\text{C.13})$$

This equation ( C.13) represents a plane, which is perpendicular to the tangent  $(\dot{x}_0, \dot{\alpha}_0)$  at a distance  $\Delta s$  from  $(x_0, \alpha_0)$ . Superscript  $T$  is the transpose.

Then the continuation can be formulated as:

$$f(x_1, \alpha_1) = 0, \quad (\text{C.14})$$

$$(x_1 - x_0)^T \dot{x}_0 + (\alpha_1 - \alpha_0) \dot{\alpha}_0 - \Delta s = 0, \quad (\text{C.15})$$

known as pseudo-arclength continuation.

Geometrically interpreted, this method is to find a solution  $(x_1, \alpha_1)$  to  $f(x, \alpha) = 0$  in a hyperplane that is at distance  $\Delta s$  from  $(x_0, \alpha_0)$  and that is perpendicular to the direction vector  $(\dot{x}_0, \dot{\alpha}_0)$ . Equation ( C.13) is one of the planes. This plane will intersect the curve (solution path)  $\Gamma$  if  $\Delta s$  is sufficiently small and the curvature of the  $\Gamma$  are not too large (see Figure C.1).

Using Newton's method for solving the equations ( C.14) and ( C.15) simultaneously for  $(x_1, \alpha_1)$  leads to the linear system:

$$\begin{pmatrix} (f_x^1)^k & (f_\alpha^1)^k \\ (\dot{x}_0)^T & \dot{\alpha}_0 \end{pmatrix} \begin{pmatrix} \Delta x_1^k \\ \Delta \alpha_1^k \end{pmatrix} = \begin{pmatrix} f(x_1^k, \alpha_1^k) \\ (x_1^k - x_0)^T \dot{x}_0 + (\alpha_1^k - \alpha_0) \dot{\alpha}_0 - \Delta s \end{pmatrix}, \quad (\text{C.16})$$

and the iterates are  $x^{k+1} = x^k + \Delta x^k$  and  $\alpha^{k+1} = \alpha^k + \Delta \alpha^k$ , and the  $k = 1, 2, \dots$ .

The next direction vector  $(\dot{x}_1, \dot{\alpha}_1)$  can be defined by the equations:

$$f_x^1 \dot{x}_1 + f_\alpha^1 \dot{\alpha}_1 = 0, \quad (\text{C.17})$$

$$(\dot{x}_0)^T \dot{x}_1 + \dot{\alpha}_0 \dot{\alpha}_1 = 1 \quad (\text{normalisation}). \quad (\text{C.18})$$

**Theorem C.1** (Doedel et al., 1991a). *The pseudo-arclength method works whenever  $(x_0, \alpha_0)$  is a regular solution point and  $\Delta s$  is sufficiently small. In particular the method works at a quadratic fold.*

Recall that such a path  $f_x^0$  may be nonsingular or singular but the  $(N + 1)$  order coefficient matrix of ( C.16) should be nonsingular (Keller, 1987).

## C.3 Singular Points and Bifurcation

### C.3.1 Simple Singular Points

A solution  $X_0 = X(s_0)$  along solution path  $X(s)$  of ( C.3) is called a singular point if  $f_X^0 = f_X(X_0)$  has rank  $n - 1$ . In terms of the parameter formulation ( C.2),  $(x_0, \alpha_0)$  is a simple singular point iff either one of the following holds: (i)  $\dim N(f_x^0) = 1$ ,  $f_\alpha^0 \in R(f_u^0)$ , (ii)  $\dim N(f_x^0) = 2$ ,  $f_\alpha^0 \notin R(f_u^0)$ .

### C.3.2 Bifurcation Theorem

Suppose we have a smooth solution branch  $X(s)$  of  $f(X) = 0$ . Differentiating the equations ( C.3) gives :  $f_X(X(s))\dot{X}(s) = 0$  at any point along the branch. Here  $\dot{X}(s)$  is the tangent to the branch. Assume that  $X_0$  be a simple singular point with  $N(f_X^0) = \text{span}\{\phi_1, \phi_2\}$  (since  $f_X$  is an  $N \times (N + 1)$  matrix,  $f_X$  has two independent null vectors) and  $N((f_X^0)^T) = \text{span}\{\psi\}$  for some nontrivial  $\psi \in \mathfrak{R}^n$ . The direction vector  $\dot{X}(s)$  lies in  $N(f_X^0)$  since the equation  $f_X(X_0)\dot{X}_0 = 0$ . Hence,  $\dot{X}_0$  has the form  $\dot{X}_0 = \beta\phi_1 + \gamma\phi_2$  for some  $\beta, \gamma \in \mathfrak{R}$ .

Differentiating the equations ( C.3) twice and evaluating at  $X_0$  we have:

$$f_X(X_0)\ddot{X}_0 + f_{XX}(X_0)\dot{X}_0\dot{X}_0 = 0 \quad (\text{C.19})$$

Now multiplying this relation on the left by  $\psi^T$ , the first term vanishes and we get:

$$\psi^T f_{XX}(X_0)\dot{X}_0\dot{X}_0 = 0. \quad (\text{C.20})$$

Substituting  $\dot{X}_0 = \beta\phi_1 + \gamma\phi_2$  gives:

$$a_{11}\beta^2 + 2a_{12}\beta\gamma + a_{22}\gamma^2 = 0, \quad (\text{C.21})$$

where  $a'_{ij}$ s are given by  $a_{ij} = \psi^T f_{XX} \phi_i \phi_j$ ,  $i, j = 1, 2$ . This equation (C.21) is called the algebraic bifurcation equation (ABE) (Keller, 1977).

Since the equation (C.21) is a quadratic equation, the roots are governed by the discriminant:

$$\Delta = a_{12}^2 - a_{11}a_{22}. \quad (\text{C.22})$$

Thus, it can be seen that there are two distinct real solutions for the equation if  $\Delta > 0$ . The discriminant  $\Delta$  cannot be negative since one real root already exists corresponding to the direction vector  $\dot{X}_0$ . If  $\Delta > 0$  then there exist two distinct "direction vector", and a bifurcation is expected, i.e. a second solution branch passes through  $X_0$ .

### C.3.3 Detection of Bifurcation Points

Let

$$F(X, s) = \begin{pmatrix} f(X) \\ (X - X_0)^T \dot{X}_0 - s \end{pmatrix}, \quad (\text{C.23})$$

and let  $X_0$  be a simple singular point. Then,

$$F_X^0 = F_X(X_0) = \begin{pmatrix} f_X^0 \\ (\dot{X}_0)^T \end{pmatrix}. \quad (\text{C.24})$$

**Theorem C.2** . (Keller, 1987) Let  $X_0 = X(s_0)$  be a simple singular point on a smooth solution branch  $X(s)$  of  $f(X) = 0$ . Assume that the discriminant  $\Delta$  is positive and that 0 is an algebraically simple eigenvalue of  $F_X^0$ . Then the determinant of  $F_X$ ,  $\det[F_X]$ , changes sign at  $X_0$ .

**Theorem C.3** . (Doedel et al., 1991a) Let  $X(s)$  be a smooth solution branch  $X(s)$  of  $F(X, s) = 0$ , where  $F : \mathbb{R}^{n+1} \times \mathbb{R}^n \rightarrow \mathbb{R}^{n+1}$  is  $C^1$ , and assume that  $\det[F_X(X(s); s)]$  changes sign at  $s = s_0$ . Then  $X(s_0)$  is a bifurcation point, i.e. every open neighbourhood of  $X(s_0)$  contains a solution of  $F(X, s) = 0$  that does not lie on  $X(s)$ .

In AUTO, the determinant of the Jacobian  $F_X$  is monitored along the solution branch  $X(s) = (x(s), \alpha(s))$ . Solution points at which the determinant changes sign are located by a secant iteration scheme and are treated as potential bifurcation points. Once the bifurcation point is detected, the solution branch can be continued in the new direction using the pseudo-arclength continuation.

## C.4 Summary

In this chapter, numerical techniques utilised in AUTO are briefly discussed. The pseudo-arclength as a fundamental tool in the AUTO was addressed. The details for the numerical method in bifurcation problems and implementation in AUTO can be seen in the lecture notes of Keller (1987) and the papers of

Doedel *et al.* (1991a, b). The codes of AUTO are available from the web site:  
<http://indy.cs.concordia.ca/auto/main.html>.